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Matrix Representation of the Resolvent Operator in Square-integrable Basis and Physical Application

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Abstract

We derive simple formulas for the matrix elements of the resolvent operator (also known as, the Green's function) in any finite set of square integrable basis. These formulas are suitable for numerical computations whether the basis elements are orthogonal or not. The formulas are written in terms of the eigenvalues and normalized eigenvectors of the matrix representation of the associated operator on the said basis. To reduce the computational cost, we also present a version of the same formulas using only matrix eigenvalues without the need for the sumptuous calculation of normalized eigenvectors. A byproduct of our findings is an expression for the normalized eigenvectors of a matrix in terms of its eigenvalues. We give a physical application of how useful these results can be. As an illustration, we use our findings to locate the resonances of a quantum mechanical system, obtain its bound states energies, and plot its energy density of states.

Keywords

Resolvent operator; basis sets; eigenvalues and eigenvectors; Green's function

1. Introduction

The resolvent operator, crucial in various scientific and engineering fields, lacks a concise technical treatment in the literature suitable for use in practical numerical calculations [1-3]. This study fills this gap, providing a detailed yet brief treatment suitable for researchers and practitioners familiar with linear algebra and matrix manipulations.

In many branches of science and engineering, one frequently comes across various operators that represent certain processes and/or actions in some space. An important object associated with such an operator is the resolvent that captures its spectral property. If we designate the operator as $\mathcal{L}$, then its resolvent is written formally as the inverse operator $(\mathcal{L}-z\mathcal{I})^{-1}$ where $\mathcal{I}$ is the identity and z is generally a complex number. It should be obvious that there exist a set of numbers in the complex z-plane on which the resolvent operator cannot be defined or realized. Such a set of values, $\{\xi\}$, are those where the action of the operator on an element of its domain $|\phi\rangle$ becomes $\mathcal{L}:|\phi\rangle \mapsto \xi|\phi\rangle$. The set $\{\xi\}$ is called the "spectral set" of $\mathcal{L}$, which can be discrete or continuous, or a combination of both. Moreover, the discrete set can either be finite or countably infinite whereas the continuous set generally consists of several disconnected but continuous regions of space in the complex plane. These regions might be curves or areas. However, the intersection of all of these spectral sets is null. Nonetheless, if the set $\{\xi\}$ is "too large" then one may not be able to find a region in the complex plane in which the resolvent could be realized. However, in this work, we will assume that such a scenario does not occur and we'll be able to define a resolvent for $\mathcal{L}$ in some large enough region of the complex plane and thus gain knowledge about its spectral property. A physical example is the Hamiltonian operator in quantum mechanics with z being the energy, $\{\xi\}$ the energy spectrum and $\{|\phi\rangle\}$ the discrete bound states or continuous scattering states. For such

systems, the resolvent is usually referred to in the physics literature as the "Green's function".

In the following section, we take $\mathcal{L}$ to be a self-adjoint operator whose action on a discrete set $\{|\psi_n\rangle\}$ is well-defined. Then, we derive the matrix elements of the resolvent on the conjugate set $\{|\bar{\psi}_n\rangle\}$. In Section 3, we obtain an alternative but equivalent representation of the resolvent that is more suitable numerically because it reduces the computational cost. In Section 4, we derive expressions for the normalized eigenvector of a matrix in terms of its eigenvalues. In Section 5, we present a physical application where our findings prove to be very useful in locating resonance energies of a given quantum mechanical system, obtaining its bound states energies and the density of states. Finally, we conclude in Section 6.

2. Theoretical Framework and Matrix Representation

Let $\{\psi_n\}_{n=0}^{\infty}$ be a complete set of square-integrable functions in configuration space that supports a Hermitian matrix representation for a self-adjoint operator H. The conjugate space is spanned by $\{\bar{\psi}_n\}_{n=0}^{\infty}$, where $\langle\bar{\psi}_n|\psi_m\rangle = \langle\psi_n|\bar{\psi}_m\rangle = \delta_{n,m}$ and $\sum_n |\bar{\psi}_n\rangle\langle\psi_n| = \sum_n |\psi_n\rangle\langle\bar{\psi}_n| = 1$. The first of these two relations is called the "orthogonality" relation and the second the "completeness" statement. The resolvent, which is also known as the Green's function $G(z)$, is formally defined by $G(z)(H-z)=1$ where z is a real number. Since the matrix elements of H are given in the basis $\{\psi_n\}_{n=0}^{\infty}$ as $H_{n,m} = \langle\psi_n|H|\psi_m\rangle$, then those of $G(z)$ are given in the conjugate basis as follows:

$$G_{n,m}(z) = \langle\bar{\psi}_n|(H-z)^{-1}|\bar{\psi}_m\rangle \tag{1}$$

Now, numerical manipulation of the resolvent, which involves taking the inverse of operators, is carried out most appropriately and efficiently in an orthonormal basis set $\{\chi_n\}_{n=0}^{\infty}$ (i.e., $\langle\chi_n|\chi_m\rangle = \delta_{n,m}$) in which the representation of those operators is diagonal. That is to say, we start by solving the eigenvalue problem

$$H|\chi_n\rangle = \varepsilon_n|\chi_n\rangle \tag{2}$$

From now on, we work in a finite subspace of dimension N and obtain the finite N-dimensional representation of the Green's function $G^N_{n,m}(z)$ where $G_{n,m}(z) = \lim_{N\to\infty} G^N_{n,m}(z)$. Since the matrix representations of the relevant operators are in the basis $\{\psi_n\}$ rather than $\{\chi_n\}$, then we can rewrite Eq. (2) as follows

$$\sum_{k=0}^{N-1}\langle\psi_m|H|\psi_k\rangle\langle\bar{\psi}_k|\chi_n\rangle = \varepsilon_n\sum_{k=0}^{N-1}\langle\psi_m|\psi_k\rangle\langle\bar{\psi}_k|\chi_n\rangle \quad ;n,m=0,1,..,N-1 \tag{3}$$

where we have used the completeness property of the basis in the finite N dimensional subspace,

$$\sum_k |\psi_k\rangle\langle\bar{\psi}_k| = \sum_k |\bar{\psi}_k\rangle\langle\psi_k| = I\,, \tag{4}$$

