Finite-element method for computing scattering phase shifts from discrete models

R. K. Nesbet*
IBM Research Laboratory, San Jose, California 95193
(Received 9 February 1981)

A method is described which converts the dense distribution of pole singularities given by a discrete representation of a Green's function or resolvent operator into an approximation to the smooth function defined by the continuum limit of such a representation. The method uses a finite-element approximation to the pole-strength distribution function, equivalent to the width function in a scattering problem. Three distinct applications of this method are provided by a model scattering problem, making use of Feshbach resonance theory, the Schwinger variational principle, and the theory of the Fredholm determinant, respectively.

I. INTRODUCTION

Hazi[1] has applied Stieltjes moment theory[2,3] to the problem of calculating widths of electron-scattering resonances. In this method, a continuous approximation to the width function $\Gamma_d(E)$ is obtained from a discrete representation of the background energy continuum. The background eigenfunctions are constrained to be orthogonal to a discrete state ϕ_d (L^2 normalized). The interaction of ϕ_d with the background continuum is described by the resonance theory of Feshbach.[4] The resonant phase shift $\eta_1(E)$, defined relative to a background phase shift $\eta_0(E)$, is given by

$$\tan\eta_1(E) = -\tfrac{1}{2}\Gamma_d(E)/[E - E_d - \Delta_d(E)]. \tag{1}$$

The energy-shift function $\Delta_d(E)$ can be obtained by a numerical Hilbert transform of $\Gamma_d(E)$. Together, these functions define a complex energy-shift function

$$W_d(z) = \Delta_d(z) - \frac{i}{2}\Gamma_d(z), \tag{2}$$

which should be analytic for values of z in the upper half of the complex energy plane.

The mathematical situation to which Hazi's method applies can be described in terms of a finite Hamiltonian matrix in bordered diagonal form. A discrete representation of the background continuum is given by $N-1$ orthonormal functions $\{\phi_l\}$, all orthogonal to ϕ_d. The matrix elements are

$$H_{ll'} = E_l\delta_{ll'}, \quad l \neq d \tag{3}$$

together with transition elements H_{dl} and the diagonal element $E_d = H_{dd}$. The eigenvalues of this matrix are obtained by solving the secular equation

$$\lambda - E_d - \sum_l \frac{H_{dl}^2}{\lambda - E_l} = 0 \tag{4}$$

or

$$\lambda - E_d - \Delta_d(\lambda) = 0, \tag{5}$$

where

$$\Delta_d(\lambda) = \sum_l \frac{H_{dl}^2}{\lambda - E_l}. \tag{6}$$

As N increases, the eigenvalue spectrum $\{E_l\}$ becomes dense, and the limit of Eq. (6) cannot be taken directly. Hazi's method, originally applied to the special case of Feshbach resonance theory, can be considered in a more general context as a numerical method for estimating the complex function $W_d(z)$ of Eq. (2), taken to be the true limit of Eq. (6). The same mathematical structure occurs in the original application of Stieltjes moment theory to oscillator strength distributions.[2,3]

The basis of Hazi's method is the observation that the cumulative width function

$$F_d(E) = \int_0^E \Gamma_d(E')dE' \tag{7}$$

must be approximated by the sum

$$F_d(E) \cong \sum_{E_l \leq E} 2\pi H_{dl}^2. \tag{8}$$

It is assumed that the discrete spectrum $\{E_l\}$ approximates the complete continuum density of states orthogonalized to ϕ_d. Equation (8) is a consequence of Feshbach resonance theory, taking into account the relationship between the normalization of continuum wave functions and the density of states with respect to energy.

Equation (8) defines a histogram, which approaches the smooth function of Eq. (7) as the eigenvalue spectrum becomes dense. Moment theory[1,2] is used to define a smooth approximation to $F_d(E)$, which can then be differentiated to get $\Gamma_d(E)$. Equation (6) is replaced by the principal-

value integral

$$\Delta_d(E)=\frac{\mathcal{P}}{2\pi}\int_0^\infty \frac{\Gamma_d(E')dE'}{E-E'}, \tag{9}$$

equivalent to a Hilbert transform.

Equation (6) is a special case of the operator expression

$$\Delta H_{QQ}(z)=H_{QP}(z-H)^{-1}_{PP}H_{PQ} \tag{10}$$

involving the Green's function or resolvent operator $(z-H)^{-1}_{PP}$. In the partitioned Q space, ΔH_{QQ} is the effective Hamiltonian or generalized optical potential that describes interaction with the P-space continuum. The Stieltjes moment technique cannot be used for nondiagonal expressions such as

$$\Delta_{dd'}(\lambda)=\sum_l H_{dl}(\lambda-E_l)^{-1}H_{ld'}, \tag{11}$$

relevant to Eq. (10). Moment theory is not applicable because the distribution function $H_{dl}H_{ld'}$ is not in general positive definite.

In the present paper, a new computional method is proposed, applicable in principle to Eq. (11). Given a discrete representation of H_{PP}, in Eq. (10), this method provides an approximation to matrix elements of ΔH_{QQ}, valid in the continuum limit.

The computational method described in Sec. II is applied to a model scattering problem, described in Sec. III. Feshbach resonance theory is used in Sec. IV. The Schwinger variational principle is used in Sec. V. Section VI describes use of this method to evaluate the Fredholm determinant or Jost function.

