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# On an "Equivalent Quadrature" Calculation of Matrix Elements of $(z - p^2/2m)^{-1}$ Using an $L^2$ Expansion Technique

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The problem of interpreting the $L^2$ discretization of an operator with a continuous spectrum is partially solved for the $s$-wave kinetic energy, $H^0$. It is shown that matrix elements of the resolvent operator $(z - \bar{H}^0)^{-1}$ where $\bar{H}^0$ is a matrix representation of $H^0$ in an $L^2$ basis, may be interpreted as quadrature approximations to the actual spectral representation of the resolvent, allowing the $z \to E + i\epsilon$ limit to be taken for $E$ in the continuous spectrum of $H^0$ with no residual error due to the poles of $(z - \bar{H}^0)^{-1}$. Specifically it is shown that diagonalization of $H^0$ in a Laguerre-type basis is equivalent to a Chebyschev quadrature of the second kind, allowing resolution of the problem of interpreting matrix elements of $(z - \bar{H}^0)^{-1}$ in the entire cut $z$-plane.

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## 1. Introduction

The Rayleigh–Ritz variational principle provides a simple procedure for numerical calculation of approximations to the discrete eigenvalues and eigenfunctions of a Hamiltonian operator $H$: The matrix representation $\bar{H}$ is formed in a subspace of the full Hilbert space defined by choice of a finite basis of square integrable ($L^2$) functions and the matrix eigenvalues and eigenvectors computed. On the other hand, if we are interested in the continuous spectrum of $H$ it is not immediately clear what information is contained in the discrete eigenvalues and normalizable eigenvectors of $\bar{H}$, although the "stabilization" technique has made progress in this direction [1]. For example, in application of the standard variational principles of scattering theory one constructs $(z - \bar{H})^{-1}$ as an approximation to $(z - H)^{-1}$. Analysis of the problems caused by this representation, which does not preserve the analytic properties of the operator inverse was begun by Schwartz [2] and has been continued by Nesbet *et al.* [3] in a detailed analysis of the computational singularities of the Kohn and inverse Kohn principles.

In this paper we take up the challenge given by Schwartz [2] of learning to directly interpret the eigenvalues and eigenvectors of $\bar{H}$ which correspond to those of $H$. We have not been able to solve the problem in any generality; however, in the simple case that

$$H = H^0 = -\frac{1}{2}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}, \tag{1.1}$$

the radial $s$-wave kinetic energy, progress can be made and some idea of how to approach the general problem obtained. Specifically, we present a technique for calculation of matrix elements of $(z - H^0)^{-1}$, the unperturbed $s$-wave Green's function for the partial wave Lippmann–Schwinger equation, using finite $L^2$ expansions in such a way that the approximation is valid for all $z$ in the cut complex energy plane, including in the $z \to E + i\epsilon$ limit. The direct motivation for considering this restricted problem was to gain an understanding of the process of extracting scattering information from approximations to the Fredholm determinant calculated entirely in a finite $L^2$ basis [4]. Application of the present results to this problem are given elsewhere [5]. The principle results of the present work are that diagonalization of $H^0$ in a basis of $L^2$ functions is equivalent to a specific numerical quadrature approximation to the ordinary spectral representation of $(z - H^0)^{-1}$, and that this equivalence allows construction of an approximation to $\langle (z - H^0)^{-1} \rangle$ valid for all $z$. That is, we develop a formalism which allows us to embed a finite matrix approximation $\langle (z - \bar{H}^0)^{-1} \rangle$ in an approximation which preserves the analytic properties of the actual matrix element.

In Section 2 we introduce, in a qualitative manner, the idea of an "equivalent quadrature" and show how this idea allows interpretation of an $L^2$ approximation to $(z - H^0)^{-1}$ in such a way as to obtain results in the $z \to E + i\epsilon$ limit. In Sections 3 and 4 two different $L^2$ basis sets are considered and shown to give results which may be interpreted as numerical quadratures. In particular, it is shown that the results obtained by diagonalization of $H^0$ in a basis of Laguerre-type functions is equivalent to a Chebyschev quadrature of the second kind. A discussion and a statement of a more general version of this problem are given in Section 5.