and I is the $N\times N$ unit matrix. In matrix notation, Eq. (3) reads

$$\sum_{k=0}^{N-1} H_{m,k}\Gamma_{k,n} = \varepsilon_n\sum_{k=0}^{N-1}\Omega_{m,k}\Gamma_{k,n} \quad ;n,m=0,1,..,N-1 \tag{5}$$

where $\Gamma_{k,n} := \langle\bar{\psi}_k|\chi_n\rangle$ and Ω is the basis overlap matrix whose elements are $\Omega_{n,m} = \langle\psi_n|\psi_m\rangle$. Thus, $\{\Gamma_{k,n}\}_{k=0}^{N-1}$ is the generalized eigenvector associated with the generalized eigenvalue ε_n. This is so because Eq. (5) could be written in matrix notation as the following generalized eigenvalue equation in the $\{\psi_n\}$ basis

$$H|\Gamma_n\rangle = \varepsilon_n\Omega|\Gamma_n\rangle\,. \tag{6}$$

Moreover, Eq. (5) reads $(H\Gamma)_{m,n} = \varepsilon_n(\Omega\Gamma)_{m,n}$ which when multiplied from left by $\Gamma^{\dagger}$, where $\Gamma^{\dagger}{}_{n,m} = \langle\chi_n|\bar{\psi}_m\rangle$, becomes

$$(\Gamma^{\intercal} H \Gamma)_{m,n} = \varepsilon_n (\Gamma^{\intercal} \Omega \Gamma)_{m,n} \qquad ; n,m = 0,1,..,N-1 \tag{7}$$

Being the generalized eigenvectors associated with the matrices H and Ω, the normalized eigenvector matrix Γ simultaneously diagonalizes H and Ω. That is,

$$(\Gamma^{\intercal} H \Gamma)_{n,m} = \eta_n \delta_{n,m} \quad \text{and} \quad (\Gamma^{\intercal} \Omega \Gamma)_{n,m} = \sigma_n \delta_{n,m} \tag{8}$$

Henceforth, we deduce that $\varepsilon_n = \eta_n / \sigma_n$ and equation (1) could be written as

$$\begin{aligned} G^N_{n,m}(z) &= \sum_{i,j,k,l=0}^{N-1} \langle \bar{\psi}_n | \chi_i \rangle \langle \chi_i | \bar{\psi}_k \rangle \langle \psi_k | (H - z)^{-1} | \psi_l \rangle \langle \bar{\psi}_l | \chi_j \rangle \langle \chi_j | \bar{\psi}_m \rangle \\ &= \sum_{i,j,k,l=0}^{N-1} \Gamma_{n,i} \left\{ \Gamma^{\intercal}_{i,k} \left[(H - z\Omega)^{-1} \right]_{k,l} \Gamma_{l,j} \right\} \Gamma^{\intercal}_{j,m} \end{aligned} \tag{9}$$

Now,

$$\sum_{k,l=0}^{N-1} \Gamma^{\intercal}_{i,k} \left[(H - z\Omega)^{-1} \right]_{k,l} \Gamma_{l,j} = \frac{\delta_{i,j}}{\eta_i - z\sigma_i} = \frac{1}{\sigma_i} \frac{\delta_{i,j}}{\varepsilon_i - z} \tag{10}$$

Therefore, we can write (9) as follows

$$G^N_{n,m}(z) = \sum_{i=0}^{N-1} \frac{\Gamma_{n,i} \Gamma_{m,i}}{\eta_i - z\sigma_i} = \sum_{i=0}^{N-1} \frac{1}{\sigma_i} \frac{\Gamma_{n,i} \Gamma_{m,i}}{\varepsilon_i - z} . \tag{11}$$

For orthonormal basis (when $\bar{\psi}_n = \psi_n$) the overlap matrix Ω is just the unit matrix I, hence $\sigma_i = 1$, $\eta_i = \varepsilon_i$. In this orthonormal basis, we can write

$$G^N_{n,m}(z) = \sum_{i=0}^{N-1} \frac{\Gamma_{n,i} \Gamma_{m,i}}{\varepsilon_i - z} . \text{ (in orthonormal basis)} \tag{12}$$

The terms “orthonormal” and “non-orthogonal” in the language of bases correspond (in the language of matrix equations) to the terms “eigenvalue equation” and “generalized eigenvalue equation”, respectively.

3. Computationally Efficient Representation

To avoid the sumptuous calculation of eigenvectors of matrices and reduce the computational cost, it is preferred that we work with eigenvalues of matrices rather than their eigenvectors. Here we give an alternative formula to (11) and (12) where only eigenvalues are involved. Let $H^{(n,m)}$ and $\Omega^{(n,m)}$ be the $(N-1)\times(N-1)$ submatrices of H and Ω obtained by deleting row n and column m, respectively. The eigenvalue equation and generalized eigenvalue equation in the truncated space, which parallel equations (2) and (6), are

$$H^{(n,m)} | \tilde{\chi}_k \rangle = \varepsilon^{(n,m)}_k | \tilde{\chi}_k \rangle , \tag{13}$$

$$H^{(n,m)} | \tilde{\Gamma}_k \rangle = \varepsilon^{(n,m)}_k \Omega^{(n,m)} | \tilde{\Gamma}_k \rangle , \tag{14}$$

where $k = 0,1,..,N-2$ and $\tilde{\Gamma}_{i,j} := \langle \bar{\psi}_i | \tilde{\chi}_j \rangle$. Moreover, the matrix of the normalized eigen-vectors, $\tilde{\Gamma}$, simultaneously diagonalizes $H^{(n,m)}$ and $\Omega^{(n,m)}$. That is,

$$\left[\tilde{\Gamma}^{\intercal} H^{(n,m)} \tilde{\Gamma} \right]_{i,j} = \eta^{(n,m)}_i \delta_{i,j} \quad \text{and} \quad \left[\tilde{\Gamma}^{\intercal} \Omega^{(n,m)} \tilde{\Gamma} \right]_{i,j} = \sigma^{(n,m)}_i \delta_{i,j} , \tag{15}$$