An original purpose of this study was to examine a model problem in which a virtual state occurs. The case studied is that of scattering by a potential well with no external barrier, where the potential is too weak to support a bound state. This problem is discussed in standard works on scattering theory, for example, by Joachain.[5]

Although the Feshbach resonance theory is ordinarily applied to true resonances, there is nothing in principle to prevent use of this formalism for a virtual state. A narrow true resonance is characterized by relatively weak coupling between the postulated discrete state ϕ_d and the background scattering continuum. The effect of orthogonalizing the background wave functions to ϕ_d can be assumed to be small, so that the background phase shift $\eta_0(E)$ should be only weakly dependent on energy.

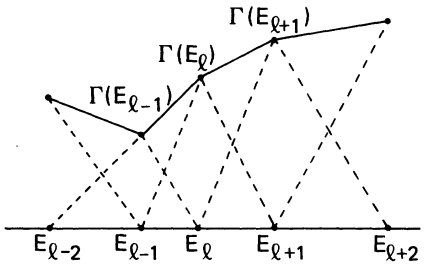

FIG. 1. Geometrical construction of $\Gamma(E)$.

In the example considered here, a natural choice of ϕ_d leads to a more complex situation: the width and shift functions are relatively large and the energy dependence of $\eta_0(E)$ is not small compared to that of the "resonant" phase shift $\eta_1(E)$. The model problem considered here provides an example of relatively strong coupling in the Feshbach theory. Methodology appropriate to such a case will be described, including methods suitable for direct calculation of the background or total phase shift.

II. NUMERICAL METHOD

In the histogram given by Eq. (8), the entire contribution $2\pi H^2_{dl}$ to the cumulative function $F_d(E)$ is concentrated at E_l. Thus $\Gamma_d(E)$ is represented by a sum of δ functions, each corresponding to one pole of $\Delta_d(E)$ in Eq. (6). When E_l represents a point in a continuous spectrum, it is much more reasonable to approximate $\Gamma(E)$ by a continuous function of E. If the pole strength H^2_{dl} associated with E_l is distributed in a continuous finite element extending only between the neighboring points E_{l-1} and E_{l+1}, the sum of such finite elements must converge to the correct $\Gamma(E)$ as the density of eigenvalues $\{E_l\}$ increases. A numerical method based on this construction is described here. The geometric construction of $\Gamma(E)$ is illustrated in Fig. 1.

A piecewise linear continuous approximation to $\Gamma(E)$ is given by a sum of triangular finite elements

$$\Gamma(E)=\sum_l \Gamma(l;E), \tag{12}$$

where

$$\Gamma(l;E)=\Gamma(l;E_l)\times\begin{cases}0, & E<E_{l-1}\\ (E-E_{l-1})/(E_l-E_{l-1}), & E_{l-1}\le E\le E_l\\ (E_{l+1}-E)/(E_{l+1}-E_l), & E_l\le E\le E_{l+1}\\ 0, & E_{l+1}<E\end{cases} \tag{13}$$

with

$$\Gamma(l;E_l)=4\pi H_{dl}^2/(E_{l+1}-E_{l-1}). \tag{14}$$

The area of each element is $2\pi H_{dl}^2$, as required by Eq. (8). To use these formulas for a finite grid (assuming $E_1>E_{\rm th}$ where $E_{\rm th}$ is the continuum threshold) of $N-1$ ordered values of E_l, two points must be added:

$$\begin{aligned} E_0&=E_{\rm th},\\ E_N&=2E_{N-1}-E_{N-2}. \end{aligned} \tag{15}$$

Equation (13) corresponds to a finite-element approximation to the complex energy-shift function of Eq. (2):

$$W(z)=\sum_l W(l;z), \tag{16}$$

where

$$W(l;z)=C(l;E_l)\left[\frac{z-E_{l-1}}{E_l-E_{l-1}}\ln\left(\frac{z-E_l}{z-E_{l-1}}\right)+\frac{E_{l+1}-z}{E_{l+1}-E_l}\ln\left(\frac{z-E_{l+1}}{z-E_l}\right)\right], \tag{17}$$

with

$$C(l;E_l)=-2H_{dl}^2/(E_{l+1}-E_{l-1}). \tag{18}$$

If the branches of the logarithms are taken so that $W(l;z)$ vanishes for large $|z|$ in the upper half-plane, Eq. (2) implies Eq. (13) for $\Gamma(l;E)$ on the real E axis. On this axis, the real part of W is

$$\Delta(E)=\sum_l \Delta(l;E), \tag{19}$$

where

$$\Delta(l;E)=C(l;E_l)\left(\frac{E-E_{l-1}}{E_l-E_{l-1}}\ln\left|\frac{E-E_l}{E-E_{l-1}}\right|+\frac{E_{l+1}-E}{E_{l+1}-E_l}\ln\left|\frac{E-E_{l+1}}{E-E_l}\right|\right). \tag{20}$$

Equation (20) can be obtained directly from Eq. (13) by evaluating the Hilbert transform as in Eq. (9). For $E=E_l$, the limiting value of Eq. (20) is

$$\Delta(l;E_l)=C(l;E_l)\ln[(E_{l+1}-E_l)/(E_l-E_{l-1})]. \tag{21}$$

If $\{E_l\}$ includes a true discrete spectrum, with some values of E_l below the continuum threshold at $E_{\rm th}$, these points contribute to real pole functions in $W(z)$, in the form $H_{dl}^2/(z-E_l)$, as in Eq. (6). These pole terms must be included in Eq. (19) for $\Delta(E)$ but omitted from Eq. (12) for $\Gamma(E)$, since they have no imaginary part for real E.

