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Jost Function Interpolation of Scattering Cross Sections*

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The analytic properties of the Jost function or Fredholm determinant for single- and many-channel scattering problems suggest that they may often be less rapidly varying functions of the energy than the S matrix or cross sections. This idea is combined with a pointwise rational-fraction interpolation to give a rapidly convergent and highly accurate method of interpolating scattering information over a continuous range of energies. Narrow resonances are easily found by examination of the zeros of the real part of the Fredholm determinant.

I. INTRODUCTION

It is often necessary to compute scattering cross sections over a range of energies in order to predict or identify interesting experimental observables such as resonances, threshold effects, and integrated cross sections. As an alternative to solving the Schrödinger equation at each desired energy it is the purpose of this paper to show that taking advantage of the underlying analytic structure of the S matrix allows accurate interpolation of detailed computations performed at relatively sparce intervals. We present a method for performing such interpolations which takes advantage of the analytic properties of the Fredholm determinant[1,2] or Jost function.[1,2] Section II A briefly reviews the well-known analytic properties of the Jost function.[1] Assuming that the Jost function is known for a series of energies, one can interpolate between these energies in many different ways: We use the pointwise rational-fraction method of Schlessinger[3] which is introduced in Sec. II B. Examples of the method for one-channel problems are presented in Secs. II C and II D.

The extension of the simple one-channel methods to several coupled channels is discussed in Sec. III. The analytic properties of the determinant of the many-channel Jost matrix,[4] or many-channel Fredholm determinant, are reviewed; the rules for computation of the S matrix via Newton's "substitution rules"[5] are given. The fact that we perform our computations for physical energies and that the individual "substituted" determinants may be continued as independent analytic functions of a single variable means that the problem of "uniformization"[6] for multichannel problems is avoided. Section III C contains a numerical application of the many-channel formalism to a problem involving four coupled channels and a narrow resonance. Section IV contains a short discussion.

II. ELASTIC SCATTERING

A. Jost Function and Fredholm Determinant

The Jost function of potential scattering theory is usually defined in terms of a Wronskian over the Jost regular and irregular solutions of the partial-wave Schrödinger equation.[1] However from a computational point of view,[7,8] it is perhaps simpler to take advantage of the fact that the Jost function is identical to the Fredholm determinant[2]

$$D(k) \equiv D(E+i\epsilon) \equiv \det[1 - G^0(E+i\epsilon)V(r)] , \qquad (1)$$

where for convenience we are considering only s waves. In Eq. (1), $G^0(E+i\epsilon)$ is the s-wave Green's function, $V(r)$ is a spherically symmetric potential, and $E=\frac{1}{2}k^2$.

The analytic properties of the Jost function $D(k)$ make it particularly well suited to analytic continuation or interpolation. For potentials which are analytic except at the origin, and which satisfy the conditions[1]

$$\int_0 r\,|V(r)|\,dr < \infty\ , \tag{2a}$$

$$\int^\infty |V(r)|\,dr < \infty\ , \tag{2b}$$

$D(k)$ is analytic for $\mathrm{Im}(k) > 0$ and is continuous with continuous first derivative onto the real k axis. In the more restrictive case that $V(r)$ is exponentially bound,[1] i.e.,

$$\int_0^\infty r\,|V(r)|\,e^{2\alpha r}\,dr < \infty\ , \tag{3}$$

the region of analyticity is extended into the lower half-plane with the result that $D(k)$ is analytic for $\mathrm{Im}(k) > -\alpha$.

The one-channel S and T matrices are given by

$$S(k) = D^*(k^*)/D(k)\ , \tag{4a}$$

$$T(k) = S(k) - 1 \tag{4b}$$

for complex k, in the region of analyticity of $D(k)$. For real k

$$S(k) = D(-k)/D(k) = D^*(k)/D(k)\ , \tag{5a}$$

$$T(k) = S(k) - 1\ , \tag{5b}$$

and

$$R(k) = -\,\mathrm{Im}[D(k)]/\mathrm{Re}[D(k)]\ , \tag{6}$$

where $R(k) = \tan\delta(k)$ is the usual R-matrix element.

