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Calculation of Substituted Fredholm Determinants Using Complex Basis Functions

Thomas N. Rescigno* and William P. Reinhardt†
Department of Chemistry, Harvard University, Cambridge, Massachusetts 02138
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Using basis functions with complex coordinates, it is possible to construct discrete approximations to the Fredholm determinant directly at real energies using only square-integrable functions. For the case of purely elastic scattering, the procedure is equivalent to an analytic continuation of the coordinate dependence of the Hamiltonian. It is shown that improved convergence is obtained by an application of the "dispersion-correction" method. The method is generalized to allow calculation of the "substituted" Fredholm determinants needed to construct the S matrix for many-channel potential-scattering problems. This generalization is not equivalent to a simple continuation of the coordinate dependence of the many-channel Hamiltonian. Results of calculations on several model problems are presented.

I. INTRODUCTION

A Fredholm technique for computing phase shifts for elastic scattering of a particle from a potential V using only square-integrable (L^2) basis functions has recently been discussed.[1] The method proceeds by construction of the matrix representations $\overline{H}$ and $\overline{H}^0$ of the operators H^0 and $H = H^0 + V$ in an L^2 set of functions, from which an approximation to the partial-wave Fredholm determinant, $D(z) = \det[1 - G^0(z)V]$, is calculated as

$$D^{\text{approx}}(z) = \det\left(\frac{z - \overline{H}}{z - \overline{H}^0}\right) = \prod_{i=1}^{N}\left(\frac{z - E_i}{z - E_i^0}\right), \qquad (1.1)$$

E_i and E_i^0 being the eigenvalues of the matrices $\overline{H}$ and $\overline{H}^0$, respectively. Phase shifts can be calculated from D^{approx} either by numerical analytic continuation to obtain the $E + i\epsilon$ limit,[1] or by working directly at real energies and making use of the relationship between the L^2 basis set and the "equivalent quadrature"[2] generated by it.

This note describes an extension of this technique to the case of many-channel potential scattering. In many-channel problems it is still possible to construct the open-channel block of the S matrix from the scalar-valued Fredholm determinant considered as a function of a single complex variable[3]; however, to accomplish this we must consider $D(z)$ as a multisheeted function of the complex variable z. Specifically we require knowledge of the "substituted"[4] determinants which may be thought of as arising from simultaneously taking the $E - i\epsilon$ limit in some channels and the more usual $E + i\epsilon$ limits in the others.[5] Using a technique which is a simple generalization of the method of complex coordinates described by Nuttall and Cohen[6] it will be shown that there is a simple and natural way to obtain these "substituted" determinants within the framework of an L^2 computational scheme.

The outline of the paper is as follows: The method of complex basis functions is introduced within the context of potential scattering in Sec. II. The results of application to several simple potentials are given. The extension to many-channel problems is outlined in Sec. III, where the results of application of the complex basis method to compute elastic and inelastic cross sections for the model problem of two coupled square wells are presented. Section IV contains a brief discussion.

II. POTENTIAL SCATTERING

A. Complex Basis Functions

The method of complex coordinates (i.e., considering the potential to be a function of complex position) is well known in the theory of potential scattering as it may be used to extend the region of analyticity[7] of the Jost function into the lower half k plane. More recently the method has been used as the basis for several new theoretical[8] and computational advances.[6,9] As specific computational methods[6] have been given for the calculation of T-matrix elements we will simply summarize the results which are needed in Fredholm theory, where it will be seen that for potential scattering the technique is equivalent to computation with complex basis functions. We postpone until Sec. III the extension to multichannel problems, where it will be shown that the technique of complex basis functions represents a generalization which is *not* equivalent to the use of a Hamiltonian with complex coordinates.

We begin with the Fredholm series[10]

$$D(z) = \det\left(\frac{z - H(r)}{z - H^0(r)}\right) = 1 - \int_0^\infty \frac{k_1\, dk_1 \langle k_1 | V | k_1 \rangle}{z - \frac{1}{2}k_1^2} \cdots . \qquad (2.1)$$