In applications to scattering theory, the finite elements of $\Gamma(E)$ should be modified to have correct analytic behavior for E near the continuum threshold $E_{\rm th}$. For this purpose, it is preferable to use the wave number or momentum (in units such that mass $m=1$)

$$k=[2(E-E_{\rm th})]^{1/2} \tag{22}$$

as an independent variable, rather than E, for $E>E_{\rm th}$. Use of piecewise linear functions of k as finite elements builds in the correct threshold dependence of $\Gamma(k)$ for short-range scattering potentials.

To define Γ as a function of k, Eq. (9) must be replaced for real values of k by

$$\Delta_d(k)=\frac{\mathcal{P}}{2\pi}\int_{-\infty}^{+\infty}\frac{\Gamma_d(k')dk'}{k-k'}+\cdots. \tag{23}$$

The pole terms here (denoted by ellipses) are the sum, Eq. (6), taken only for bound eigenstates with

$$E_b=E_{\rm th}-\kappa_b^2/2. \tag{24}$$

The poles occur at $\pm i\kappa_b$ in the complex k plane. Since $\Gamma_d(k)$ is required by threshold laws to be an odd function of real k, Eq. (23) implies that $\Delta_d(k)$ is an even function of real k.

For real positive k a piecewise linear continuous approximation to $\Gamma(k)$ is given by

$$\Gamma(k)=\sum_l \Gamma(l;k), \tag{25}$$

where

$$\Gamma(l;k)=\Gamma(l;k_l)\times\begin{cases}0, & k<k_{l-1}\\ (k-k_{l-1})/(k_l-k_{l-1}), & k_{l-1}\le k\le k_l\\ (k_{l+1}-k)/(k_{l+1}-k), & k_l\le k\le k_{l+1}\\ 0, & k_{l+1}<k\end{cases}. \tag{26}$$

The required normalization is

$$\int_0^\infty \Gamma(l;E)dE = \int_0^\infty \Gamma(l;k)k\,dk = \Gamma(l;k_l)A_l = 2\pi H_{dl}^2, \tag{27}$$

where the area of the second factor in Eq. (26) is

$$A_l = \tfrac{1}{6}(k_{l+1}+k_l+k_{l-1})(k_{l+1}-k_{l-1}). \tag{28}$$

Hence

$$\Gamma(l;k_l) = 2\pi H_{dl}^2/A_l. \tag{29}$$

The threshold law is built into Eq. (26) by taking $k_{l-1}=0$ for the first E_l above the continuum threshold.

Omitting bound-state poles, the complex energy-shift function corresponding to Eq. (26) is

$$W(k) = \sum_l W(l;k), \tag{30}$$

where, with

$$B(l;k_l) = -H_{dl}^2/A_l, \tag{31}$$

$$W(l;k) = B(l;k_l)\left[\frac{k-k_{l-1}}{k_l-k_{l-1}}\ln\left(\frac{k-k_l}{k-k_{l-1}}\right) - \frac{k+k_{l-1}}{k_l-k_{l-1}}\ln\left(\frac{k+k_l}{k+k_{l-1}}\right) + \frac{k_{l+1}-k}{k_{l+1}-k_l}\ln\left(\frac{k-k_{l+1}}{k-k_l}\right) - \frac{k_{l+1}-k}{k_{l+1}-k_l}\ln\left(\frac{k+k_l}{k+k_{l+1}}\right)\right]. \tag{32}$$

For real values of k, $\Delta(l;k)$ is given by Eq. (32) with the arguments of all logarithms replaced by their absolute values. This result can be obtained directly from Eqs. (23) and (26). For $k=k_l$ the limiting value is

$$\Delta(l;k_l) = B(l;k_l)\left[\ln\left(\frac{k_{l+1}-k_l}{k_l-k_{l-1}}\right) + \frac{k_l+k_{l-1}}{k_l-k_{l-1}}\ln\left(\frac{k_l+k_{l-1}}{2k_l}\right) + \frac{k_{l+1}+k_l}{k_{l+1}-k_l}\ln\left(\frac{k_l+k_{l+1}}{2k_l}\right)\right]. \tag{33}$$

The full expression for the energy shift for real k is

$$\Delta(k) = \sum_l \Delta(l;k) + \sum_b \frac{2H_{db}^2}{k^2+\kappa_b^2}, \tag{34}$$

where the sum over l excludes bound states, indicated by the index b in the second sum. For complex k, the branches of the logarithms in Eq. (32) are to be chosen so that $W(l;k)$ vanishes for large $|k|$ in the upper half-plane.

III. DESCRIPTION OF THE MODEL PROBLEM

The Schrödinger equation

$$\left(-\frac{1}{2}\frac{d^2}{dr^2}+V(r)-E\right)\phi(r)=0, \tag{35}$$

$$\phi(0)=0, \tag{36}$$

for the square-well potential function

$$V(r) = \begin{cases} -V_0, & 0\le r<r_0 \\ 0, & r_0<r \end{cases} \tag{37}$$

has simple analytic solutions. As discussed, for example, by Joachain,[5] Eq. (35) provides an example of a virtual state if the parameter $(2V_0r_0^2)^{1/2}$ is less than $\pi/2$. For larger values of this parameter the potential supports at least one bound state. Parameter values in dimensionless units

$$V_0 = 1.2,\quad r_0 = 1.0, \tag{38}$$

are used here, in the virtual-state regime.