It is evident from Eqs. (4) and (5) that if $D(k)$ has a zero in the complex plane, $S(k)$ and $T(k)$ will have poles there. If a zero lies in the lower half k plane close to the real k axis, we identify the corresponding pole in $S(k)$ or $T(k)$ as a resonance pole. For real k in the vicinity of such a pole the S and T matrices undergo a rapid variation returning quickly to the preresonance values. The R matrix has a pole at $k = k^{\mathrm{res}}$ and also returns to previous behavior. This makes it quite possible that a narrow resonance will go unnoticed unless a fine-meshed search is made.

On the other hand, the Fredholm determinant is often a slowly varying function of real k whose only distinction at a resonance is that its real part $d(k) = \mathrm{Re}[D(k)]$ changes sign and the imaginary part is small. These properties allow easy identification of resonances. More generally the analytic properties of $D(k)$ are simpler than those of $S(k)$, $T(k)$, and $R(k)$, so we may expect that, except in pathological cases, $D(k)$ is the more convenient quantity to continue or interpolate.

B. Pointwise Rational-Fraction Interpolation

Given an analytic or other smooth function of k at a set of input points k_i, $i = 1, 2, \ldots$, there are many ways to interpolate[9] between these points to obtain the function over a continuous range of the variable. Schlessinger[3] has investigated the use of rational-fraction methods. We define a pointwise rational-fraction interpolation of a known function $f(x)$ as

$$R_{[N,M]}(x) = P_N(x)/Q_M(x)\ , \tag{7}$$

where

$$P_N(x) = p_0 + \sum_{i=1}^{N} p_i x^i\ , \tag{8a}$$

$$Q_M(x) = 1 + \sum_{i=1}^{M} q_i x^i\ , \tag{8b}$$

by requiring that

$$R_{[N,M]}(x_i) = f(x_i)$$

at $N+M+1$ points x_i; this uniquely determines the constants p_i and q_i. The rational fraction $R_{[N,M]}(x)$ is referred to as the $[N, M]$ approximant by analogy with the better known Padé[10] approximants which may also be expressed as rational fractions. After investigating several continuation methods Schlessinger has found that pointwise expansion of the type of Eq. (7) give superior representations of known and computed functions.

The "diagonal" rational fraction $R_{[N,N]}(x)$ which is equal to $f(x)$ at $2N+1$ points x_i ($i = 1, 2, \ldots, 2N+1$) is easily determined by the method of Wall.[11] The continued fraction

$$C_{2N}(x) = \frac{f(x_1)}{1+\cdots}\ \frac{(x-x_1)a_1}{1+\cdots}\cdots\frac{(x-x_{2N})a_{2N}}{1}\ , \tag{9}$$

where the coefficients a_l ($l = 1, 2, \ldots, 2N$) are determined recursively as

$$a_l = \frac{1}{(x_l - x_{l+1})}\left(1 + \frac{(x_{l+1}-x_{l-1})a_{l-1}}{1+\cdots}\ \frac{(x_{l+1}-x_{l-2})a_{l-2}}{1+\cdots}\cdots \times\frac{(x_{l+1}-x_1)\,a_1}{1 - f(x_1)/f(x_{l+1})}\right)\ , \tag{10a}$$

with

$$a_1 = \frac{f(x_1)/f(x_2) - 1}{x_2 - x_1}\ , \tag{10b}$$

where the dots indicate a continued fraction, is equal to $f(x)$ at the points $x_1, x_2, \ldots, x_{2N+1}$, and may be shown by direct expansion to be equivalent to $R_{[N,N]}(x)$. The rational-fraction expansion of Eqs. (7), (9), and (10) has proved to be a rapidly convergent and highly accurate method for analytic continuation and interpolation.