For analytic potentials,[7,11] the matrix element $\langle k|V|k\rangle$ is an analytic function of k allowing evaluation of the integrals in Eq. (2.1) along the distorted contour obtained by rotating the integration path into the lower half k plane:

$$D^{\theta}(z)=1-\theta^{2}\int_{0}^{\infty}\frac{k\,dk\langle k\theta^{*}|V|k\theta\rangle}{z-\frac{1}{2}k^{2}\theta^{2}}+\cdots, \tag{2.2}$$

where $\theta=e^{-i\phi}$, and $\langle k\theta^{*}|V|k\theta\rangle$ is the analytic continuation of $\langle k|V|k\rangle$ evaluated at $k\theta=ke^{-i\phi}$. A simple change of variables gives[12]

$$\theta^{2}\langle k\theta^{*}|V|k\theta\rangle=\langle k|V(r\theta^{*})|k\rangle, \tag{2.3}$$

which leads to the formal identity

$$D^{\theta}(z)=\det\left(\frac{z-H(r\theta^{*})}{z-H^{0}(r\theta^{*})}\right). \tag{2.4}$$

$D(z)$ has a branch cut along the positive energy axis, while the branch cut of $D^{\theta}(z)$ has been rotated by an angle 2ϕ into the lower half z plane. $D(z)$ and $D^{\theta}(z)$ are identical everywhere on the physical part of the complex energy plane except in the region between the two cuts, where $D^{\theta}(z)$ provides the analytic continuation of $D(z)$ onto the second Riemann sheet, as is shown in Fig. 1. In particular we note that $D^{\theta}(E)=D(E+i\epsilon)$. In the spirit of Eq. (1.1) we can now approximate $D^{\theta}(z)$ as

$$D^{\text{approx}(\theta)}(z)=\det\left(\frac{z-\bar{H}(r\theta)}{z-\bar{H}^{0}(r\theta)}\right), \tag{2.5}$$

where $\bar{H}(r\theta)$ and $\bar{H}^{0}(r\theta)$ are the matrix representations of $H(r\theta)$ and $H^{0}(r\theta)$ in an L^{2} basis $\{U_{i}(r)\}$. The cut in $D^{\theta}(z)$ has been replaced in $D^{\text{approx}(\theta)}$ by a row of simple poles, but as these poles are not on the real axis, $D^{\text{approx}(\theta)}(E)$ gives approximate values of $D(E+i\epsilon)$ and thus approximate phase shifts without the analytic continuation needed in Ref. 1.[13] However, inspection of the matrix elements of $V=H-H^{0}$ reveals by the same change of variables used in Eq. (2.3) that

$$\int_{0}^{\infty}r^{2}\,dr\,\mu_{i}(r)V(r\theta^{*})\mu_{j}(r)=\theta^{2}\int_{0}^{\infty}r^{2}\,dr\times U_{i}(r\theta)V(r)U_{j}(r\theta) \tag{2.6}$$

and thus that

$$D^{\text{approx}(\theta)}(z)=\det\left(\frac{z-\tilde{H}(r)}{z-\tilde{H}^{0}(r)}\right), \tag{2.7}$$

where the matrix representations $\tilde{H}$ and $\tilde{H}^{0}$ are defined in the complex (L^{2}) set $\{\theta U_{i}(r\theta)\}$. We will refer to the use of complex basis functions combined with the usual real Hamiltonian operators as the method of complex basis functions. For potential scattering this "new" method is entirely equivalent to the method of complex coordinates, as is shown by Eq. (2.6); however, we will see in Sec. III that the complex basis techniques will generalize in such a way as to allow solution of many-channel problems, and that this generalization will not be equivalent to simply making the coordinate dependence of the Hamilton complex.

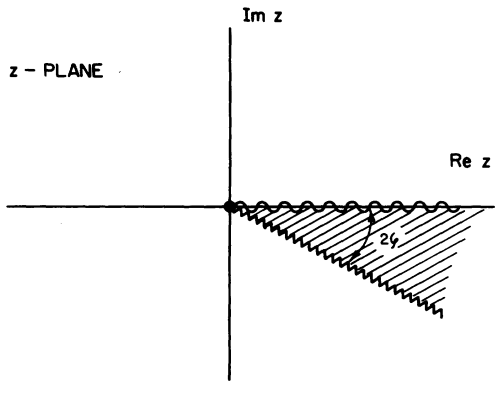

FIG. 1. $D(z)$ and $D^{\theta}(z)$ on the physical sheet. $D(z)$ is analytic except for a branch cut running out the positive real axis indicated by the Sine-wave curve. $D^{\theta}(z)$ is analytic with the rotated cut (ramp-shaped plot). $D(z)$ and $D^{\theta}(z)$ are identical, on the physical sheet, in the unshaded region. The values of $D^{\theta}(z)$ in the shaded region provide the analytic continuation of $D(z)$ onto its second sheet.