The phase shift $\eta(E)$ for any positive energy E is easily computed from continuity conditions at r_0. A complete discrete set of eigenfunctions correspond to the imposed boundary condition for $r_1 > r_0$,

$$\phi_n(r_1) = 0. \tag{39}$$

The value of r_1 used for results reported here is 10.0, in dimensionless units. The eigenvalues $\{E_n\}$ are obtained by solving the transcendental equation obtained from continuity conditions at r_0. With the parameter values of Eq. (38), all eigenvalues E_n are positive.

For a model study of the Feshbach resonance formalism, a discrete state ϕ_d is defined as the lowest-energy eigenstate of the square-well potential $V_d(r)$ obtained from $V(r)$ of Eq. (37) by placing an infinite potential barrier at r_0. Then

$$\phi_d(r)=N_d \sin(k_d r), \quad r \leq r_0, \tag{40}$$

where k_d is π/r_0 and N_d is $(2/r_0)^{1/2}$. It should be noted that ϕ_d, which vanishes outside r_0, has discontinuous slope at r_0. When ϕ_d is acted on by the operator H-E of Eq. (35), this produces an inhomogeneous term proportional to a Dirac delta function at r_0.

The background continuum functions orthogonal to ϕ_d, required in the Feshbach theory, are solutions of the projection of Eq. (35) into a function space orthogonal to ϕ_d. These solutions can be constructed in closed form by standard methods, for any positive E, and the resulting background phase shift $\eta_0(E)$ can be computed. If the boundary condition of Eq. (39) is imposed, the projected Schrödinger equation has a discrete set of normalized eigenfunctions $\phi_l(r)$ and eigenvalues E_l. The transition matrix elements H_{dl} can be evaluated from explicit formulas. The functions and matrix elements mentioned here were evaluated and used in the calculations described below.

Exact phase shifts computed for the model problem are shown in Fig. 2. The total phase shift $\eta(E)$ is characteristic of a virtual state: It rises rapidly from the origin, following an $E^{1/2}$ law, then returns gradually to zero at large E. The background phase shift $\eta_0(E)$ shows no effect of the virtual state, but descends to $-\pi$ radians over a broad energy range. This could be called an antiresonance, since it represents the effect of removing one state from the energy spectrum. The difference phase shift $\eta_1(E)$, computed as $\eta-\eta_0$, combines these two features, converting the antiresonance of $\eta_0(E)$ into a broad resonance structure.

The numerical method described in Sec. II was tested on known analytic functions, computing the real part as the Hilbert transform of the imaginary part. In the model calculations, convergence was examined by varying the number N of discrete basis functions (or energy grid points E_n) and the parameter r_1, which determines the density of energy points. Results will be reported here only for $N=50$ and $r_1=10.0$.

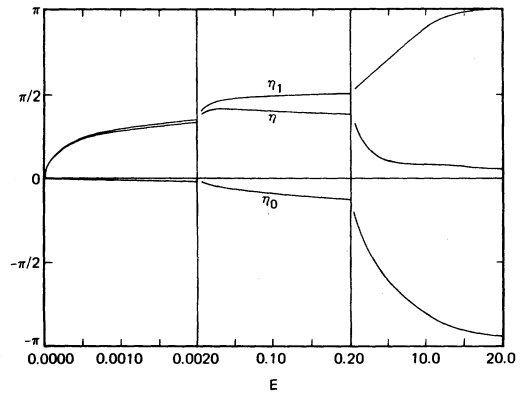

FIG. 2. Exact phase shifts.

IV. MODEL CALCULATIONS: FESHBACH THEORY

When the present method was applied to the model problem described above, it was found that the computed value of $\Delta_d(E)$ did not agree well with the value obtained directly from $\Gamma_d(E)$ and $\tan\eta_1$, which could be computed accurately from the wave function. The error in $\Delta_d(E)$ was nearly constant in E. This problem was traced to failure of the Hilbert transform relationship, Eq. (9), for the model problem, rather than to a failure of the numerical method. Specifically, as discussed by Titchmarsh,[6] the cumulative integral $F_d(E)$ of Eq. (7) must be bounded for large E for the Hilbert transform of Eq. (9) to define an integrable function $\Delta_d(E)$. In the limit of completeness (large r_1 and large N here), Eqs. (7) and (8) imply that the cumulative width function for $E\to\infty$ is proportional to the integral over r of $|(H-E_d)\phi_d|^2$. Because ϕ_d has a discontinuous slope at r_0, the integrand contains the square of a δ function, and this integral diverges. In order to use the Feshbach theory, the discrete function ϕ_d apparently should satisfy the same continuity conditions as the background functions $\{\phi_l\}$.