## 2. The Method of Equivalent Quadrature

### a. *The Idea of an Equivalent Quadrature*

Consider the following approximation scheme. To obtain an approximate value of the matrix element

$$\langle f \mid G^0(z) \mid f \rangle \tag{2.1}$$

where

$$G^0(z) = (z - H^0)^{-1}, \tag{2.2}$$

$$H^0 = -\frac{1}{2}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} \tag{2.3}$$

and $|f\rangle$ is assumed to be a well-behaved square integrable function, we consider

$$\left\langle f \left| \frac{1}{z - \bar{H}^0} \right| f \right\rangle = \sum_{i=1}^{N} \frac{\langle f \mid \chi_i \rangle \langle \chi_i \mid f \rangle}{z - E_i^0}, \tag{2.4}$$

where $\chi_i$ and $E_i^0$ are the (normalized) eigenfunctions and eigenvalues of the matrix $\bar{H}^0$ which is the matrix representation of $H^0$ taken in a set of $N$ square integrable basis functions $\{\psi_i\}$, and $\langle \chi \mid f \rangle = \int_0^\infty r^2 \chi(r) f(r)\, dr$, it being assumed that all the functions are real. That is, we replace

$$\langle f \mid (z - H^0)^{-1} \mid f \rangle \tag{2.5}$$

by

$$\langle f \mid (z - \bar{H}^0)^{-1} \mid f \rangle, \tag{2.6}$$

$\bar{H}^0$ being a matrix representation of $H^0$. The question now arises as to what extent such a replacement is possible, or even well defined; in particular how are we to interpret $\langle f \mid (z - \bar{H}^0)^{-1} \mid f \rangle$ in the limit as $z \to E + i\epsilon$ for real positive $E$ in the continuous spectrum of $H^0$, where $(z - H^0)^{-1}$ has a cut and $(z - \bar{H}^0)^{-1}$ has simple poles?

To answer this question we examine an alternate method for calculating the matrix element $\langle f|(z - H^0)^{-1}|f\rangle$. The normal spectral representation of $(z - H^0)^{-1}$ is given by [6]

$$\frac{1}{z - H^0} = \int_0^\infty \frac{dE\,|E\rangle\langle E|}{z - E} \tag{2.7}$$

where $|E\rangle = (2k/\pi)^{1/2} j_0(kr)$ the $j_0(kr)$ being the usual spherical bessel function, and $E = k^2/2$. In terms of this spectral representation we may write,

$$\langle f|(z - H^0)^{-1}|f\rangle = \int_0^\infty \frac{dE\langle f|E\rangle\langle E|f\rangle}{z - E} \tag{2.8}$$

where

$$\langle f|E\rangle = (2k/\pi)^{1/2} \int_0^\infty r^2 dr f(r)\, j_0(kr). \tag{2.9}$$

If we now introduce a numerical quadrature approximation of the type[1]

$$\int_0^\infty dEg(E) \approx \int_0^{E^{\max}} dEg(E) \cong \sum_{i=1}^{N} \omega_i g(E_i), \tag{2.10}$$

$\omega_i$ and $E_i$ being a set of quadrature weights and abscissas, we have

$$\langle f|(z - H^0)^{-1}|f\rangle^{\text{quad}} = \sum_{i=1}^{N} \frac{\omega_i\langle f|E_i\rangle\langle E_i|f\rangle}{z - E_i}. \tag{2.11}$$

If by some coincidence, or arrangement, the quadrature abscissas $E_i$ of Eq. (2.11) are the same as the eigenvalues $E_i^0$ of $\bar{H}^0$, we would be tempted to equate the residues of Eqs. (2.4) and (2.11) with the result that

$$|\langle f|\chi_i(E_i^0)\rangle|^2 = |\langle f|E_i^0\rangle|^2\, \omega_i\,. \tag{2.12}$$

Avoiding for the moment a detailed discussion of the validity of Eq. (2.12), which will certainly be an approximation in most cases (e.g., $f(r)$ might extend beyond the range of the basis $\{\psi_i(r)\}$), we have the suggestion that the approximation of Eq. (2.4) is related, in some way, to the quadrature approximation of Eq. (2.11). That is, use of a $L^2$ basis to define the matrix $\bar{H}^0$ implies a quadrature approximation to the spectral representation of Eq. (2.8). We call this quadrature the "equivalent quadrature" generated by the basis $\{\psi_i\}$. In the following section we will give two explicit examples of "equivalent quadratures" generated by different choices of the $L^2$ basis. Before doing this we show that the assumption of an equivalent