with $\varepsilon^{(n,m)}_k = \eta^{(n,m)}_k / \sigma^{(n,m)}_k$. An identity for an $N \times N$ non-singular matrix C, which is very useful in such calculation reads

$$(C^{-1})_{n,m} = (-1)^{n+m} \frac{|C^{(n,m)}|}{|C|} = (-1)^{n+m} \frac{\prod_{i=0}^{N-2} c^{(n,m)}_i}{\prod_{j=0}^{N-1} c_j} , \tag{16}$$

where we have also used the determinant identity for C that reads $|C| = |\Lambda^{\intercal} C\, \Lambda| = \prod_{n=0}^{N-1} c_n$ with $\{c_n\}_{n=0}^{N-1}$ being the set of its eigenvalues and $\{\Lambda_{m,n}\}_{n,m=0}^{N-1}$ the corresponding normalized eigenvectors. Then, it is easy to show that the following is an alternative but equivalent form for $G_{n,m}^{N}(z)$ in a non-orthogonal basis

$$\begin{aligned} G_{n,m}^{N}(z) &= (-1)^{n+m} \frac{\left|\Omega^{(n,m)}\right|}{|\Omega|} \left[\prod_{i=0}^{N-2} \left(\varepsilon_i^{(n,m)} - z\right) \Big/ \prod_{j=0}^{N-1} \left(\varepsilon_j - z\right) \right] \\ &= (-1)^{n+m} \left[\prod_{i=0}^{N-2} \tau_i^{(n,m)} \left(\varepsilon_i^{(n,m)} - z\right) \Big/ \prod_{j=0}^{N-1} \tau_j \left(\varepsilon_j - z\right) \right] \end{aligned} \quad \text{(in non-orthogonal basis)} \tag{17}$$

where $\{\tau_j\}_{j=0}^{N-1}$ and $\{\tau_i^{(n,m)}\}_{i=0}^{N-2}$ are the eigenvalues of the overlap matrices Ω and $\Omega^{(n,m)}$, respectively. For an orthonormal basis, $\Omega^{(n,m)} = I^{(n,m)}$ and (17) is not valid if $n \neq m$ because then $I^{(n,m)}$ is singular. However, a valid formula for orthonormal bases that replaces Eq. (17) is obtained using the identity (16) and reads

$$G_{n,m}^{N}(z) = (-1)^{n+m} \frac{\prod_{i=0}^{N-2} \omega_i^{(n,m)}(z)}{\prod_{j=0}^{N-1} \varepsilon_j - z}, \quad \text{(in orthonormal basis)} \tag{18}$$

where $\{\omega_i^{(n,m)}(z)\}_{i=0}^{N-2}$ are the eigenvalues of the matrix function $H^{(n,m)} - z\, I^{(n,m)}$. For $n = m$, Eq. (18) becomes

$$G_{n,n}^{N}(z) = \frac{\prod_{i=0}^{N-2} \varepsilon_i^{(n,n)} - z}{\prod_{j=0}^{N-1} \varepsilon_j - z}. \quad \text{(in orthonormal basis)} \tag{19}$$

For $n \neq m$, an alternative formula to (18) is preferred to avoid the functional dependence of the eigenvalue $\omega_i^{(n,m)}(z)$ that greatly increases the computational cost. Due to the fact that $I^{(n,m)}$ is singular for $n \neq m$, a formula similar to (19) is not possible. However, because of the product $\prod_{j=0}^{N-1} \varepsilon_j - z$ in the denominator of $G_{n,m}^{N}(z)$ as shown in (18), we can recast $G_{n,m}^{N}(z)$ as the sum $G_{n,m}^{N}(z) = \sum_{k=0}^{N-1} \frac{A_k^{(n,m)}}{\varepsilon_k - z}$, where

$$A_k^{(n,m)} = (-1)^{n+m} \frac{\prod_{i=0}^{N-2} \omega_i^{(n,m)}(\varepsilon_k)}{\prod_{\substack{j=0 \\ j\neq k}}^{N-1} \varepsilon_j - \varepsilon_k}, \tag{20}$$

which is obtained by multiplying (18) by $\varepsilon_k - z$ then evaluating at $z = \varepsilon_k$. Therefore, we obtain the following formula in an orthonormal basis

$$G_{n,m}^{N}(z) = (-1)^{n+m} \sum_{k=0}^{N-1} \frac{\prod_{i=0}^{N-2} \varepsilon_{i,k}^{(n,m)}}{(\varepsilon_k - z) \prod_{j\neq k}^{N-1} (\varepsilon_j - \varepsilon_k)}, \quad \text{(in orthonormal basis)} \tag{21}$$

where $\{\varepsilon_{i,k}^{(n,m)} = \omega_i^{(n,m)}(\varepsilon_k)\}_{i=0}^{N-2}$ are the $N-1$ eigenvalues of the matrix $H^{(n,m)} - \varepsilon_k\, I^{(n,m)}$. For $n = m$, one can use the equivalent but simpler formula (19).

4. Deriving Normalized Eigenvectors from Eigenvalues

A by-product of formulas (12) and (18) is an interesting recipe for calculating the square of the elements of the normalized eigenvectors of a square Hermitian matrix in terms of its set of eigenvalues (i.e., where $H\left|\Gamma_n\right\rangle=\varepsilon_n\left|\Gamma_n\right\rangle$ with $\Omega=I$) as follows

$$\Gamma_{n,k}\Gamma_{m,k}=(-1)^{n+m}\frac{\prod_{i=0}^{N-2}\varepsilon_{i,k}^{(n,m)}}{\prod_{\substack{j=0\\ j\neq k}}^{N-1}\varepsilon_j-\varepsilon_k}, \quad \text{(in orthonormal basis)} \tag{22}$$

which is obtained by multiplying (12) and (18) by ε_k-z then evaluating at $z=\varepsilon_k$. However, for $n=m$, we can use (19) instead of (18) to write

$$\Gamma_{n,k}^2=\frac{\prod_{i=0}^{N-2}\varepsilon_i^{(n,n)}-\varepsilon_k}{\prod_{\substack{j=0\\ j\neq k}}^{N-1}\varepsilon_j-\varepsilon_k}. \quad \text{(in orthonormal basis)} \tag{23}$$