Referring to the function defined by Eq. (40) as $\phi_{(0)d}$, this function was modified to remove the discontinuity in slope at r_0 by adding another function $\phi_{(1)d}$, described below, then orthogonalizing to the first $N-1$ functions $\{\phi_l\}$ and renormalizing the resulting function, which will be called ϕ_d in the subsequent discussion. To minimize the modification of $\phi_{(0)d}$, the augmenting function was taken to be

$$\phi_{(1)d}=\begin{cases}0, & r<r_0\\ C\sin[k(r_1-r)], & r_0<r\end{cases}$$

where k was chosen to be the value nearest k_d of

$$k=n_d\pi/(r_1-r_0),$$

where n_d is an integer. Since $\phi_{(1)d}$ vanishes at r_0, the coefficient C is determined by matching the slope of ϕ_d at r_0. The effect of orthogonalizing $\phi_{(1)d}$ to all ϕ_l for $l<N$ is to reduce the norm of $\phi_{(1)d}$ to a very small quantity, without affecting the exact matching condition. For $N=50$, the resulting change of E_d is still substantial, 0.2 energy units, although this energy correction should vanish in the limit of large N. The renormalization of the modified ϕ_d multiplies all transition matrix elements H_{dl} by a common fac-

TABLE I. Values of $\Gamma_d(E)$ and $\Delta_d(E)$ computed in the Feshbach formalism.

E_l	$\Gamma_d(E_l)$ (1)[a]	$\Gamma_d(E_l)$ (2)[b]	$\Gamma_d(E_l)$ Exact	$\Delta_d(E_l)$ (1)[a]	$\Delta_d(E_l)$ (2)[b]	$\Delta_d(E_l)$ Exact
0.056 16	0.919 65	0.919 65	0.919 58	−3.443 67	−3.443 51	−3.449 58
0.224 61	1.817 14	1.817 14	1.817 00	−3.335 85	−3.335 68	−3.341 59
0.505 24	2.670 40	2.670 40	2.670 18	−3.158 33	−3.158 16	−3.163 80
0.897 87	3.457 44	3.457 43	3.457 13	−2.914 45	−2.914 28	−2.919 52
1.402 25	4.156 45	4.156 44	4.156 06	−2.609 00	−2.608 82	−2.613 55
2 018 02	4.745 91	4.745 89	4.745 43	−2.248 36	−2.248 18	−2.252 24
2.744 71	5.204 68	5.204 65	5.204 09	−1.840 72	−1.840 54	−1.843 77
3.581 72	5.512 28	5.512 24	5.511 57	−1.396 39	−1.396 21	−1.398 41
4.528 27	5.649 29	5.649 24	5.648 46	−0.928 24	−0.928 05	−0.928 97
5.583 35	5.598 25	5.598 18	5.597 29	−0.452 30	−0.452 11	−0.451 43
6.745 72	5.345 15	5.345 06	5.344 07	0.011 37	0.011 56	0.014 27
8.013 74	4.882 33	4.882 22	4.881 18	0.437 81	0.437 99	0.443 25
9.385 37	4.213 59	4.213 47	4.212 44	0.796 24	0.796 41	0.804 80
10.858 06	3.362 76	3.362 64	3.361 74	1.050 07	1.050 23	1.062 25
12.428 70	2.386 92	2.386 81	2.386 18	1.159 48	1.115 96	1.175 20
14.093 70	1.392 68	1.392 60	1.392 30	1.089 84	1.089 99	1.107 45
15.849 36	0.546 56	0.546 52	0.546 48	0.829 78	0.829 94	0.844 78
17.692 61	0.055 60	0.055 60	0.055 60	0 418 20	0.418 39	0.423 06
19.622 17	0.087 92	0.087 91	0.087 95	−0.036 36	−0.036 13	−0.048 19
21.639 64	0.643 99	0.643 92	0.644 30	−0.376 77	−0.376 50	−0.403 46

[a] Computed using modified ϕ_d.
[b] Computed from true eigenfunctions.

tor. The shift of E_d very nearly compensates the systematic error found in $\Delta_d(E)$ in calculations with the unmodified $\phi_{(0)d}$.

The method of Sec. II, in its k-dependent version, was applied to the modified function ϕ_d in the Feshbach formalism. Computed values of $\Gamma_d(E)$ and $\Delta_d(E)$ are listed in Table I, columns (1), and compared with exact values. This method appears to be capable of giving quantitative results.

An alternative method of constructing a function ϕ_d with satisfactory continuity properties was also implemented. In this method, N exact eigenfunctions $\{\phi_n\}$ and the overlap matrix elements $(\phi_n|\phi_{(0)d})$ are computed. The particular $\phi_{n'}$ with maximum overlap element is selected and denoted by ϕ_d. The remaining $N-1$ eigenfunctions are orthogonalized to $\phi_{(0)d}$ by successive 2×2 rotations with the current ϕ_d, which is updated by each rotation. The final function ϕ_d is the least-square approximation to $\phi_{(0)d}$ in the basis of N eigenfunctions. This process is organized as a modified Jacobi algorithm, and is completed by diagonalizing the Hamiltonian matrix among the orthogonalized functions. The final matrix is in bordered diagonal form as in Eq. (3).

The method of Sec. II was applied to this matrix using the Feshbach formalism. Computed values of $\Gamma_d(E)$ and $\Delta_d(E)$ are listed in Table I, columns (2). The results agree closely with method (1), and represent an excellent approximation to exact values.

To compute $\tan\eta_1$ from the data given in Table I, using Eq. (1), values of E_d are required. These are 3.532 481 for method (1) and 3.532 279 for method (2). The value of E_d for the unmodified function $\phi_{(0)d}$ is 3.734 802.