B. Dispersion Correction of $D^{\theta}(z)$

The result of application of the method of complex basis functions to the problem of computing s-wave phase shifts for elastic scattering from a square well are shown in Fig. 2. The oscillatory results are evidently due to the proximity of the poles to the real axis. Attempting to avoid this source of error by choosing a larger rotation angle ϕ slows convergence, as has been discussed in detail by Nuttall and co-workers,[14] who have shown that the leading term in the error in the phase computed from $D^{\theta}(E)$ is of order $1/\sqrt{N}$, N being the dimension of the L^{2} basis. However, the oscillating errors shown in Fig. 2 may be systematically removed using the dispersion correction technique of Refs. 2 and 15, allowing use of small rotation angles.

The Fredholm determinant satisfies the dispersion relation

$$D(z)=1+\int_{0}^{\infty}k\,dk\,\frac{A(k)}{z-\frac{1}{2}k^{2}}, \tag{2.8}$$

where $E=\frac{1}{2}k^{2}$ and $A(k)=-\text{Im}\,D(E+i\epsilon)/\pi$ gives the discontinuity across the cut along the real axis. The contour rotation of II A gives the equivalent

result:

$$D^{\theta}(z) = 1 + \theta^2 \int_0^{\infty} \frac{k\, dk\, A(k\theta)}{z - \frac{1}{2}k^2\theta^2}, \qquad (2.9)$$

where $A(k\theta)$ gives the discontinuity across the rotated cut. The use of a discrete L^2 basis to approximate $D^{\theta}(z)$ gives

$$D^{\text{approx}(\theta)}(z) = 1 + \theta^2 \sum_i \frac{A(k_i\theta)k_i\omega_i}{z - \frac{1}{2}k_i^2\theta^2}, \qquad (2.10)$$

where the k_i and ω_i are, respectively, the "equivalent-quadrature" abscissas and weights associated with diagonalization of H^0 in an L^2 basis. For small ϕ and real z the integrand of Eq. (2.9) is nearly singular and thus the approximation of Eq. (2.10) will not be accurate for real z. This error can be compensated for by subtracting $A(k)$ from the integrand before carrying out the quadrature approximations giving the dispersion-correction formula[15]

$$D^{\text{corrected}(\theta)}(E) = D^{\text{approx}(\theta)}(E) + A(k)C(E), \qquad (2.11)$$

where

$$C(E) = \theta^2 \left\{ \int \frac{dE'}{E - E'\theta^2} - \sum_i \frac{k_i\omega_i}{E - \frac{1}{2}k_i^2\theta^2} \right\}. \qquad (2.12)$$

To utilize this formula we need the explicit "equivalent-quadrature"[2] weights associated with our choice of L^2 basis, and also knowledge of $A(k)$.

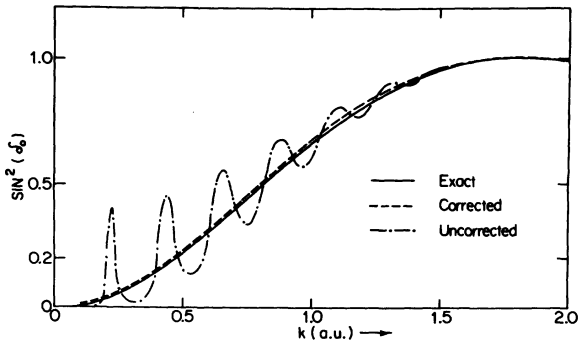

FIG. 2. $\sin^2(\delta_0)$ for s-wave scattering from an attractive square well computed by construction of $D^{\text{approx}(\theta)}(E)$ with (dashed lines) and without (dot-dashed lines) the dispersion-correction terms of Eq. (2.11). For this example, the rotation angle ϕ ($\theta = e^{-i\phi}$) was 0.1 rad, and the uncorrected values of $\sin^2(\delta_0)$ oscillate about the exact values (solid lines). Dispersion correction removes these oscillations, allowing use of small rotation angles. For this problem, the basis set consisted of 50 odd harmonic-oscillator functions,

$$e^{-\lambda r^2/2} H_{2n+1}(\lambda r), \quad \text{with } \lambda = 0.95e^{-i\phi},$$

which generated an equivalent quadrature of the Laguerre type [H. Yamani (unpublished)]. The potential depth was 5 a.u. and the range 1 a.u.