[1] The cutoff $E^{\max}$ is introduced purely to simplify the notation — an alternative, explored in Section 4, is to map $[0, \infty]$ onto the finite interval $[-1, +1]$.

quadrature will allow us to embed the $L^2$ approximation to $\langle f|(z - H^0)^{-1}|f\rangle$ in an approximation which is valid in the $z \to E + i\epsilon$ limit, providing only that $\langle f | E\rangle$ is a smooth function of $E$.

b. *A Dispersion Correction Formula*

The approximation

$$\langle f|(z - H^0)^{-1}|f\rangle^{\text{quad}} = \sum_{i=1}^{N} \frac{\omega_i\langle f | E_i\rangle\langle E_i | f\rangle}{z - E_i} \tag{2.13}$$

apparently suffers from the same problem that Eq. (2.4) does; in replacing the cut by a row of poles we have lost the ability to take the $z \to E + i\epsilon$ limit. However, in the case of a numerical quadrature approximation to $(z - H^0)^{-1}$ this is easily remedied. In the $z \to E + i\epsilon$ limit we have

$$\int_0^\infty \frac{\langle f | E\rangle\langle E | f\rangle}{E_0 + i\epsilon - E} = P\int_0^\infty \frac{\langle f | E\rangle\langle E | f\rangle}{E_0 - E} - i\pi\,|\langle f | E_0\rangle|^2. \tag{2.14}$$

The principal value integration may be performed numerically with no error due to the singularity [7] as

$$\begin{aligned} &P\int_0^\infty \frac{\langle f | E\rangle\langle E | f\rangle}{E_0 - E}\,dE \\ &\approx P\int_0^{E^{\max}} dE\,\frac{\langle f | E\rangle\langle E | f\rangle}{E_0 - E} \\ &= \int_0^{E^{\max}} \frac{(|\langle f | E\rangle|^2 - |\langle f | E_0\rangle|^2)}{E_0 - E}\,dE + |\langle f | E_0\rangle|^2 \int_0^{E^{\max}} \frac{dE}{E_0 - E} \\ &\cong \sum_{i=1}^{N} \frac{\omega_i\,|\langle f | E_i\rangle|^2}{E_0 - E} + |\langle f | E_0\rangle|^2 \left\{\int_0^{E^{\max}} \frac{dE}{E_0 - E} - \sum_{i=1}^{N} \frac{\omega_i}{E_0 - E_i}\right\} \end{aligned} \tag{2.15}$$

provided there is a $C$ such that the Lipschitz condition

$$\big|\,|\langle f | E\rangle|^2 - |\langle f | E_0\rangle|^2\,\big| < C\,|E - E_0|$$

holds. In this case the "correction" term

$$|\langle f | E_0\rangle|^2 \left\{\int_0^{E^{\max}} \frac{dE}{E_0 - E} - \sum_{i=1}^{N} \frac{\omega_i}{E_0 - E_i}\right\} \tag{2.16}$$

allows computation of approximations to

$$P\int_0^\infty \frac{|\langle f | E\rangle|^2}{E_0 - E}\,dE$$

over a continuous range of $E^0$ using a fixed set of quadrature weights and abscissas $(\omega_i, E_i)$ provided that $\langle f | E_0\rangle$ is interpolable from the discrete set $\{\langle f | E_i\rangle\}_{i=1,n}$. Assuming that this is the case we have

$$\langle f | (E + i\epsilon - H^0)^{-1} | f\rangle$$
$$\approx \sum_{i=1}^{N} \frac{\omega_i |\langle f | E_i\rangle|^2}{E_0 - E_i} + |\langle f | E_0\rangle|^2 \left\{ \int_0^{E^{\max}} \frac{dE}{E_0 - E} - \frac{\omega_i}{E_0 - E_i} \right\} - i\pi |\langle f | E_0\rangle|^2 \tag{2.17}$$

which is valid in a numerical quadrature sense for all $E_0 < E^{\max}$. We have thus embedded the numerical approximation of Eq. (2.11) which appeared to be valid only for complex $z$, into an approximation which allows direct construction of the $E + i\epsilon$ limit. Using the "equivalent quadrature" idea introduced in Section 2(a) we now do the same for the $L^2$ approximation of Eq. (2.4).