This formula has been rediscovered recently by D. Mitnik and S. Mitnik [4]. However, we have been utilizing it since the early days of the *J*-matrix method (see, for example, Ref. [5] and citations therein). A version of (22) for non-orthogonal basis (i.e., for generalized eigenvectors where $H\left|\Gamma_n\right\rangle=\varepsilon_n\Omega\left|\Gamma_n\right\rangle$) could be obtained by combining (11) and (17) where we get

$$\Gamma_{n,k}\Gamma_{m,k}=(-1)^{n+m}\sigma_k\frac{\left|\Omega^{(n,m)}\right|}{|\Omega|}\frac{\prod_{i=0}^{N-2}\varepsilon_i^{(n,m)}-\varepsilon_k}{\prod_{\substack{j=0\\ j\neq k}}^{N-1}\varepsilon_j-\varepsilon_k}. \quad \text{(in non-orthogonal basis)} \tag{24}$$

Moreover, for $n=m$, this gives

$$\Gamma_{n,k}^2=\frac{\sigma_k}{\tau_k}\frac{\prod_{i=0}^{N-2}\tau_i^{(n,n)}\left(\varepsilon_i^{(n,n)}-\varepsilon_k\right)}{\prod_{\substack{j=0\\ j\neq k}}^{N-1}\tau_j\left(\varepsilon_j-\varepsilon_k\right)}. \quad \text{(in non-orthogonal basis)} \tag{25}$$

5. Physical Application

As an example, we use the matrix representation of the Green's function derived above to calculate the scattering matrix of a given physical system, obtain its resonance energies, bound state energies, and compute the energy density of states. We consider a system with the Hamiltonian $H=H_0+V$ where H_0 stands for the Hamiltonian operator associated with the Coulomb problem in three dimensions, which has the following realization in the radial coordinate *r*

$$H_0=\frac{1}{2}\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{2r^2}+\frac{Z}{r}, \tag{26}$$

where $\ell=0,1,2,...$ is the angular momentum quantum number, $Z\in\mathbb{R}$ is the electric charge coupling, and we have adopted the atomic units $\hbar=M=e=1$ in which distances are measured in units of the Bohr radius $4\pi\in_0$. The added potential V is taken as a non-singular short-range radial function such that $V(r>R)\approx 0$, where R is some finite range. Now, we take the basis elements as

$$\psi_n(r)=\sqrt{\frac{\lambda\Gamma(n+1)}{\Gamma(n+2\ell+2)}}(\lambda r)^{\ell+1}e^{-\lambda r/2}L_n^{2\ell+1}(\lambda r), \tag{27}$$

where $L_n^{2\ell+1}(x)$ is the Laguerre polynomial and λ is a real scale parameter of inverse length dimension. The orthogonality of the Laguerre polynomials gives $\bar{\psi}_n(r)=(\lambda r)^{-1}\psi_n(r)$ and the three-term recursion relation gives

$$\Omega_{n,m}=\langle\psi_n|\psi_m\rangle=2(n+\ell+1)\delta_{n,m}-\sqrt{n(n+2\ell+1)}\,\delta_{n,m+1}-\sqrt{(n+1)(n+2\ell+2)}\,\delta_{n,m-1}, \tag{28}$$

making Ω a tridiagonal symmetric matrix. Moreover, using the differential equation of the Laguerre polynomial, its differential property, and recursion relation we obtain the following matrix elements of H_0

$$\begin{aligned}(H_0)_{n,m}=\langle\psi_n|H_0|\psi_m\rangle&=\left[\lambda Z+\frac{\lambda^2}{4}(n+\ell+1)\right]\delta_{n,m}\\ &+\frac{\lambda^2}{8}\sqrt{n(n+2\ell+1)}\delta_{n,m+1}+\frac{\lambda^2}{8}\sqrt{(n+1)(n+2\ell+2)}\delta_{n,m-1}\end{aligned} \tag{29}$$

Therefore, the matrix elements of H in the basis $\{\psi_n\}$ is $H_{n,m}=(H_0)_{n,m}+V_{n,m}$ and since the potential function $V(r)$ is short-range, then its matrix elements $V_{n,m}=\langle\psi_n|V|\psi_m\rangle\approx 0$ if n and/or m is greater than or equal to some large enough integer N that depends on the dimensionless range λR. Consequently, the infinite Hermitian matrix H will consist of an $N\times N$ block on the top-left corner that represents H_0+V and an infinite tridiagonal symmetric tail representing H_0. That is, the matrix representation of H will look like the following

$$H=\begin{pmatrix}
\times & \times & \times & \times & \times & \times & \times & & & & & & \\
\times & \times & \times & \times & \times & \times & \times & & & & & & \\
\times & \times & \times & \times & \times & \times & \times & & & & & & \\
\times & \times & \times & \times & \times & \times & \times & & & & & & \\
\times & \times & \times & \times & \times & \times & \times & & & & & & \\
\times & \times & \times & \times & \times & \times & \times & & & & & & \\
\times & \times & \times & \times & \times & \times & \times & b_{N-1} & & & & & \\
 & & & & & & b_{N-1} & a_N & b_N & & & & \\
 & & & & & & & b_N & a_{N+1} & b_{N+1} & & & \\
 & & & & & & & & b_{N+1} & a_{N+2} & \times & & \\
 & & & & & & & & & \times & \times & \times & \\
 & & & & & & & & & & \times & \times & \times \\
 & & & & & & & & & & & \times & \times
\end{pmatrix}, \tag{30}$$

where $a_n=\lambda Z+\frac{\lambda^2}{4}(n+\ell+1)$ and $b_n=\frac{\lambda^2}{8}\sqrt{(n+1)(n+2\ell+2)}$.