The residues of the approximation of Eq. (2.7) give $\theta^2 A(k_i\theta)k_i\omega_i$, allowing evaluation of $A(k_i\theta)$ which can be analytically continued to give $A(k)$. We note that this latter analytic continuation, in contrast to that employed in earilier work, is of a smooth function,[15] allowing computation with arbitrarily small rotation angle, or for that matter, with no rotation at all.[2]

C. Numerical Examples of Method for Potential Scattering

The method of complex basis functions coupled with the dispersion correction technique has been applied to the calculation of phase shifts for scattering from an attractive square well, and from a long-range potential with an asymptotic $1/r^2$ dependence of the type expected in inelastic electron–hydrogen-atom scattering. Figure 2 gives the corrected and uncorrected results for the square-well problem[16]; the dispersion correction of Sec. II B has gone a long way toward removing the error involved in the discrete approximation to $D^{\theta}(z)$. Results for s-wave scattering from the potential $V(r) = (e^{-r} - 1)/r^2$ are presented in Table I. As expected, convergence for this long-range potential is quite slow, as the region of coordinate space spanned by N Laguerre functions is proportional to N. However, in this case a simple semiclassical estimate[17] suggests that for a potential with a $1/r^2$ tail the error will go as $1/N$. This allowed a highly accurate extrapolation of the results, which is also shown in Table I.

TABLE I. s-wave phase shifts for elastic scattering from the potential $V(r) = (e^{-r} - 1)/r^2$. Results are given for a basis of N Laguerre functions of the type $re^{-\alpha r/2} L_n^1(\alpha r)$ with $\alpha = 2$ and $\phi = -0.1$ rad. As expected, for a potential with a $1/r^2$ tail, convergence was slow, but extrapolation[a] yielded highly accurate results.[b]

	N					
k	20	30	40	45	Extrap[a]	Exact[c]
0.4	2.949	2.970	2.981	2.985	3.017	3.016
0.6	2.453	2.469	2.478	2.481	2.504	2.506
0.8	2.112	2.126	2.133	2.136	2.156	2.158
1.0	1.861	1.874	1.882	1.888	1.916	1.905
1.2	1.668	1.681	1.688	1.690	1.708	1.712

[a] Extrapolated phase shifts were obtained from extrapolation of the lower order results in $1/N$.

[b] For the Laguerre basis used here the equivalent quadrature weights are modified Chebyschev weights of the second kind, see Ref. 2.

[c] Exact phase shifts were obtained by diagonalizations of the potential in a basis of 172 Bessel functions as per the prescriptions of W. P. Reinhardt and A. Szabo, Phys. Rev. A 1, 1162 (1970).

D. Range of Applicability of the Method

The derivation of Eqs. (2.3) and (2.4), as outlined in Ref. 12, assumes that the potential $V(r)$ is analytic in the interval $(0,\infty)$, in addition to satisfying the usual Fredholm conditions[10]

$$\lim_{r\to\infty} rV(r)=0\,, \tag{2.13a}$$

$$\lim_{r\to 0} r^2V(r)=0\,. \tag{2.13b}$$

This implies that the rotated-coordinate method can be used with the Fredholm techniques for potentials which behave asymptotically as C/r^{ζ}, $\zeta>1$, allowing the technique to be applied in the presence of the long-range potential occuring in atomic and molecular scattering. This is in contrast to T-matrix techniques where the use of contour distortion by use of complex coordinates of the type $r\theta$ in the Hamiltonian is restricted to exponentially bounded analytic potentials.[18] Of course, if more-complicated contour distortions are permitted, the analyticity conditions may be relaxed (provided that appropriate moments of the potential exist) as discussed in Ref. 11.

However, we note that for numerical work to proceed these conditions are unnecessarily restrictive. The numerical results of Sec. II C show that, for at least the square-well case,[16] we can relax the analyticity condition, as it is actually only the properties of the "potential"

$$\sum_{i,j} |U_i(\theta r)\rangle\langle U_i(\theta r'')|V(r'')|U_j(\theta r'')\rangle\langle U_j(\theta r')|\,, \tag{2.14}$$

which is implicit in the use of an L^2 basis, which will determine the range of applicability of the method. We note that for $\theta=1$, the potential of Eq. (2.14) is analytic and exponentially bounded in r and r' for the types of basis sets used here, assuming the existence of the matrix elements $\langle U_i|V|U_j\rangle$. The question of convergence thus depends both on the potential and the basis set used.[19] Minimal conditions on the potential and basis would seem to be the existence of the matrix elements $\langle U_i(\theta r'')|V(r'')|U_j(\theta r'')\rangle$ and the corresponding equivalent quadrature approximations to the traces $\mathrm{tr}(GV)^n$, $n=1,\ldots,N$, where N is the the number of terms in the L^2 basis.