Assuming that the $L^2$ diagonalization of $H^0$ gives a set of abscissas $E_i^0$ and that, in some sense,

$$|\langle f | \chi_i\rangle|^2 = |\langle f | E_i^0\rangle|^2 \omega_i^{\mathrm{Eq}}$$

as suggested by Eq. (2.12), we interpret

$$\sum_{i=1}^{N} \frac{|\langle f | \chi_i\rangle|^2}{z - E_i^0}$$

as a quadrature approximation to $\langle f |(z - H^0)^{-1} | f\rangle$ with "equivalent quadrature" weights $\omega_i^{\mathrm{Eq}}$ and abscissas $E_i^0$. Now using Eq. (2.17) in the $z \to E + i\epsilon$ limit we have

$$\langle f | (E_0 + i\epsilon - H^0)^{-1} | f\rangle \tag{2.18}$$
$$= \sum_{i=1}^{N} \frac{|\langle f | \chi_i\rangle|^2}{E_0 - E_i^0} + |\langle f | E_0\rangle|^2 \left\{ \int_0^{E^{\max}} \frac{dE}{E_0 - E} - \sum_{i=1}^{N} \frac{\omega_i^{\mathrm{Eq}}}{E_0 - E_i^0} \right\} - i\pi |\langle f | E_0\rangle|^2$$

where we obtain $\langle f | E_0\rangle$ from the results of our $L^2$ calculation by use of Eq. (2.12):

$$|\langle f | E_i^0\rangle|^2 \equiv |\langle f | \chi_i\rangle|^2 / \omega_i^{\mathrm{Eq}} \tag{2.19}$$

followed by interpolation to obtain $|\langle f | E_0\rangle|^2$. Note that the construction of $|\langle f | E_i^0\rangle|^2$ requires *explicit* knowledge of the "equivalent quadrature" weights $\omega_i^{\mathrm{Eq}}$.

In summary, given an $L^2$ approximation to $(z - H^0)^{-1}$ if we assume the existence of a set of "equivalent quadrature" weights, and if these weights are explicitly known, we can embed $\langle f |(z - \bar{H}^0)^{-1} | f\rangle$ into an approximation which retains the actual cut structure of the matrix element. We now construct some "equivalent quadratures."

## 3. An "Equivalent Quadrature" Generated by Box Quantization

Consider the set of orthogonal $L^2$ functions which are eigenfunctions of

$$H^0 = -\frac{1}{2}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}$$

in a spherical box of radius $R$. These functions satisfy the boundary conditions

$$\psi_n(0) = \psi_n(R) = 0 \tag{3.1}$$

and are,

$$\psi_n^{\text{box}}(r) = c_n j_0(k_n r) \tag{3.2a}$$

where

$$k_n = n\pi/R; \quad E_n{}^0 = k_n{}^2/2. \tag{3.2b}$$

If we require

$$\int_0^R r^2\, dr \psi_n(r)\, \psi_m(r) = \delta_{nm} \tag{3.2c}$$

the $c_n$ are determined as

$$c_n = ((2/R)\, k_n{}^2)^{1/2}. \tag{3.3}$$

Using this $L^2$ basis we have

$$\left\langle f \left| \frac{1}{z - \overline{H}^0} \right| f \right\rangle = \sum_{i=1}^{N} \frac{|\langle f \mid \psi_n\rangle^{\text{box}}|^2}{z - E_i^0}, \tag{3.4}$$

where

$$\langle f \mid \psi_n\rangle^{\text{box}} = \int_0^R r^2\, dr\, f(r) \left(\frac{2k_n}{R}\right)^{1/2} j_0(k_n r) \tag{3.5}$$

as the $L^2$ approximation to

$$\langle f | (z - H^0)^{-1} | f\rangle.$$

To see what "equivalent quadrature" is implicit in the approximation of Eq. (3.4) we consider a numerical approximation with as yet undetermined weights $\omega_i^{\mathrm{Eq}}$ to the exact spectral representation

$$\int_0^{E^{\max}} dE \frac{\langle f \mid E\rangle\langle E \mid f\rangle}{z - E} = \sum_{i=1}^{N} \frac{\omega_i^{\mathrm{Eq}} \, |\langle f \mid E_i\rangle|^2}{z - E_i} \tag{3.6}$$

where now

$$| E_i\rangle = (2k_i/\pi)^{1/2} j_0(k_i r) \tag{3.7}$$

and we require that the numerical quadrature have the same abscissas as Eq. (3.4); that is, $E_n = k_n^2/2$. Equating the residues of Eq. (3.7) with those of Eq. (3.4) gives