The solution of the wave equation $H|\Phi\rangle=E|\Phi\rangle$ for all energies (discrete bound states and continuous scattering states) in such a configuration is handled more effectively by using the J-matrix method [6]. In this method, the solution is written as $|\Phi\rangle=\sum_{n=0}^{\infty}f_n|\psi_n\rangle$ and one obtains the coefficients $\{f_n\}$ that depend on $\{E,\ell,Z,\lambda\}$ and the parameters of the potential V. The asymptotic coefficients $\{f_n\}_{n=N-1}^{\infty}$ are solutions of the reference wave equation where $V=0$. They satisfy the following symmetric three-term recursion relation that results from the infinite tail of the matrix wave equation $(H_0-E\,\Omega)|\Phi\rangle=0$ and reads

$$\left[a_n-2E(n+\ell+1)\right]f_n+\left(1+\frac{8E}{\lambda^2}\right)b_{n-1}f_{n-1}+\left(1+\frac{8E}{\lambda^2}\right)b_nf_{n+1}=0, \tag{31}$$

for $n=N,N+1,N+2,\ldots$. This recursion relation has two independent solutions, which we call $c_n(E)$ and $s_n(E)$, and $f_n(E)$ becomes a linear combination of both with energy dependent factors [5, 6]. The boundary conditions give

$$f_n(E)=\left[c_n(E)-\mathrm{i}s_n(E)\right]-e^{2\mathrm{i}\delta(E)}\left[c_n(E)+\mathrm{i}s_n(E)\right], \tag{32}$$

for $n=N-1,N,N+1,..$ and where $\delta(E)$ is the scattering phase shift angle. This phase shift and the $N-1$ coefficients $\{f_n\}_{n=0}^{N-2}$ are determined from the solution of the remaining N equations (after removing the infinite tail from the matrix wave equation) that read

$$\begin{pmatrix} \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \\ \times & \times & \times & \times & \times & \times & \times \end{pmatrix}\begin{pmatrix} f_0 \\ f_1 \\ \times \\ \times \\ \times \\ f_{N-2} \\ f_{N-1} \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \\ \times \\ \times \\ \times \\ 0 \\ -J_{N-1,N}f_N \end{pmatrix} \tag{33}$$

where the $N\times N$ symmetric matrix on the left side is $\left(H_0+V-E\,\Omega\right)$ and $J_{n,m}(E)=\left(H_0-E\,\Omega\right)_{n,m}$. We multiply both sides of Eq. (33) by the inverse of this matrix which is the finite $N\times N$ Green's functional matrix $\left(H-E\,\Omega\right)^{-1}$ (i.e., the resolvent of H). The last row (row $N-1$) of the resulting matrix equation gives a special relation that determines $\delta(E)$ by using $f_N(E)$ and $f_{N-1}(E)$ from Eq. (32) and reads

$$e^{2\mathrm{i}\delta(E)}=T_{N-1}(E)\frac{1+G_{N-1,N-1}(E)J_{N-1,N}(E)R_N^-(E)}{1+G_{N-1,N-1}(E)J_{N-1,N}(E)R_N^+(E)} \tag{34}$$

where $T_n(E)=\dfrac{c_n(E)-\mathrm{i}s_n(E)}{c_n(E)+\mathrm{i}s_n(E)}$ and $R_n^{\pm}(E)=\dfrac{c_n(E)\pm\mathrm{i}s_n(E)}{c_{n-1}(E)\pm\mathrm{i}s_{n-1}(E)}$. To calculate these coefficients, we start with $T_0(E)$ and $R_1^{\pm}(E)$ then use the recursion relation (31) to obtain the rest[1]. Now, since the basis set $\{\psi_n\}$ with the elements given by Eq. (27) are not orthogonal, then the finite Green's function $G_{N-1,N-1}^N(E)$ are obtained by using either formula (11) or formula (17). Thus, we can write

$$G_{N-1,N-1}^N(E)=\sum_{j=0}^{N-1}\frac{1}{\sigma_j}\frac{\Gamma_{N-1,j}^2}{\varepsilon_j-E}=\frac{\prod_{i=0}^{N-2}\tilde{\tau}_i\left(\tilde{\varepsilon}_i-E\right)}{\prod_{j=0}^{N-1}\tau_j\left(\varepsilon_j-E\right)}, \tag{35}$$

where $\tilde{\tau}_i=\tau_i^{(N-1,N-1)}$ and $\tilde{\varepsilon}_i=\varepsilon_i^{(N-1,N-1)}$.

Figure 1 is a plot of $\left|1-S(E)\right|$, where $S(E)$ is the scattering matrix $e^{2\mathrm{i}\delta(E)}$ associated with the short-range potential $V(r)=7.5r^2e^{-r}$ for $\ell=0$ and $Z=0$. We took the computational parameters $\lambda=1.0$ and $N=60$. The figure clearly shows a resonance activity near $E=3.4$. Figure 2 is a plot of the real part (solid curve) and imaginary part (dashed curve) of $S(E)$ for the same system. Figure 3 is a zoom plot of Figure 2 showing that the imaginary part peaks at $E=3.425$, which agrees well with the findings in the literature [7-11] where $E_{res}=3.426-\mathrm{i}0.0128$.

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[1] Using Eq. (A26) in the Appendix of Ref. [6], we can write $T_0(E)=e^{2\mathrm{i}\theta}\dfrac{\ell+1+\mathrm{i}t}{\ell+1-\mathrm{i}t}\dfrac{{}_2F_1\left(-\ell-\mathrm{i}t,1;\ell+2-\mathrm{i}t;e^{2\mathrm{i}\theta}\right)}{{}_2F_1\left(-\ell+\mathrm{i}t,1;\ell+2+\mathrm{i}t;e^{-2\mathrm{i}\theta}\right)}$ and $R_1^+(E)=\dfrac{e^{-\mathrm{i}\theta}\sqrt{2\ell+2}}{\ell+2+\mathrm{i}t}\dfrac{{}_2F_1\left(-\ell+\mathrm{i}t,2;\ell+3+\mathrm{i}t;e^{-2\mathrm{i}\theta}\right)}{{}_2F_1\left(-\ell+\mathrm{i}t,1;\ell+2+\mathrm{i}t;e^{-2\mathrm{i}\theta}\right)}$, where $t=Z/\sqrt{2E}$ and $\cos\theta=\dfrac{8E-\lambda^2}{8E+\lambda^2}$ with $0<\theta\le\pi$. However, we had to take care of the normalization of the basis element adopted in [6] that differs from ours in Eq. (27).