III. MANY-CHANNEL SCATTERING

A. Calculation of Substituted Determinants

The S-matrix elements needed to compute cross sections for many-channel scattering processes are given in terms of the "substituted" Fredholm determinants as[3]

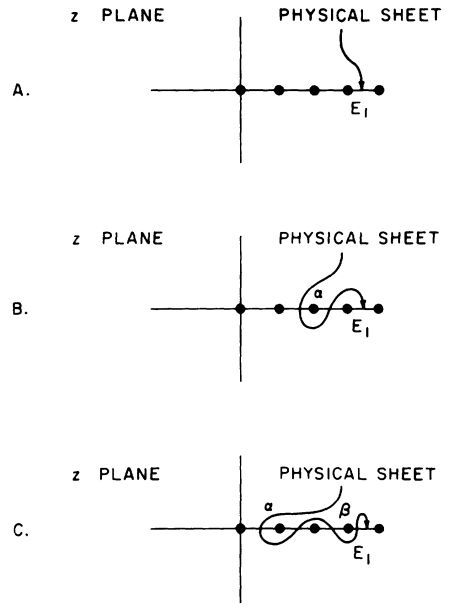

FIG. 3. Continuation paths for construction of the various substituted Fredholm determinants needed to construct the open-channel block of the S matrix. For clarity, only the branch points corresponding to thresholds are shown. It is assumed that the cuts run out the positive real axis. Continuation path A represents construction of $D(E+i\epsilon)$; continuation path B shows the analytic continuation needed to construct $D_\alpha(E+i\epsilon)$; $D_\alpha(E+i\epsilon)$ may thus be interpreted as corresponding to taking the $E-i\epsilon$ limit in channel α and the $E+i\epsilon$ limit in all other channels. Path C shows continuation needed for $D_{\alpha\beta}(E+i\epsilon)$.

$$S_{\alpha\alpha}(E)=\frac{D_\alpha(E+i\epsilon)}{D(E+i\epsilon)}\,, \tag{3.1a}$$

$$S^2_{\alpha\beta}(E)=\frac{D_\alpha(E+i\epsilon)D_\beta(E+i\epsilon)-D_{\alpha\beta}(E+i\epsilon)D(E+i\epsilon)}{D(E+i\epsilon)^2}\,, \tag{3.1b}$$

where

$$D(E+i\epsilon)=D(k_1\ldots k_\alpha\ldots k_\beta\ldots)\,, \tag{3.2a}$$

$$D_\alpha(E+i\epsilon)=D(k_1\ldots -k_\alpha\ldots)\,, \tag{3.2b}$$

$$D_{\alpha\beta}(E+i\epsilon)=D(k_1\ldots -k_\alpha\ldots -k_\beta\ldots)\,, \tag{3.2c}$$

k_1, k_α, k_β being the channel momenta. An alternate interpretation[5] of the substituted determinants is that they may be obtained by analytic continuation of $D(z)$ from the physical sheet via the prescriptions of Fig. 3. These continuations are easily performed, using the contour distortions implicit in the method of complex basis functions, even in the case of degenerate thresholds, where simple analytic continuation in complex energy fails.[20]

Consider the Fredholm series for the many-channel Fredholm determinant[10]:

$$D(z)=1-\sum_{\alpha}\int_0^{\infty}\frac{k_1^{\alpha}\,dk_1^{\alpha}V_{11}^{\alpha\alpha}}{z-E_1^{\alpha}}\cdots$$
$$+\frac{(-1)^n}{n!}\sum_{\alpha,\beta,\ldots,n}\int_0^{\infty}k_1^{\alpha}\,dk_1^{\alpha}\int_0^{\infty}k_2^{\beta}\,dk_2^{\beta}\cdots\int_0^{\infty}k_n^{\eta}\,dk_n^{\eta}\frac{1}{(z-E_1^{\alpha})\cdots(z-E_n^{\eta})}\begin{vmatrix}V_{11}^{\alpha\alpha} & V_{11}^{\alpha\beta}\cdots V_{1n}^{\alpha\eta}\\ \cdots & \\ V_{n1}^{\eta\alpha}\cdots & V_{nn}^{\eta\eta}\end{vmatrix}\cdots, \tag{3.3}$$

where $E_i^{\gamma}=\frac{1}{2}(k_i^{\gamma})^2$, and

$$V_{ij}^{\alpha\beta}=2\pi(k_i^{\alpha}k_j^{\beta})^{1/2}\langle j_l(k_ir^{\alpha})\,|\,V^{\alpha\beta}\,|\,j_l(k_jr^{\beta})\rangle\,.$$