$$(2k_i^2/R) \, |\langle f \mid j_0(k_i r)\rangle^{\mathrm{box}}|^2 = \omega_i^{\mathrm{Eq}}(2k_i/\pi) \, |\langle f \mid j_0(k_i r)\rangle|^2, \tag{3.8}$$

which is exact if $f(r) = 0$ for $r > R$, and certainly becomes exact as $R \to \infty$ in the more general case. Assuming that it is at least a reasonable approximation to assume that

$$\langle f \mid j_0(k_n r)\rangle^{\mathrm{box}} = \langle f \mid j_0(k_n r)\rangle,$$

we conclude

$$\omega_n^{\mathrm{Eq}} = \pi k_n/R = n\pi^2/R^2, \tag{3.9}$$

which are the weights for the equivalent quadrature generated by the box-normalized $L^2$ basis.

We can easily check that this set of weights does define a quadrature by taking

$$E_{\max} = \sum_n \omega_n^{\mathrm{Eq}} = \frac{\pi^2}{R^2} \frac{N(N+1)}{2} \tag{3.10a}$$

and then performing the first moment of $E$ as

$$\sum_n \omega_n E_n = \frac{1}{2} \frac{\pi^4}{R^4} \sum_n n^3 = \frac{1}{2} \frac{\pi^4}{R^4} \left(\frac{N(N+1)}{2}\right)^2 = E_{\max}^2/2, \tag{3.10b}$$

which is, indeed, the correct result. Higher moments contain errors, which means that the quadrature is essentially trapezoidal.

The essence of the equivalent quadrature method now becomes clear; over a restricted region of space, in this case $0 < r < R$, $| \chi_i\rangle \cong | E_i\rangle$, to within a normalization factor. The difference between the unit normalization of the $L^2$ function $| \chi_i\rangle$ and the continuum normalization of $| E_i\rangle$ being related to the weight for the "equivalent quadrature."

## 4. Laguerre Functions and Chebyschev Quadrature

### a. *Diagonalization of $H^0$ in a Laguerre Basis*

The $s$-wave kinetic energy can be diagonalized in the (nonorthogonal) basis of Laguerre type functions

$$e^{-\alpha r/2}\, \alpha L_n{}^1(\alpha r), \quad n = 0,\ldots, N-1, \tag{4.1}$$

following the technique outlined by Schwartz [2]. The resulting eigenvalues are

$$E_n^{(N)} = \frac{k_n{}^2}{2} = \frac{\alpha^2}{8}\frac{1 + x_n^{(N)}}{1 - x_n^{(N)}} \tag{4.2a}$$

$$x_n^{(N)} = \cos((n+1)\pi/(N+1)) \qquad n = 0, 1, 2,\ldots, N-1, \tag{4.2b}$$

and the normalized, square integrable, eigenfunctions are [8]

$$\chi_i^{\mathrm{Lag}(N)} = A_i e^{-\alpha r/2}(\alpha) \sum_{n=0}^{N-1} \frac{1}{(n+1)}\, U_n(x_i^{(N)})\, L_n{}^1(\alpha r), \qquad n = 0,\ldots, N-1, \tag{4.3a}$$

where

$$A_i = \left(\frac{\alpha(1 + x_i^{(N)})}{N+1}\right)^{1/2} \frac{1}{U_{N-1}(x_i^{(N)})} \tag{4.3b}$$

and $U_N(x)$ is a Chebyschev polynomial of the second kind (the $U_N(x)$ are orthogonal on $[-1, +1]$ with the weight function $(1 - x^2)^{1/2}$).

We now note the rather striking fact that under the mapping

$$E \to \frac{\alpha^2}{8}\frac{1+x}{1-x} \qquad \text{or} \qquad x = \frac{E - \alpha^2/8}{E + \alpha^2/8} \tag{4.4}$$

the transformed eigenvalues

$$x_n^{(N)} = \cos((n+1)\pi/(N+1)), \qquad n = 0, 1,\ldots, N-1, \tag{4.5a}$$

are the roots of the $N$-th order Chebyschev polynomials of the second kind [9, 10]. This immediately suggests that calculation of $\langle f|(z - \bar{H}^0)^{-1}|f\rangle$ where $\bar{H}^0$ is the representation of $H^0$ in the basis of Eq. (4.1) may be interpreted, with an appropriate change of variables, as a Chebyschev quadrature of the second kind, and that the "equivalent quadrature" weights are the Chebyschev weights [11]

$$\omega_n^{\mathrm{Ch}}(N) = \frac{\pi}{N+1} \sin^2\left(\frac{(n+1)\pi}{N+1}\right) \tag{4.5b}$$

appropriate to a Chebyschev quadrature of the second kind. The proof of this conjecture is given in the following subsection. In what follows we will write $x_i = x_i^{(N)}$, $\omega_i^{\mathrm{Ch}} = \omega_j^{\mathrm{Ch}}(N)$, it being understood that we are referring to an $N$-th order quadrature.