C. Example: Computation of Resonance Parameters

We consider the elastic s-wave scattering of a particle from a square well coupled to a second square well which is energetically inaccessible, but causes a resonance in the elastic scattering. The (attractive) diagonal square-well depths are $V_{11} = V_{22} = 1.7429$ a.u. and the off-diagonal potentials are $V_{12} = V_{21} = 0.02$ a.u. All the square wells have a range of 1.0 a.u. The threshold energy for the second channel is 0.25 a.u. above the first threshold at 0.0 a.u. Figure 1 shows $-\mathrm{Im}[D(k)]$ and

TABLE I. Computation of resonance parameters for elastic scattering in the coupled square-well problem described in Sec. II C. Re[$D(k)$] and Im[$D(k)$] are shown in Fig. 1; it is evident that they are both smooth functions of k, and thus the interpolation converges rapidly. To compute the determinant at the initial 15 energies, 42 Fredholm quadrature points per channel were used. The analytic results for this model problem[a] give $\frac{1}{2}\Gamma = 7.67 \times 10^{-4}$ and $E^{res} = 0.1504$ a.u.

Approximant	[2, 2][b]	[3, 3][c]	[4, 4][d]	[7, 7][e]
E^{res}	0.149974	0.149811	0.149813	0.149813
$\frac{1}{2}\Gamma$	9.68×10^{-4}	7.52×10^{-4}	7.67×10^{-4}	7.67×10^{-4}

[a]R. G. Newton, Ref. 1, p. 543.

[b]Input Energies: 0.075, 0.100, 0.125, 0.185, 0.215.

[c]Input Energies: 0.115, 0.195, in addition to those in footnote b above.

[d]Input Energies: 0.135, 0.165, in addition to those in footnote c above.

[e]Input Energies: 0.050, 0.145, 0.150, 0.155, 0.175 0.205, in addition to those in footnote d above.

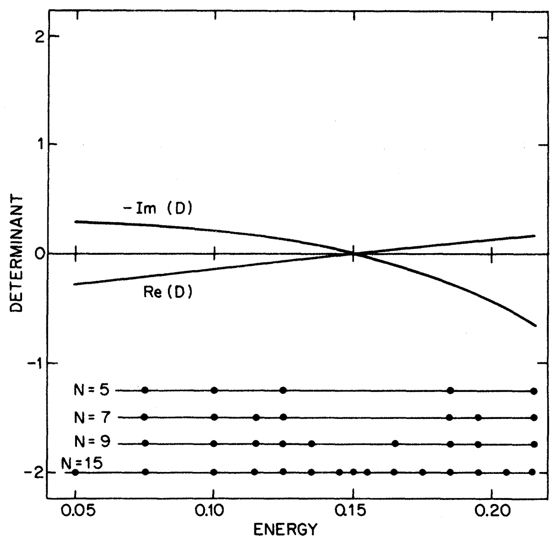

FIG. 1. Real and imaginary parts of $D(E+i\epsilon)$ (times a factor of 10) for elastic scattering from two coupled square wells. The fact that near the energy $E=0.15$ Re(D) has a zero while Im(D) is small implies the existence of a narrow resonance. The postion and width of the resonance has been determined by rational-fraction interpolating of $D(E+i\epsilon)$ using varying numbers of input points as shown. Results of the interpolations are given in Table I.

Re[$D(k)$] as computed by the pointwise rational-fraction method; as anticipated they are slowly varying functions of the energy. The real and imaginary parts of $D(k)$ both pass through zero near $E=\frac{1}{2}k^2 = 0.15$ a.u. corresponding to a resonance. The width of the resonance is given by

$$\tfrac{1}{2}\Gamma = \mathrm{Im}[D(k)] / (d/db)\,\mathrm{Re}[D(k)]\big|_{E=E^{res}}, \tag{11}$$

where $\mathrm{Re}[D(E^{res}+i\epsilon)]=0$, showing that the condition for a narrow resonance is not only that $\mathrm{Re}[D(k)]=0$ but that $\mathrm{Im}[D(k)]$ be "small" compared to $d\mathrm{Re}[D(k)]/dE$. To give some indication of the accuracy of the interpolation Table I shows the position and the half-width of the resonance for a series of approximants ranging from the [2, 2] to the [7, 7]. The input values of $D(k)$ were computed using essentially the numerical Fredholm techniques of Ref. 7.