As in the one-channel case, we can distort the integration contours. To evaluate $D(E+i\epsilon)$ without computing any principle-value integrals we rotate all the cuts down by making the variable change $k_i^{\alpha}\to k_i^{\alpha}e^{-i\phi}$, which rotates all the cuts "down" into the lower half z plane by an angle 2ϕ taken with respect to the individual threshold branch points, giving rise to a new function $D^{\theta}(z)$ such that $D(E+i\epsilon)=D^{\theta}(E)$. To evaluate $D_{\alpha}(E+i\epsilon)$ we take $k_i^{\alpha}\to k_i^{\alpha}e^{+i\phi}$ and $k_i^{\beta}\to k_i^{\beta}e^{-i\phi}$ $(\beta\neq\alpha)$. The effect of such a contour rotation on $D(z)$ is shown in Fig. 4 when the branch structure of the new determinant $D_{\alpha}^{\theta}(z)$ is shown. Above the threshold for channel α we have $D_{\alpha}(E+i\epsilon)=D_{\alpha}^{\theta}(E)$, allowing computation of the substituted determinant. $D_{\alpha\beta}^{\theta}(z)$ may be defined in an analogous manner allowing calculation of $D_{\alpha\beta}(E+i\epsilon)$ as $D_{\alpha\beta}^{\theta}(E)$. We note that in contrast to the potential-scattering case, there is no simple analytic continuation of the coordinate dependence of the Hamiltonian which gives rise to the determinants $D_{\alpha}^{\theta}(z)$ and $D_{\alpha\beta}^{\theta}(z)$, although of course $D^{\theta}(z)$, the determinant with all cuts rotated down, is equivalent to use of a Hamiltonian with complex coordinates.

The L^2 analog of the contour distortions needed to calculate D_{α}^{θ} is to rotate the coordinates of the (one-particle) basis functions representing the unperturbed channels: If the various unperturbed channel wave functions are expanded in L^2 sets $\{U_i^{\gamma}(r)\}$, we construct $D_{\alpha}^{\theta}(z)$ by taking $\{U_i^{\alpha}(r)\}\to\{e^{i\phi}U_i^{\alpha}(re^{+i\phi})\}$ and $\{U_i^{\gamma}(r)\}\to\{e^{-i\phi}U_i^{\gamma}(re^{-i\phi})\}$, $\gamma\neq\alpha$. As in the potential-scattering case this use of L^2 basis sets replaces the cuts of $D_{\alpha}^{\theta}(z)$ by rows of poles in $D_{\alpha}^{\text{approx}(\theta)}(z)$. L^2 construction of $D_{\alpha\beta}^{\text{approx}(\theta)}(z)$ proceeds in a similar way. In principle the prescription allows construction of $D^{\theta}(E)$, $D_{\alpha}^{\theta}(E)$, $D_{\alpha\beta}^{\theta}(E)$, and thus inelastic S-matrix elements, directly at real energies using only square-integrable functions. However, for calculations using a small number of basis functions, necessitating use of small rotation angles, a dispersion-correction technique is needed to "smooth out" the calculated results.

B. Multichannel Dispersion Correction

An appropriate generalization of dispersion correction is needed to obtain accurate scattering information from the approximate determinants $D^{\theta}(E)$ and $D_{\alpha}^{\theta}(E)$.

We can use Cauchy's integral theorem to derive a dispersion relation for $D_{\alpha}^{\theta}(E)$ analogous to the one given for potential scattering

$$D_{\alpha}^{\theta}(z)-1=\frac{1}{2\pi i}\oint_C\frac{[D(z')-1]z'}{z-z'}\,, \tag{3.4}$$

where the contour used is shown in Fig. 5.

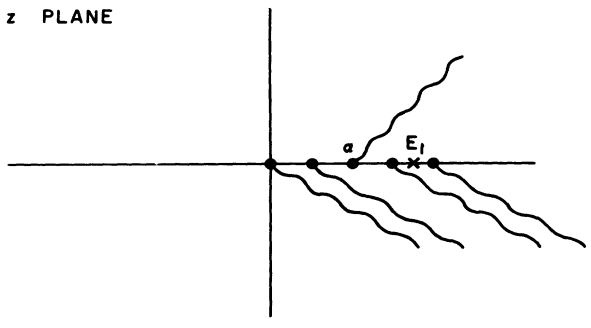

FIG. 4. Branch structure of the determinant $D_{\alpha}^{\theta}(z)$. The cut corresponding to channel α has been rotated "up" by angle 2ϕ while all other cuts have been rotated "down" by angle 2ϕ $(\theta=e^{-i\phi})$. Above the threshold for channel α, $D_{\alpha}(E+i\epsilon)=D_{\alpha}^{\theta}(E)$.