b. *A Chebyschev Equivalent Quadrature*

Consider the approximation of

$$\langle f \mid (z - H^0)^{-1} \mid f \rangle = \int_0^\infty \frac{\langle f \mid E \rangle \langle E \mid f \rangle}{z - E}\, dE \tag{4.6a}$$

by

$$\langle f \mid (z - \bar{H}^0)^{-1} \mid f \rangle = \sum_{i=0}^{N-1} \frac{\langle f \mid \chi_i^{\mathrm{Lag}} \rangle \langle \chi_i^{\mathrm{Lag}} \mid f \rangle}{z - E_i} \tag{4.6b}$$

where the $E_i$ are given by Eq. (4.2a). We show that if $f(r)$ is representable in the form

$$f(r) = \sum_{i=0}^{N-1} a_i L_i^1(\alpha r)\, e^{-\alpha r/2}$$

where the $a_i$ are arbitrary coefficients, that the sum of Eq. (4.6b) is *identical* to a Chebyshev approximation to the integral of Eq. (4.6a); in the case that $f(r)$ is not given exactly by a finite Laguerre expansion we will see that Eq. (4.6b) represents an *approximate* Chebyschev quadrature approximation to the integral of Eq. (4.6a).

To demonstrate these results we first rewrite Eq. (4.6) as

$$\int_0^\infty dE\, \frac{|\langle f \mid E \rangle|^2}{z - E} = \frac{\alpha^2}{4} \int_{-1}^{+1} \frac{dx}{(1-x)^2}\, \frac{1}{z - E(x)}\, |\langle f \mid E(x) \rangle|^2 \tag{4.7}$$

where

$$E(x) = ((1 + x)/(1 - x))\, \alpha^2/8. \tag{4.4}$$

We now approximate the integral of Eq. (4.7) by a quadrature with as yet unspecified weights, $\omega_i^{\mathrm{Eq}}$, but choosing the $x_i$ to be given by Eq. (4.5a), that is corresponding to the transformed eigenvalues of $\bar{H}^0$ as defined in Eq. (4.4). Thus we take

$$\frac{\alpha^2}{4} \int_{-1}^{+1} \frac{dx}{(1-x)^2}\, \frac{1}{z - E(x)}\, |\langle f \mid E(x) \rangle|^2$$
$$\approx \frac{\alpha^2}{4} \sum_{i=0}^{N-1} \frac{\omega_i^{\mathrm{Eq}}}{(1-x_i)^2}\, \frac{1}{(z - E(x_i))}\, |\langle f \mid E(x_i) \rangle|^2 \tag{4.8}$$

Equating residues of Eqs. (4.6b) and (4.8) gives:

$$(\alpha^2/4\omega_i^{\mathrm{Eq}}/(1-x_i)^2)\,|\langle f\,|\,E(x_i)\rangle|^2 = |\langle f\,|\,\chi_i^{\mathrm{Lag}}\rangle|^2 \tag{4.9}$$

Using the representation [12]

$$\left(\frac{2}{\pi}\right)^{1/2}\sin(k(x)r) = 2\left(\frac{2}{\pi}\right)^{1/2}\left(\frac{2\alpha k(x)}{4k(x)+\alpha^2}\right)e^{-\alpha r/2}(\alpha r)\sum_{n=0}^{\infty}\frac{1}{n+1}\,U_n(x)\,L_n^{1}(\alpha r), \tag{4.10}$$

where $x$ is given by Eq. 4.4, we see that it is reasonable to equate the matrix elements

$$\left\langle f\left|\sum_{n=0}^{\infty}(\alpha)\,e^{-\alpha r/2}\frac{1}{n+1}\,U_n(x)\,L_n^{1}(\alpha r)\right.\right\rangle \tag{4.11a}$$