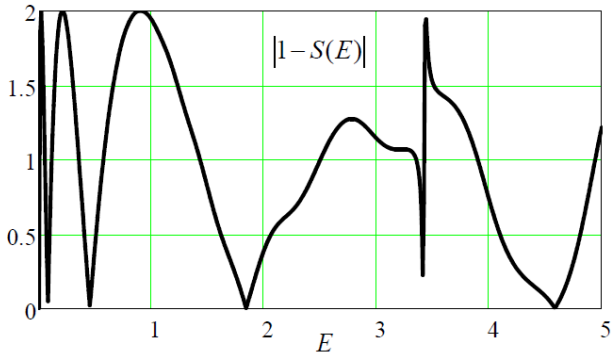

Figure 1. Plot of $|1-S(E)|$ for the system associated with $V(r)=7.5r^2e^{-r}$ for $\ell=0$ and $Z=0$. We took the computational parameters $\lambda=1$ and $N=60$. The figure shows a resonance activity at $E=3.4$.

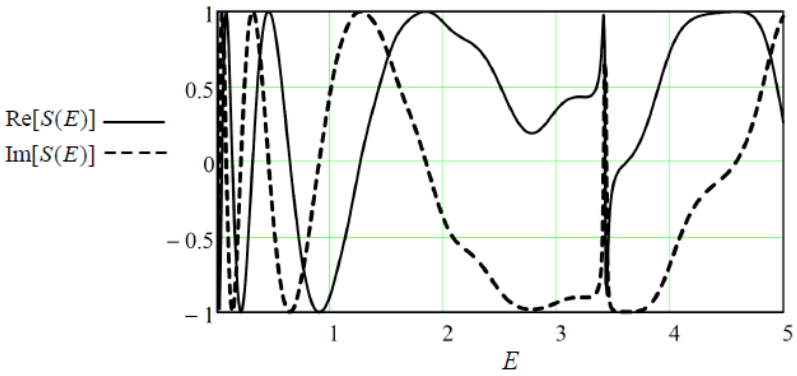

Figure 2. A reproduction of Figure 1 but for the real part (solid curve) and imaginary part (dashed curve) of $S(E)$.

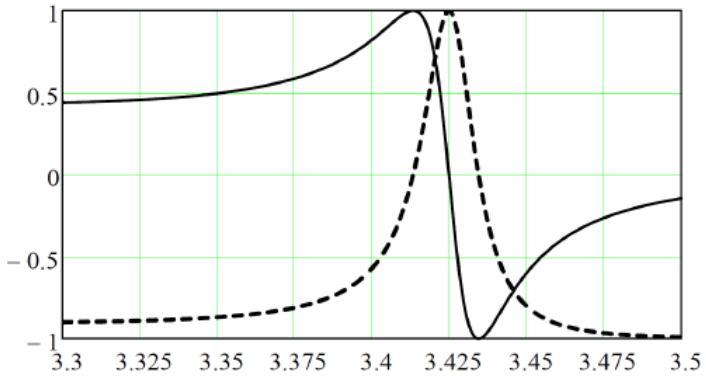

Figure 3. Zoom plot of Figure 2 showing that the imaginary part peaks at $E=3.425$, which agrees well with the location of this resonance found elsewhere [7-11]. The horizontal axis is the energy in atomic units.

Figure 4 is a plot of $|1-S(E)|$ associated with the short-range potential $V(r)=5e^{-(r-3.5)^2/4}-8e^{-r^2/5}$ for $\ell=0$ and $Z=0$. We took the computational parameters $\lambda=20$ and $N=20$. The figure clearly shows resonance activities near $E=2.2$ and $E=4.6$. Figure 5, which is a zoom plot of the real and imaginary parts of $S(E)$ with $N=100$, gives a better resolution showing that these resonances occur at $E=2.2524$ and $E=4.51$. These are in good agreement with the findings in the literature [8, 11, 12] where $E_{res}=2.2524-\mathrm{i}0.00005913$ and $E_{res}=4.5010-\mathrm{i}0.12398$. Figure 6 shows six zoom plots of $S(E)$ for the same system with $\ell=0,1,2$ and $Z=\pm1$. The six resonance energies are in good agreement with the findings in Ref. [12] as shown in Table 1.

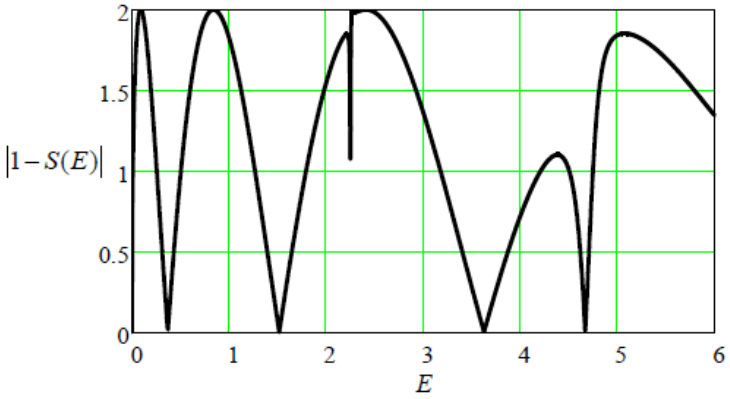

Figure 4. Plot of $|1-S(E)|$ associated with the short-range potential $V(r)=5e^{-(r-3.5)^2/4}-8e^{-r^2/5}$ for $\ell=0$ and $Z=0$. We took the computational parameters $\lambda=20$ and $N=20$. The figure shows resonance activities at $E=2.2$ and $E=4.6$.