D. Comparison of Rational-Fraction Continuation of $D(k)$ and $R(k)$

The rational fraction of Eq. (7) can represent simple poles if $Q_M(x)$ has simple zeros. The interpolation scheme can thus be used to interpolate the R matrix in addition to the Fredholm determinant, even though the former has poles on the real k axis. However, as might be expected, convergence of $R_{[N,N]}(x)$ to a function with a singularity is slow, as is shown by the results of Table II, where values of $\tan\delta(k)$ are given for s-wave scattering from the potential $V=-\frac{1}{2}\lambda\delta(r-a)$,[12] for $\lambda=15$, and $a=1$. In this case the analytic solutions[12]

$$\tan\delta(k) = \frac{k\lambda[j_0(k)]^2}{1+k\lambda j_0(k)h_0(k)} \tag{12}$$

and

$$D(k) = 1 - ikj_0(k)[j_0(k)+ih_0(k)] \tag{13}$$

were used as input for the continuation. As is clear from Table II the interpolated values of $\tan\delta(k)$ obtained from the R matrix converge more slowly than those interpolated for $D(k)$. For fixed input points as λ becomes larger the resonance at $k\approx\pi\times(1+1/\lambda)$ becomes very narrow, and the R-matrix interpolation becomes considerably less accurate

TABLE II. Convergence of $\tan\delta$ as computed by rational-fraction interpolation of the R matrix itself, and as computed by interpolation of $D(E+i\epsilon)$ and construction of $\tan\delta$ as $-\mathrm{Im}D/\mathrm{Re}[D(E+i\epsilon)]$. The results shown are for the s-wave scattering of a particle of unit mass from a δ-shell potential as discussed in Sec. II D. $D(E+i\epsilon)$ interpolates more easily than $\tan\delta(k)$ itself. The [8, 8] interpolation of both $R(E)$ and $D(E+i\epsilon)$ are within ±2 in the last reported significant figure of the exact result.

Approximant	[5, 5][a]		[6, 6][a]		[8, 8][a]	
	R	$-\mathrm{Im}D/\mathrm{Re}D$	R	$-\mathrm{Im}D/\mathrm{Re}D$	R	$-\mathrm{Im}D/\mathrm{Re}D$
$k=3.30$	0.817	0.376	0.398	0.387	0.3874	0.3875
$k=3.32$	1.79	0.652	0.695	0.674	0.6745	0.6746
$k=3.34$	9.23	1.26	1.37	1.32	1.320	1.320
$k=3.36$	-4.95	3.46	4.09	3.76	3.763	3.764
$k=3.38$	-2.39	-17.25	-11.20	-13.46	-13.48	-13.47
$k=3.40$	-1.75	-3.33	-3.10	-3.20	-3.203	-3.203

[a]The $2N+1$ points needed for an $[N, N]$ interpolation were chosen to be evenly spaced between $k=0.1$ and $k=6.1$ a.u.

and eventually misses the resonance altogether; in contrast, the results obtained from the continued determinant retain their accuracy.