and

$$\left\langle f\left|\sum_{n=0}^{N-1}(\alpha)\,e^{-\alpha r/2}\frac{1}{n+1}\,U_n(x)\,L_n^{1}(\alpha r)\right.\right\rangle, \tag{4.11b}$$

which is exact if

$$f(r) = \sum_{n=0}^{N-1} a_n L_n^{1}(\alpha r)\,e^{-\alpha r/2}.$$

as

$$\int_0^{\infty} d(\alpha r)(\alpha r)\,e^{-\alpha r}L_n^{1}(\alpha r)\,L_m^{1}(\alpha r) = 0, \qquad m \neq n,$$

and becomes exact as $N \to \infty$ in the general case provided that the $L^2$ function $f(r)$ is not pathological.

Assuming the validity of equating the matrix elements of Eqs. (4.11a and b), we have immediately

$$\omega_n^{\mathrm{Eq}} = |\langle f\,|\,\chi_n^{\mathrm{Lag}}\rangle|^2 \Big/ \frac{1}{(1-x_n)^2}\frac{\alpha^2}{4}|\langle f\,|\,E_n\rangle|^2$$

$$= \frac{\left|\left(\dfrac{\alpha(1+x_n)}{N+1}\right)^{1/2}\dfrac{1}{U_{N-1}(x_n)}\right|^2\dfrac{1}{k(x_n)}}{\dfrac{\alpha^2}{4}\dfrac{1}{(1-x_n)^2}\left|\dfrac{2}{k(x_n)}\left(\dfrac{2}{\pi}\right)^{1/2}\left(\dfrac{2\alpha k(x_n)}{4k(x_n)^2+\alpha^2}\right)\right|^2}. \tag{4.13}$$

Using the fact that [9]

$$U_{N-1}(\cos\psi_n)^2 = \left(\sin N\frac{(n+1)\pi}{N+1}\Big/\sin\frac{(n+1)\pi}{N+1}\right)^2 = 1 \tag{4.14}$$

and

$$x_n = \cos\psi_n = \cos((n+1)\pi/(N+1))\ n = 0, 1,..., N-1,$$

Eq. 4.13 may be simplified using standard trigonometric identities, giving

$$\omega_n^{\mathrm{Eq}} = \frac{\pi}{N+1}\sin^2\left(\frac{(n+1)\pi}{N+1}\right)\frac{1}{(1-x_n^2)^{1/2}} \tag{4.15}$$

which is the appropriate Chebyschev weight for the Chebyschev quadrature of the second kind [11]:

$$\int_{-1}^{+1}(1-x^2)^{1/2}\,g(x)\,dx = \sum_{n=0}^{N-1}\omega_n^{\mathrm{Ch}}g(x_n) \tag{4.16a}$$

where

$$\omega_n^{\mathrm{Ch}} = \frac{\pi}{N+1}\sin^2\left(\frac{(n+1)\pi}{N+1}\right) \tag{4.16b}$$

and

$$x_n = \cos((n+1)\pi/(N+1)) \tag{4.16c}$$

which is exact if $g(x)$ is a polynomial degree $2N-1$ or less. Equations (4.16a and b) make the origin of the $(1-x_n^2)^{-1/2}$ factor in Eq. 4.15 clear.

We have thus shown explicitly that the differences in normalization of $|\chi_n^{\mathrm{Lag}}\rangle$ and $|E_n\rangle$ implies that the $L^2$ approximation to $\langle f|(x-H^0)^{-1}|f\rangle$ is a Chebyschev quadrature if $f$ is of the form of Eq. 4.12, and an approximation to such a Chebyschev quadrature to the extent that the matrix element of Eq. (4.11b) only approximates that of Eq. (4.11a). This identification implies the Chebyschev interpolation scheme discussed in the following subsection.