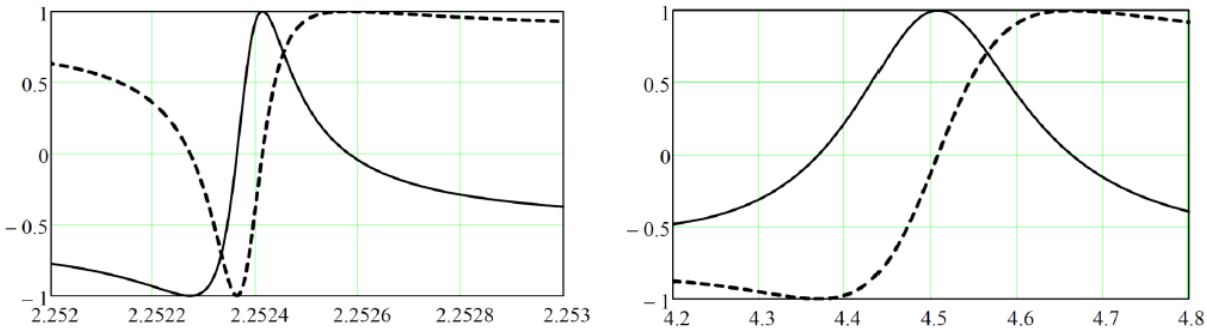

Figure 5. Zoom plots of Figure 4 for the real and imaginary parts of $S(E)$ showing resonance activities at $E=2.2524$ and $E=4.51$. We took the computational parameters $\lambda=20$ and $N=100$. The horizontal axis is the energy in atomic units.

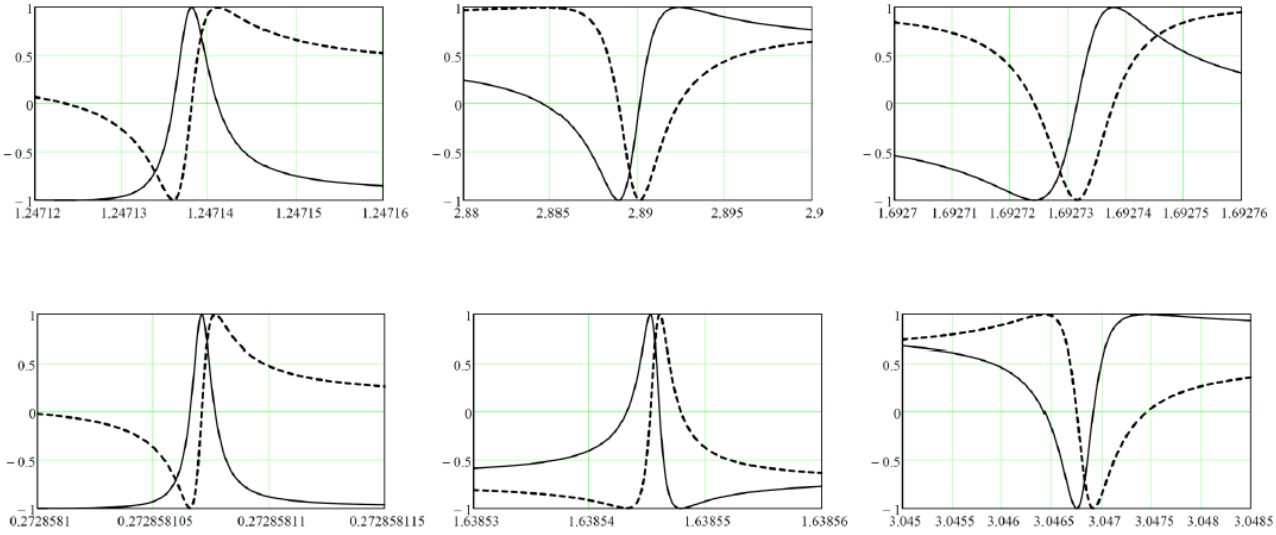

Figure 6. Zoom plots of the real and imaginary parts of $S(E)$ for the system associated with the potential $V(r)=5e^{-(r-3.5)^2/4}-8e^{-r^2/5}$ for $Z=-1$ (top row) and $Z=+1$ (bottom row). The angular momenta were taken as $\ell=0,1,2$ (from left to right columns). The horizontal axis is the energy in atomic units.

Table 1. Resonance energies associated with the potential $V(r)=5e^{-(r-3.5)^2/4}-8e^{-r^2/5}$ for the given electric charge and angular momentum. These results are obtained from Figure 6 and compared to those in the Table of Ref. [12]. Uncertainty in the numbers obtained from Figure 6 is in the last decimal digit. The smaller the imaginary part of the resonance energy, the sharper the resonance, and the larger the number of significant digits.

Z	ℓ	$\mathrm{Re}(E_{res})$ (Fig. 6)	E_{res} (Ref. [12])
	0	1.247137	1.247137679 – i0.0000023985
–1	1	2.889	2.889663069 – i0.0014603245
	2	1.69273	1.692732086 – i0.000006761
	0	0.272858107	0.272858107 – i0.0000000006
+1	1	1.638546	1.638545711 – i0.000000971
	2	3.0467	3.046808400 – i0.000100441

Finding the bound states energies, on the other hand, is much easier than resonances and requires much less calculation cost. For example, we can choose any desired (n,m) component of the Green's function and just plot $\left|G^N_{n,m}(E)\right|$ for $E<0$. The plot will show very sharp divergences at the bound state energies even for small N. Increasing N will increase the accuracy. This is so, because the poles of $G^N_{n,m}(E)$ are at the eigenvalues $\{\varepsilon_n\}_{n=0}^{N-1}$ of the Hamiltonian matrix that get more accurate and stable at the bound state energies by increasing N. Figure 7 is such a plot for $\left|G^N_{N-1,N-1}(E)\right|$ associated with the potential $V(r)=5e^{-(r-3.5)^2/4}-8e^{-r^2/5}$ for $\ell=0$, $Z=0$, and $N=5$. The plot shows bound state energies at $E=-4.6$ and $E=-0.8$. Increasing the basis size to $N=15$ and zooming into the figure, we obtain $E=-4.571182831$ and $E=-0.8842806$ which agrees very well with the results in [11] and [12].