III. CONTINUATION AND INTERPOLATION FOR MANY-CHANNEL SCATTERING

A. Many-Channel Determinant and the Substitution Rules

For many-channel potential-scattering problems the Jost function of one-channel theory becomes a Jost matrix.[4] The determinant of the Jost matrix,

$$D(E+i\epsilon)=D(k_1,\ k_2,\ldots,\ k_\eta)\ , \tag{14}$$

where η is the number of open channels, is analytic in the independent-channel momenta in their respective upper half-planes for potentials satisfying the conditions of Eq. (2) and in extended regions under more restrictive conditions. The determinant of the Jost matrix is the Fredholm determinant for the corresponding coupled Lippmann-Schwinger equations.[4]

Thus, for real k

$$D(k_1,\ k_2,\ldots,\ k_\eta)=\det[\underline{1}-\underline{G}^0(E+i\epsilon)\underline{V}]\ . \tag{15}$$

As was shown in Ref. 8, $D(k_1,\ldots,k_\eta)$ may be factored as

$$D(k_1,\ k_2,\ldots,\ k_\eta)=\det[\underline{1}-\mathcal{P}\underline{G}^0(E+i\epsilon)\underline{V}]\det(\underline{1}-i\underline{R})\ , \tag{16}$$

where the real symmetric matrix $\underline{R}$ is the usual R matrix of principal-value Lippman-Schwinger theory and has the dimensionality of the number of open channels. Since the cross section can be constructed from R, the real factor $\det[\underline{1}-\mathcal{P}\underline{G}^0(E+i\epsilon)\underline{V}]$ has no effect on the scattering; however, it is responsible for the well-behaved properties of $D(k_1,\ldots,k_\eta)$ since the R-matrix elements can have polar singularities.

Scattering information is extracted from $D(k_1,\ldots,k_\eta)$ using the substitution rules of Newton,[5]

$$S_{\alpha\alpha}=D_\alpha^-/D\ , \tag{17a}$$

$$(S_{\alpha\beta})^2=(D_\alpha^-D_\beta^- - DD_{\alpha\beta}^-)/D\ , \tag{17b}$$

where

$$D_\alpha^-=D(k_1,\ldots,\ -k_\alpha,\ldots,\ k_\eta)\ , \tag{18a}$$

$$D_{\alpha\beta}^-=D(k_1,\ldots,\ -k_\alpha,\ldots,\ -k_\beta,\ldots,\ k_\eta)\ . \tag{18b}$$

TABLE III. Potential parameters for the many-channel square-well problem discussed in Sec. III C. All the wells have a range of 1 a.u. The parameters below are well depths in a.u.

Channel[a]	1	2	3	4
1	1.742 904	0.15	0.15	0.015
2	0.15	1.742 904	0.15	0.015
3	0.15	0.15	1.742 904	0.015
4	0.015	0.015	0.015	1.742 904

[a]Thresholds were at $E=0$, 0.25, 0.50, 0.75 (a.u.).

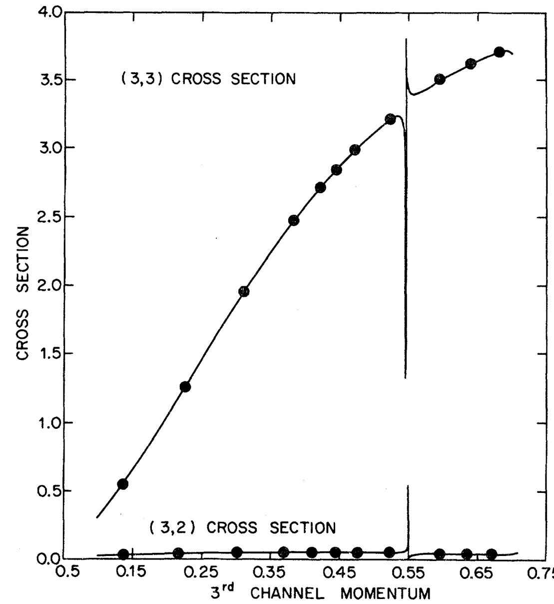

FIG. 2. The (3, 3) and (3, 2) cross sections (multiplied by k_3^2) for the four-channel problem discussed in Sec. III. The dots indicate the energies at which $D(k_1, k_2, k_3)$ and the substituted determinants were computed. The solid line gives the interpolated cross sections. Note that the interpolation procedure has "found" the resonance at $k_3 \simeq 0.55$ a.u. even though none of the input points is at the resonance energy.