V. MODEL CALCULATIONS: SCHWINGER FUNCTIONAL

It is evident from Fig. 2 that beyond the threshold region, the principal energy dependence of $\eta_1(E)$ simply compensates the antiresonance behavior of the "background" phase shift $\eta_0(E)$. Hence, for practical applications, the background phase shift cannot be assumed to be less strongly energy dependent than η_1. It is necessary to compute either η_0 or the total phase shift η directly. It will be shown here that the Schwinger variational principle can be adapted to this purpose, using the numerical method of Sec. II, but still requiring only data computed from discrete eigenfunctions.

The variational method of Schwinger,[7] as discussed, for example, by Nesbet,[8] can be based on the stationary functional

$$[\tan\eta] = -2(w_0|\Delta V|f)(f|\Delta V + \Delta V G \Delta V|f)^{-1}(f|\Delta V|w_0). \quad (41)$$

TABLE II. Calculations using the Schwinger variational functional.

E_n	$\Gamma_n(E_n)$	$\Delta_n(E_n)$	$(n\|V\|n)$	$\tan\eta$ Schwinger	Exact
0.017 02	0.032 26	−0.107 68	−0.112 93	3.073 18	3.553 00
0.126 48	0.092 99	−0.108 90	−0.124 89	2.908 25	3.047 21
0.344 75	0.139 12	−0.089 38	−0.123 57	2.034 89	2.072 31
0.671 42	0.165 05	−0.063 87	−0.119 89	1.473 21	1.485 42
1.105 61	0.170 00	−0.038 03	−0.114 85	1.106 45	1.110 63
1.646 07	0.157 66	−0.016 20	−0.108 92	0.850 19	0.851 40
2.291 11	0.134 64	−0.001 00	−0.102 65	0.662 30	0.662 38
3.038 63	0.108 28	0.006 96	−0.096 82	0.521 69	0.521 45
3.886 14	0.084 58	0.008 72	−0.092 51	0.417 73	0.417 51
4.831 05	0.067 05	0.006 25	−0.090 98	0.344 81	0.344 76
5.871 08	0.056 77	0.001 64	−0.093 30	0.299 01	0.299 17
7.004 96	0.053 12	−0.003 29	−0.099 64	0.275 63	0.275 98
8.233 07	0.054 47	−0.007 07	−0.108 73	0.267 89	0.268 39
9.557 38	0.058 46	−0.008 69	−0.118 00	0.267 42	0.268 02
10.980 70	0.062 26	−0.007 84	−0.124 71	0.266 35	0.266 97
12.505 49	0.063 42	−0.005 12	−0.127 28	0.259 59	0.260 14
14.132 95	0.060 91	−0.001 78	−0.125 71	0.245 75	0.246 18
15.862 86	0.055 36	0.000 92	−0.121 25	0.226 56	0.226 86
17.693 82	0.048 46	0.002 27	−0.115 71	0.205 37	0.205 58
19.623 88	0.042 02	0.002 16	−0.110 95	0.185 76	0.185 91

Here f is an approximation to a true scattering wave function, and w_0 is the exact solution of a model scattering problem, with model Hamiltonian H_0. The difference potential $H-H_0$ is ΔV, and G is the principal-value Green's function of the model equation, symbolically $\mathcal{P}(H_0-E)^{-1}$.

In the present context, f can be taken to be the discrete eigenfunction ϕ_n at E_n. Then w_0 is the free scattering wave function at the same energy if ΔV is the full scattering potential function of Eq. (37). The required normalization of w_0 is given by

$$w_0(E_n)=k_n^{-1/2}\sin(k_n r), \tag{42}$$

where

$$k_n^2=2E_n. \tag{43}$$

Instead of evaluating the Green's-function integral in Eq. (41) directly, the method of Sec. II can be used to approximate it from a formula involving only bound-free integrals $(\phi_k^0|V|\phi_n)$ where ϕ_k^0 is an L^2 normalized eigenfunction of H_0 with the boundary condition of Eq. (39). The eigenvalue is E_k^0. Equation (41) is equivalent to an expression similar to Eq. (1) of the Feshbach theory:

$$[\tan\eta]=-\tfrac{1}{2}\Gamma_n(E_n)/[E_n-E_{n0}-\Delta_n(E_n)]. \tag{44}$$

Here

$$\Gamma_n(E)=4(w_0(E)|V|\phi_n)^2, \tag{45}$$

$$E_n-E_{n0}=(n|H-H_0|n)=(\phi_n|V|\phi_n), \tag{46}$$

and

$$\Delta_n(E)\cong\sum_k(\phi_n|V|\phi_k^0)\frac{\mathcal{P}}{E-E_k^0}(\phi_k^0|V|\phi_n). \tag{47}$$

Equation (47), evaluated for $E=E_n$, is an approximation to the Green's-function integral $-(f|\Delta V G\Delta V|f)$ required in Eq. (41), with exactly the same structure as Eq. (6). The principal-value integral over energy E_k^0 is replaced by summation over the discrete eigenvalue spectrum of H_0. Since ϕ_k^0 and w_0 at E_k^0 differ only by a normalization constant, the same bound-free integrals occur in Eqs. (45) and (47). The method of Sec. II essentially computes this normalization constant if Eqs. (45) and (47) are evaluated by this method.