c. *A Chebyschev interpolation*

Once it is realized that diagonalization of $H^0$ in a Laguerre function basis is equivalent to a Chebyschev quadrature with weight

$$\omega_n^{\mathrm{Ch}} = \pi/(N+1)\sin^2((n+1)\pi/(N+1))$$

and abscissa

$$x_n^{(N)} = \cos((n+1)\pi/(N+1))$$

we can apply the technique of Section 2b to embed the approximation of Eq. (4.6b) into a form which allows an interpolative construction of the $z \to E + i\epsilon$ limit. The appropriate formula is

$$\left\langle f \left| \frac{1}{E_0 + i\epsilon - H^0} \right| f \right\rangle = \sum_{n=0}^{N-1} \frac{\langle f \mid \chi_n^{\mathrm{Lag}} \rangle \langle \chi_n^{\mathrm{Lag}} \mid f \rangle}{E_0 - E(x_n)} + \frac{\alpha^2}{4} \frac{\langle f \mid E_0 \rangle \langle E_0 \mid f \rangle}{(1 - x_0)^2 (1 - x_0^2)^{1/2}}$$

$$\times \left\{ \int_{-1}^{+1} \frac{(1 - x^2)^{1/2}}{E_0 - E(x)} dx - \sum_{n=0}^{N-1} \frac{\omega_n^{\mathrm{Ch}}}{E_0 - E(x_n)} \right\}$$

$$- i\pi \, |\langle f \mid E_0 \rangle|^2, \tag{4.17}$$

where

$$x_0 = (E_0 - \alpha^2/8)/(E_0 + \alpha^2/8)$$

and the $|\langle f \mid E_0 \rangle|^2$ are calculated by interpolating the $|\langle f \mid E(x_i) \rangle|^2$ which are obtained as

$$|\langle f \mid E(x_i) \rangle|^2 = \frac{(1 - x_i^2)^{1/2} (1 - x_i)^2}{\omega_i^{\mathrm{Ch}}} \frac{4}{\alpha^2} |\langle f \mid \chi_i^{\mathrm{Lag}} \rangle|^2. \tag{4.18}$$

Application of Eqs. (4.17) and (4.18) to extraction of elastic scattering information from $L^2$ approximations to the partial wave Fredholm determinant is considered in [5].

## 5. Discussion

We have shown, for two specific cases, that calculation with an $L^2$ discretized matrix representation of an operator with a continuous spectrum is equivalent to a numerical quadrature approximation to the spectral representation of the operator. This realization permits the embedding of the discrete representation into an approximation which retains the correct spectral properties of the operator being considered. In this sense the problem, posed by Schwartz [2], of learning to squarely face the singularities of an $L^2$ discretized operator inverse has been solved for the simplest case, namely $H = H^0$. The work presented here may be generalized to higher partial waves and to the use of more general $L^2$ basis sets related to the classical orthogonal polynomials [13]. However, we have not been able to make satisfactory progress in finding the equivalent quadratures in two interesting more general cases.

(1) If $H^0$ is formed in a basis *not* simply related to the classical orthogonal

polynomials, e.g., in the basis of Slater-type functions, $r^{n_i}e^{-\xi_i r}$ with several different $\xi_i$, $H^0$ probably cannot be diagonalized analytically and the comparison of Eqs. (4.11a and b) is not directly possible.

(2) Even using well understood basis functions the potential scattering Hamiltonian $H = H^0 + V$ will probably not admit analytic diagonalization unless it is soluble anyway, and thus of limited interest, except in defining a distorted wave Green's function.

In each of these cases one could proceed numerically and construct the eigenfunctions of $H$ and $\bar{H}$, normalize them according to

$$\langle E \mid E' \rangle = \delta(E - E') \qquad \text{and} \quad \langle E_i \mid E_j \rangle = \delta_{ij},$$

respectively, and determine the weights from direct comparison of the functions over a limited region of coordinate space, in analogy with the methods of Section 3, or by comparison of coordinate space generalized moments within the subspace defined by the basis set (as done in Section 4), and then construct the "equivalent quadrature" weights directly in the spirit of Eq. (3.8) or (4.9). At first glance one might expect that his sort of procedure is the best one can hope for, as it appears to be the natural generalization of the method used in Sections 3 and 4, appropriate in those cases where analytic results are not available.

It is possible, however, to approach the problem in an alternate way, without explicit comparison of the eigenfunctions of $H$ and $\bar{H}$. Equivalent quadrature weights may be extracted by direct examination of the pole density of $\langle f \mid (z - \bar{H})^{-1} \mid f \rangle$ defining weights by a variety of pole spacing averaging techniques [14]. This works well for large basis sets in the case where the poles are roughly evenly spaced, but is not as accurate as the Chebyschev results. It may also prove possible to extract information directly from the energy moments [15] of $\langle f \mid (z - \bar{H})^{-1} \mid f \rangle$, but at present this implicitly requires "equivalent quadrature" weights obtained by a pole spacing averaging technique.

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