The computational significance of Eqs. (18a) and (18b) is that the value of D_α^- is computed by taking the complex conjugate of the αth column of the matrix $(1-i\underline{R})$ before evaluating its determinant. Thus computation of the various substituted determinants D_α^- and $D_{\alpha\beta}^-$ needed for construction of the S matrix does *not* involve repeated evaluations of large determinants; once the factorization of Eq. (16) has been performed by the partial triangularization procedure of Ref. 8, the only further determinants needed to apply the rules of Eqs. (17a) and (17b) have the dimensionality of the number of open channels.

B. Analytic Continuation and/or Interpolation

The determinant $D(E+i\epsilon)=D(k_1,\ k_2,\ldots,\ k_\eta)$ may be regarded as the $E+i\epsilon$ limit of a multisheeted function of a single complex energy z and the substitution rule of Eqs. (17) and (18) interpreted as analytic continuations around the cuts for each channel. Such a procedure has been discussed by Blankenbecler.[13] To implement such a continuation procedure using the rational-fraction continuation method of Sec. II B would require a uniformization technique[6] of the type used by Schlessinger.[3] Such procedures are cumbersome for more than one channel and cannot be carried out globally, in analytic form, on a plane for more than two open channels.[14] We avoid this problem by noting that the substituted determinants D_α^-, $D_{\alpha\beta}^-$, etc., are each analytic functions of $k_1, \ldots, k_\alpha, \ldots, k_n$ in the upper half k planes and at least possess a continuous derivative on the real axis. If we consider *each* of these substituted determinants as a separate function of a single complex energy defined on a single Riemann sheet there is no need to worry about uniformization. Computationally this procedure leads to very little extra work since the construction and continuation of the substituted determinants is almost instantaneous compared to the time required to carry out the partial triangularizations.

As in the one-channel case we expect the individual substituted determinants to be far smoother functions of the energy than the S, T, or R matrices, and thus more useful for continuation or interpolation. That this can be the case is borne out by the following example.

C. Many-Channel Interpolation

As an illustration of the above methods we consider a problem involving four coupled channels. The potential matrix consists of square wells with the parameters shown in Table III. Figure 2 shows results for the case of three open channels with a resonance produced by the (closed) fourth channel. To compute the 3×3 open-channel S matrix, the substituted determinants D_1^-, D_2^-, D_3^-, D_{12}^-, D_{23}^-, D_{13}^- in addition to D itself are needed. However, for the three-channel problem we find $D_{12}^- = (D_3^-)^*$, $D_{23}^- = (D_1^-)^*$, $D_{13}^- = (D_2^-)^*$, and only four determinants need be computed. The determinants were calculated numerically (even though an exact solution is available) using the techniques of Ref. 8; the substituted determinants were continued independently using the pointwise rational-fraction interpolation of Sec. II B. The real and imaginary parts of D and D_3^- are shown in Figs. 3 and 4; the zeros of ReD and ReD_3^- indicate the position of the resonances shown in Fig. 2.

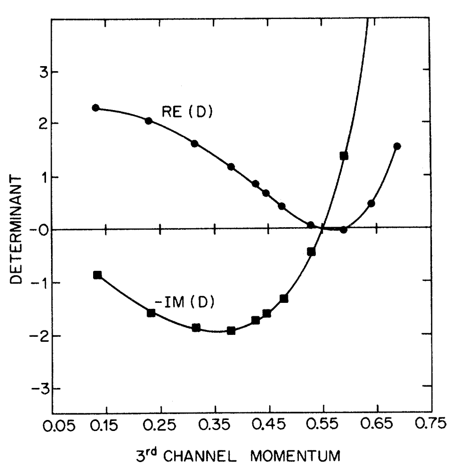

FIG. 3. The real and imaginary parts of the determinant $D(k_1,k_2,k_3)$ (times a factor of 100) for the four-channel problem discussed in Sec. III C. The resonance shown in Fig. 2 corresponds to the zero of Re(D) near $k_3 = 0.55$ a.u. The zero of Re(D) near $k_3 = 0.59$ a.u. does not correspond to a resonance as Im(D) is not small near $k_3 = 0.59$ a.u.