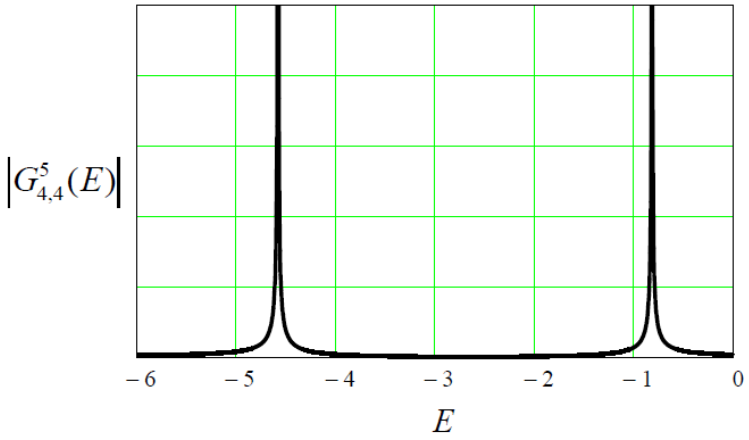

Figure 7. Plot of $\left|G^N_{N-1,N-1}(E)\right|$ for the system with $V(r)=5e^{-(r-3.5)^2/4}-8e^{-r^2/5}$ and for $\ell=0$, $Z=0$ and $N=5$. The plot blows up at the two bound state energies: $E=-4.6$ and $E=-0.8$.

Finally, we calculate the energy density of states $\rho(E)$ using its definition as the discontinuity of the $(0,0)$ component of the Green's function across the real axis in the complex energy plane. That is,

$$\rho(E)=\frac{1}{2\pi\mathrm{i}}\lim_{\varepsilon\to 0}\left[G_{0,0}(E+\mathrm{i}\varepsilon)-G_{0,0}(E-\mathrm{i}\varepsilon)\right]=\frac{1}{\pi}\mathrm{Im}\,G_{0,0}(E+\mathrm{i}\varepsilon)\,. \tag{36}$$

Several techniques have been developed to obtain a good approximation of $\rho(E)$ using this definition but with the finite Green's function $G^N_{0,0}(E)$. See, for example, the three techniques outlined in Ref. [13]. For this calculation, we use an alternative orthonormal basis set with the elements.

$$\psi_n(r)=\sqrt{\frac{2\lambda\Gamma(n+1)}{\Gamma\left(n+\ell+\frac{3}{2}\right)}}(\lambda r)^{\ell+1}e^{-\lambda^2r^2/2}L_n^{\ell+\frac{1}{2}}(\lambda^2r^2)\,. \tag{37}$$

In this orthonormal basis, the finite Green's function is written using either formula (12) or formula (19) as follows

$$G_{0,0}^N(E)=\sum_{i=0}^{N-1}\frac{\Gamma_{0,i}^2}{\varepsilon_i-E}=\frac{\prod_{i=0}^{N-2}\varepsilon_i^{(0,0)}-E}{\prod_{j=0}^{N-1}\varepsilon_j-E}\,. \tag{38}$$

Figure 8 shows $\rho(E)$ for the system corresponding to the potential $V(r)=7.5r^2e^{-r}$ with $Z=0$ and $\ell=0,1,2$ (left to right) obtained by employing the analytic continuation procedure. In that procedure, $G_{0,0}^N(z)$ is evaluated using (38) in the upper half of the complex energy plane far away from the discontinuity where it is fitted to a complex analytic function $F(z)$. Subsequently, the function $F(z)$ is analytically continued to the real energy axis to replace $G_{0,0}(z)$ in (36) for evaluating $\rho(E)$.

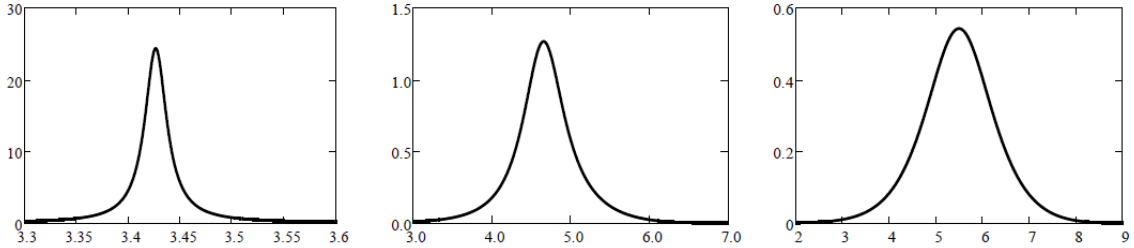

Figure 8. Energy density of states $\rho(E)$ for the system corresponding to $V(r)=7.5r^2e^{-r}$ with $Z=0$ and $\ell=0,1,2$ (from left to right). The horizontal axis is the energy *E* in atomic units.

In closing this section, we add a few technical notes. The first is about calculating the matrix elements of the potential function, $V_{n,m}=\langle\psi_n|V|\psi_m\rangle$, which is needed for the evaluation of the total Hamiltonian matrix $H_{n,m}=(H_0)_{n,m}+V_{n,m}$. We have used Gauss quadrature integral approximation associated with the Laguerre polynomials (see, for example, Section 2 of Ref. [14] for details of this technique). The second note is that physical results do not change significantly (within the desired accuracy) if the scale parameter λ varies within a certain range of values called the "plateau of stability". The size of this plateau increases with the size of the basis *N* becoming infinite when $N\to\infty$ (i.e., physical results will then be independent of λ). The third note is about the calculation of deep resonances (those with large negative imaginary parts). One could use complex scaling/rotation where the scale parameter λ is replaced by $\lambda e^{-i\varphi}$ with $\varphi\gtrapprox-\frac{1}{2}\arg(E_{res})$ but such that $\varphi<\pi/4$.

6. Conclusion

In this work, we made a detailed and complete calculation of the finite matrix representation of the resolvent operator in any square-integrable basis. The work is useful for scientist and engineers who are looking for such treatment in one place and whether the basis chosen is orthogonal or not. Formulas (17) and (21) are particularly valuable because of the associated reduction in computational cost. An interesting byproduct of this study is an expression for the elements of the normalized eigenvectors (generalized eigenvectors) in terms of its eigenvalues (generalized eigenvalues) as given by (23) and (25), respectively.

As a physical application, we showed how to use these findings is calculating the resonance structure, bound state energies, and density of states in quantum mechanics.

Acknowledgement

I am grateful to Prof. H. A. Yamani for assistance in obtaining formula (21) for the finite Green's function $G_{n,m}^N(z)$ in an orthonormal basis with $n\neq m$.

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