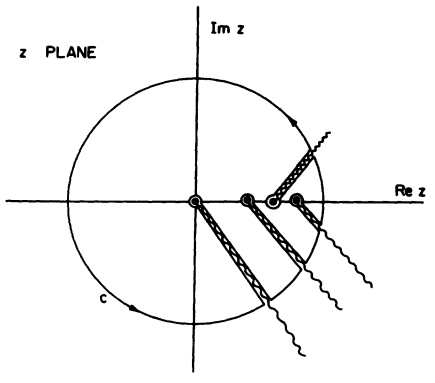

FIG. 5. Integration contour used for derivation of the dispersion-correction formula of Eq. (3.7), needed to compute accurate approximations to $D_{\alpha}^{\theta}(E)$ from $D_{\alpha}^{\text{approx}(\theta)}(E)$.

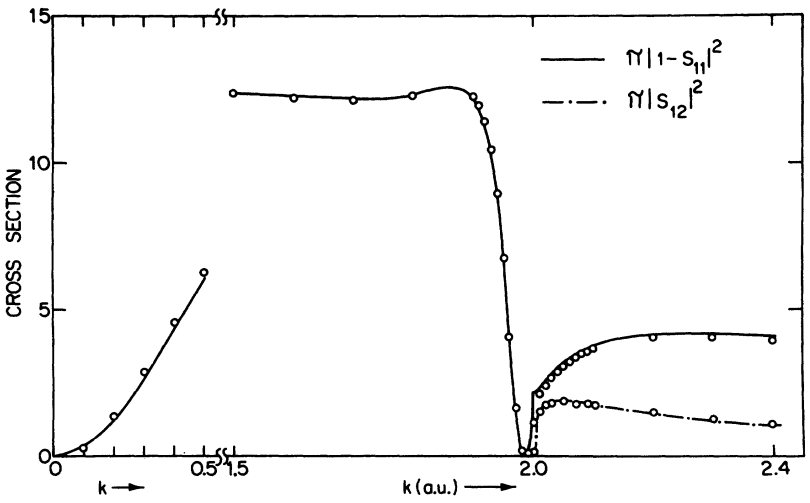

FIG. 6. Unnormalized elastic and inelastic cross sections for s-wave scattering from two coupled square wells. Exact results for the elastic cross section are indicated as solid lines; for the inelastic by dot-dashed lines. Potential parameters are those of Eq. (3.9). The basis set consisted of 30 odd harmonic oscillator functions for each channel. Basis parameters are the same as those of Fig. 2. The two determinants needed to construct these cross sections were obtained using the complex basis function technique of Section III A, and coupled with the dispersion correction of Eq. (3.7); the calculated cross sections are indicated by the open circles.

Since $D_\alpha^\theta(z) \to 1$ as $z \to \infty$, we have the result

$$D_\alpha^\theta(z) = 1 + \sum_{i=\alpha,\beta,\ldots} \theta_i^2 \int_0^\infty \frac{k_i A_{\theta_i}^i(\theta_i k_i) k_i \, dk_i}{z - k_i^2/2\theta^2}, \tag{3.5}$$

where $A_{\theta_i}^i(\theta_i k_i)$ is the discontinuity in $D(z)$ across the ith rotated branch cut. The L^2 approximation to (3.5) is

$$D_\alpha^{\text{approx}(\theta)}(z) = 1 + \sum_{i=\alpha,\ldots} \theta_i^2 \sum_{j=1,N_i} \frac{A_{\theta_i}(\theta_i k_i^j) k_i^j \omega_i^j}{z - k_{i/2}^{j2}\theta_i^2}, \tag{3.6}$$

where we have assumed a basis of N_i functions for each channel, the k_i^j's being simply related to the matrix eigenvalues of $\tilde{H}^0(r)$ in the various channels. We now follow the dispersion-correction procedure of II B to obtain the generalization of Eq. (2.11),

$$D^{\text{corrected}(\theta)}(E) = D^{\text{approx}(\theta)}(E) + \sum_i A_i(E_i) C_i(E_i), \tag{3.7}$$

where

$$C_i(E_i) = \theta_i^2 \int \frac{dE}{E_i - \theta_i^2 E} - \theta_i^2 \sum_j \frac{k_i^j \omega_i^j}{E_i - \theta_i^2 k_{i/2}^{j2}}, \tag{3.8}$$

where $E_i = \frac{1}{2}k_i^2$ and the index i runs over all channels. The $A_i(E_i)$'s are obtained by separate continuation of the residues of $D^{\text{approx}(\theta)}(z)$ for the various channels.