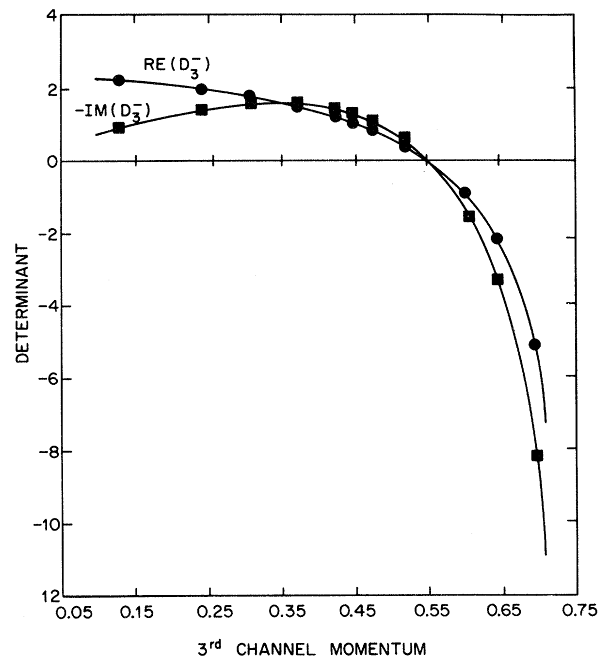

FIG. 4. The real and imaginary parts of the substituted determinant $D(k_1, k_2, -k_3)$ (times a factor of 100) for the four-channel problem discussed in Sec. III C. This determinant, $D(k_1, -k_2, k_3)$, and $D(-k_1, k_2, k_3)$, as well as $D(k_1, k_2, k_3)$, are needed to construct the whole open-channels matrix.

IV. DISCUSSION

The examples shown in Secs. II and III show that the numerical computation of the Fredholm determinant (or Jost function) followed by rational-fraction analytic continuation can provide a rapidly convergent and highly accurate method for obtaining scattering cross sections over a continuous range of energies from detailed computations at a relatively small number of energies.

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Effect of Charge Polarization on Inelastic Scattering: Differential and Integral Cross Sections for Excitation of the 2^1S State of Helium by Electron Impact*

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Experimental differential scattering cross sections for excitation of helium by electron impact from its ground state to its $2\,^1S$ state are presented at four incident electron energies in the range 26–55.5 eV for scattering angles between 10° and 70° and at 81.6 eV for scattering angles between 10° and 80°. These differential cross sections are normalized by using previously determined $2\,^1P$ cross sections and measured $2\,^1S/2\,^1P$ cross-section ratios. These experimental cross sections and cross-section ratios are compared with results predicted by the Born approximation, the polarized Born approximation, and several other first-order approximations in which direct excitation is calculated in the Born approximation and exchange scattering in various Ochkur-like approximations. Calculations based on these approximations are also compared to the data of other experimenters at energies up to 600 eV. The effect on the small-angle scattering of several nonadiabatic dipole-polarization potentials is examined. For the 34–81.6-eV energy range, it is shown that the inclusion of polarization is necessary for accurate predictions of the angle dependence of the $2\,^1S$ cross sections at small angles. Cross sections resulting from the use of analytic self-consistent-field wave functions for both the ground and excited states are presented. They agree well with those obtained from more accurate correlated wave functions.

I. INTRODUCTION

In many cases, the first Born approximation has been successful in explaining the differential cross sections for electronic excitation of atoms and molecules by electron impact at high energies (E greater than about 150 eV) and small scattering angles (less than about 15°).[1–5] This is the region