This version of the Schwinger method was used to evaluate $\tan\eta$, where η is the total scattering phase shift, for the model problem considered here. Results of these calculations are given in Table II, with $[\tan\eta]$ listed in the column labeled Schwinger. The method appears to be quite accurate. It should be noted that Eq. (44) is, in principle, exact, since ϕ_n is an exact eigenfunction of H within the range of V. The approximation enters through Eq. (47), which tests the method of Sec. II as a numerical Hilbert transform, and through use of the discrete eigenvalue distribution to compute the relative normalization constant of Eq. (45).

Because the sum in Eq. (47) approximates a function $\Delta_n(E)$ which is different for each index n,

each value $\Delta_n(E_n)$ requires separate use of the method of Sec. II. The arrays of values $\Delta_n(E_n)$ and $\Gamma_n(E_n)$ do not necessarily correspond to a function of complex energy analytic in the upper half-plane.

VI. MODEL CALCULATIONS: FREDHOLM DETERMINANT

Reinhardt and collaborators[9,10] have shown that the Fredholm theory of integral equations can be used to derive scattering information from quadratically integrable wave functions. The technique is to evaluate the Fredholm determinant $D(z)$ for complex energy z. For single-channel scattering, the phase shift $\eta(E)$ is equal to minus the phase of $D(E+i\epsilon)$ in the limit $\epsilon \to 0+$. Diagonalization of the matrices of H_0 and H in an N-term quadratically integrable basis gives the approximate expression

$$D(z) \cong \prod_{n=1}^{N} \frac{z-E_n}{z-E_n^0}, \tag{48}$$

valid for values of z sufficiently far from the real axis. Here E_n is an eigenvalue of H and E_n^0 in an eigenvalue of H_0, evaluated here by imposing the boundary condition of Eq. (39). H_0 will be taken here to be the free scattering Hamiltonian, as in Sec. V.

Along the real z axis, $D(z)$ as given by Eq. (48) is a real function with an artificial structure of closely spaced poles and zeroes due to the discrete representation. The true limit of $D(E+i\epsilon)$ is a complex-valued function with continuous phase. Reinhardt *et al.*[10] estimate this limit by evaluating Eq. (48) at points displaced from the real axis, then use a rational approximation of lower order than N to smooth this function and to extrapolate back to the real axis. It was found necessary to use an approximation of order roughly $N/2$ in order to avoid the coarse-grained structure inherent in Eq. (48).

The numerical method described in Sec. II here provides an alternative estimate of the continuum limit of Eq. (48). The residue of Eq. (48) at E_n^0 is

$$(E_n^0 - E_n) \prod_{n' \neq n}^{N} \frac{E_n^0 - E_{n'}}{E_n^0 - E_{n'}^0}. \tag{49}$$

If this residue is used instead of H_{dl}^2 in Eqs. (6) and (14) or (29), the numerical construction of Sec. II can be used directly to give a complex function $W(z)$, as in Eq. (2), for which

$$D(z) = W(z) + 1$$
$$= \Delta(z) - \frac{i}{2}\Gamma(z) + 1. \tag{50}$$

TABLE III. Calculations using the Fredholm determinant.

E_n^0	$\Gamma(E_n^0)$	$\Delta(E_n^0)$	tanη Fredholm	tanη Exact
0.000 00	0.000 00	−0.970 41	0.000 00	0.000 00
0.049 35	0.403 07	−0.939 02	3.305 03	3.696 02
0.197 39	0.759 17	−0.849 80	2.527 23	2.616 77
0.444 13	1.030 15	−0.716 58	1.817 34	1.838 53
0.789 56	1.193 52	−0.559 15	1.353 65	1.357 40
1.233 70	1.245 70	−0.399 26	1.036 81	1.035 77
1.776 53	1.201 16	−0.256 41	0.807 68	0.805 65
2.418 05	1.087 82	−0.144 39	0.635 70	0.633 91
3.158 27	0.940 01	−0.069 36	0.505 04	0.503 84
3.997 19	0.790 81	−0.029 83	0.407 56	0.406 96
4.934 80	0.665 57	−0.018 16	0.338 94	0.338 82
5.971 11	0.578 10	−0.023 38	0.295 97	0.296 20
7.106 12	0.530 00	−0.034 17	0.274 37	0.274 83
8.339 82	0.512 99	−0.041 58	0.267 62	0.268 20
9.672 21	0.513 21	−0.040 59	0.267 46	0.268 06
11.103 31	0.516 12	−0.030 47	0.266 17	0.266 67
12.633 09	0.510 62	−0.013 89	0.258 91	0.259 27
14.261 58	0.491 51	0.004 63	0.244 62	0.244 85
15.988 76	0.459 71	0.020 55	0.225 23	0.225 38
17.814 64	0.420 78	0.030 77	0.204 11	0.204 23
19.739 21	0.382 19	0.034 38	0.184 74	0.184 88

The constant unity must be included separately here to give the correct limit of $D(z)$ for large $|z|$, while retaining the Hilbert transform relationship between Δ and Γ. From the phase property of the Fredholm determinant, the total phase shift $\eta(E)$ is given by

$$\tan\eta(E) = \tfrac{1}{2}\Gamma(E)/[1+\Delta(E)]. \tag{51}$$

This method was applied to the present model problem. Results are given in Table III, with tanη computed from Eq. (51) listed in the column labeled Fredholm. The table includes the point $E = 0$, which is not an eigenvalue of H_0. The results appear to be usefully accurate.