C. Two-Channel Numerical Example

We have tested the procedure outlined in III B by applying it in the calculation of cross sections for the model two-channel problem

$$V = \begin{pmatrix} -2\theta(r-1) & -1\theta(r-1) \\ -1\theta(r-1) & -2\theta(r-1)+2 \end{pmatrix}, \tag{3.9}$$

where

$$\theta(r) = 1 \quad r \leq 0,$$
$$= 0 \quad r > 0.$$

The L^2 basis set consisted of 30 harmonic-oscillator functions for each channel. The results for the elastic and inelastic cross section are plotted in Fig. 6 along with the exact cross section which can be obtained analytically for this problem.[21]

IV. DISCUSSION

The method introduced in Section III allows the solution of many-channel scattering problems using only bound-state computational techniques, without explicit enforcement of asymptotic boundary conditions. As the determinants are completely "off-shell" the S-matrix elements are obtained over a continuous range of energies from a single major computational step. This suggests that the method will be useful in electron-atom and electron-molecule scattering, as only standard configuration interaction techniques[1] will be needed.

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*N.S.F. predoctoral Fellow 1969-72.

†Alfred P. Sloan Fellow, Camille and Henry Dreyfus Fellow.

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[12]Consider the real matrix element

$$(*) \equiv \langle k|V|k\rangle = \frac{2}{\pi k}\int_0^\infty \sin^2(kr)V(r)r^2\,dr$$

We desire the analytic continuation of this matrix element for complex $k' = ke^{-i\phi}$. If $V(r)$ is exponentially bounded; i.e., $V(r) \sim Ce^{-\alpha r}$ as $r \to \infty$, then we can evaluate (*) directly for complex k', provided $\alpha > 2k \sin\phi$. If $V(r)$ is not exponentially bounded, (*) will diverge for any complex k'. However, *if* $V(r)$ is analytic in r, we can distort the r-space integration contour by an upward rotation $e^{+i\phi}$ before evaluating the integral at $ke^{-i\phi}$:

$$\langle k\theta^*|V|k\theta\rangle = \frac{2e^{3i\phi}}{\pi k'}\int_0^\infty \sin^2(k're^{i\phi})V(re^{i\phi})r^2\,dr$$

$$= \frac{\theta^{*2}}{\pi k}\int_0^\infty \sin^2(kr)V(r\theta^*)r^2\,dr.$$

Thus, for analytic potentials the desired continuation is equivalent to use of a complex Hamiltonian.

[13]J. Nuttall had earlier suggested this use of direct analytic continuation in r to avoid the rational fraction continuations of Ref. 1 (private communication). See also G. Doolen, M. Hidalgo, J. Nuttall, and R. Stagat, in *Proceedings of the Third International Conference on Atomic Physics, Boulder, Colorado,* edited by S. J. Smith and G. K. Walters (Plenum, New York, 1973), p. 257.

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[16]Although the square well is *not* analytic in coordinate space, the projection of this potential onto a finite L^2 set of analytic functions results in a potential which is an *approximate* square well, and *is* analytic in r.

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[19]The fact that the convergence in contour distortions method depends on the potential *and* the basis is made clear by the square-well example of Sec. IIC: Early calculations of $\int_0^\infty k\,dk\langle k|V|k\rangle(z-\frac{1}{2}k^2)^{-1}$, the 1st Fredholm trace, using a basis of spherical Bessel functions and a numerical quadrature, failed when the contour distortion $k \to k\theta$ was made. This is as expected as the square-well potential is nonanalytic and thus $\langle k|V|k\rangle$ cannot be continued in k, *even though the k-space formula for* $\langle k|V|k\rangle$ *appears to be a well-defined function of* k. This is because for complex k, the *integral* $\int_0^\infty r^2 dr\, j_0(kr)V(k)j_0(kr)$ diverges and cannot be made to converge by the coordinate rotation trick of Ref. 12. The analytic continuation of the formula for $\langle k|V|k\rangle$ thus does not represent an appropriate continuation of the integral.

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