The present results should be compared with earlier work of Langhoff and Reinhardt,[11] who used the Stieltjes imaging technique to evaluate the Fredholm determinant for static s-wave electron-hydrogen atom scattering. For a given number of basis function (50) the present method appears to be more accurate, presumably because the finite element method gives a smoother approximation to the principal-value integral of Eq. (19).

Unlike the data of Table II, the calculations summarized in Table III define a single analytic function $D(z)$ that can be used for general values of complex energy z. It can be shown[12] that $D(z)$ is identical with the Jost function $J(z)$, which can be evaluated in closed form for the present model problem. For real k, such that $k^2 = 2E$, this is

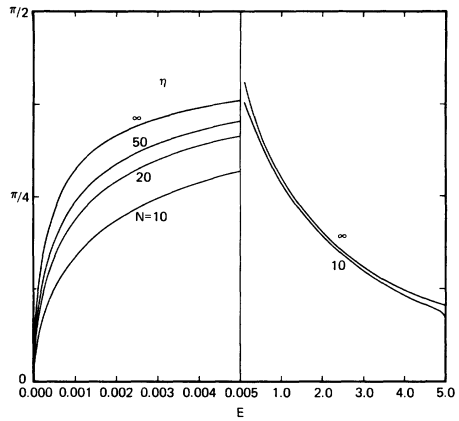

FIG. 3. Convergence of total phase shift, the Fredholm formalism.

$$J(k) = \cos(k'r_0)e^{-i\eta}/\cos(kr_0+\eta), \tag{52}$$

where

$$k'^2 = k^2 + 2V_0. \tag{53}$$

The value at $k = 0$ is

$$J(0) = 0.021\,60. \tag{54}$$

From Table III,

$$D(0) = 1 + \Delta(0) = 0.029\,59. \tag{55}$$

This close agreement indicates that the present method can be used, for example, to characterize a virtual state, which depends on the analytic behavior of $J(k)$ near the origin $k = 0$.

VII. DISCUSSION

A new computational method, described in Sec. II here, has been applied in three different ways to a model scattering problem. The method appears to be sufficiently accurate for practical use in all three applications. In the Feshbach resonance formalism, this work provides a computational procedure alternative to the Stieltjes moment theory technique of Hazi.[1] In the Schwinger variational formalism, the method makes it possible to evaluate the required Green's-function integral through use only of bound-free integrals, which can be evaluated using only quadratically integrable functions. In the Fredholm formalism, the present method provides a simple and effective alternative to the analytic continuation technique of Reinhardt *et al.*[10]

Data plotted in Fig. 3 give an indication of the relative accuracy and rate of convergence of the present method, as applied to the total phase shift in the Fredholm formalism. The results converge monotonically, so that curves for $N > 10$ lie between the $N = 10$ and exact ($N = \infty$) results. For $N > 10$, differences between the different curves are not distinctly evident except in the near-threshold region, plotted separately. The threshold results are sensitive to extrapolation below the lowest computed energy eigenvalue. For $N = 10$, the highest eigenvalue, as given in Table III, lies below 5.0 units, causing the dropoff of the curve shown in Fig. 3. This occurs at successively higher energy values as N is increased.

Unlike Stieltjes moment theory, the present method does not require pole strengths to be positive definite. Although this aspect has not been exploited in the examples given here, this should make other more complicated applications feasible. In particular, it should be possible to use this method in multichannel applications of the Fredholm formalism.

The geometric construction used here assumes that the residue at each discrete pole represents a pole-strength distribution that can be localized between the adjacent poles. A similar assumption is implicit in practical applications of Stieltjes moment theory.[13] If the discrete spectrum is a superposition of two or more weakly interacting spectra, this assumption can lead to difficulties that have been discussed and exemplified elsewhere.[13] In such cases, the weakly interacting subspectra must be separated before either the present method or the Stieltjes moment theory can be used.

ACKNOWLEDGMENT

This work was supported in part at the University of Kaiserslautern under Sonderforschungsbereich 91 by the Deutsche Forschungsgemeinschaft, and in part at IBM, San Jose, California by the Office of Naval Research.

*Visitor at University of Kaiserslautern, West Germany.

[1] A. U. Hazi, J. Phys. B 11, L259 (1978).
[2] P. W. Langhoff, Chem. Phys. Lett. 22, 60 (1973).
[3] P. W. Langhoff, C. T. Corcoran, J. S. Sims, F. Weinhold, and R. M. Glover, Phys. Rev. A 14, 1042 (1976).
[4] H. Feshbach, Ann. Phys. (N.Y.) 19, 287 (1962).
[5] C. J. Joachain, *Quantum Collision Theory*, Vol. 1 (North-Holland, New York, 1979), pp. 86–91.
[6] E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Oxford University Press, London, 1948), pp. 119–151.
[7] J. S. Schwinger, Phys. Rev. 72, 742 (1947); and unpublished.
[8] R. K. Nesbet, *Variational Methods in Electron-Atom*

Scattering Theory (Plenum, New York, 1980), pp. 64–78.
[9]W. P. Reinhardt and A. Szabo, Phys. Rev. A 1, 1162 (1970).
[10]W. P. Reinhardt, D. W. Oxtoby, and T. N. Rescigno, Phys. Rev. Lett. 28, 401 (1972).
[11]P. W. Langhoff and W. P. Reinhardt, Chem. Phys. Lett. 24, 495 (1974).
[12]R. G. Newton, *The Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), pp. 343 and 375.
[13]R. K. Nesbet, Phys. Rev. A 14, 1065 (1976).