JOURNAL OF COMPUTATIONAL PHYSICS 26, 257-276 (1978)

# Accurate Numerical Solutions of Integral Equations with Kernels Containing Poles\*

## HAROLD COHEN

Physics Department, California State University, Los Angeles, Los Angeles, California 90032 Received September 2, 1975; revised May 19, 1977

An interpolative technique is presented which yields accurate numerical solutions to various types of integral equations, the kernels of which contain poles. It is also shown that other techniques which are successful when the kernel is weakly singular are unsatisfactory when the singularities are poles. The success of the approach is illustrated by various examples of physical interest.

## 1. INTRODUCTION

Many physical problems involve integral equations which have kernels that contain pole singularities. In this paper, an interpolative procedure is presented which leads to a very straightforward, accurate numerical solution to such equations. Linear integral equations are considered first.

In general, nonsingular linear integral equations can be solved numerically by approximating the integral by a sum over a suitable set of quadrature points. That is, if the kernel, K, is nonsingular,

$$\psi(z) = \psi_0(z) + \lambda \int_a^b K(z, z') \, \psi(z') \, dz'$$
(1)

is written approximately as

$$\psi(z_i) = \psi_0(z_i) + \lambda \sum_{j=1}^{N} w_j K(z_i, z_j) \psi(z_j), \qquad (2)$$

where  $z_j$  and  $w_j$  are the abscissas and weights of the quadrature used. A solution is then achieved by matrix inversion.

$$\psi(z_i) = \sum_{j=1}^{N} \left[ 1 - \lambda M \right]_{ij}^{-1} \psi_0(z_j)$$
(3)

with  $M_{ij} = w_j K(z_i, z_j)$ .

\* Research partially supported by a grant from the Research Corporation, and by Associated Western Universities, Inc.

If K(z, z') is singular, such a straightforward scheme cannot be used. If, for example

$$\lim_{z\to z'}K(z,\,z')=\infty,$$

the diagonal elements of  $M_{ij}$  as defined above would be infinite. Thus, to obtain a numerical solution to such singular equations, techniques must be found which correctly deal with these singularities.

In this note, integral equations with kernels that have pole singularities are considered. It is illustrated, by examples, that the method presented here treats the singularities correctly and yields very accurate solutions to equations of physical interest.

In Section 2, an equation is considered in which the kernel is of the form

$$K(z, z') = T(z, z')/(z - z')_P, \qquad (4)$$

where T(z, z') is a bounded continuous function for all values of z, z', and does not vary wildly over this range. (Such functions will be called "well behaved.") P means the Cauchy principal value. The proposed method is presented in this section. As illustrative examples, equations with kernels described in Eq. (4) are considered, one inhomogeneous and one homogeneous.

In Section 3, the technique is applied to an equation in which the kernel has a fixed pole.

$$K(z, z'; E) = V(z, z')/(z' - E)_P.$$
(5)

In the illustrative example, a Lippmann-Schwinger equation is solved numerically.

In Section 4, the approach is applied to nonlinear equations such as arise from dispersion relations. Here again, it is shown by example that the technique yields accurate results in a straightforward way.

Two appendixes are also included. In the first, integral equations with infinite limits are discussed. No numerical examples are considered. In the second, other techniques presented elsewhere are compared with the approach of this paper.

## 2. LINEAR EQUATIONS WITH CAUCHY SINGULARITIES

A linear integral equation with a Cauchy singularity (with a kernel like that of Eq. (4)), has the form

$$\psi(z) = \psi_0(z) + \lambda \int_a^b \frac{T(z, z')}{(z - z')_P} \,\psi(z') \, dz'.$$
(6)

Here  $\lambda$  is a known constant, and  $\psi_0$  and T are well-behaved functions.

It is quite straightforward to show if either a or b is finite, Eq. (6) can be transformed into an equation of the form

$$\phi(x) = f(x) + \lambda \int_{-1}^{1} \frac{U(x, y)}{(x - y)_P} \phi(y) \, dy.$$
(7)

It is in this form that a solution to the integral equation is studied.

To solve Eq. (7), I propose a particular interpolative approximation to  $\phi$ . It yields a straightforward numerical system to solve and, as will be seen, accurate results.

To begin, Eq. (7) is rewritten

$$\phi(x) = f(x) + \lambda \int_{-1}^{1} \frac{[U(x, y) - U(x, x)]}{(x - y)} \phi(y) \, dy + \lambda U(x, x) \int_{-1}^{1} \frac{\phi(y)}{(x - y)_P} \, dy. \tag{8}$$

It is first noted that the first integrand is no longer singular at y = x since U is a wellbehaved function and thus has a Taylor expansion in y around x. Thus the first integral can be well approximated by a quadrature sum. With  $x = x_i$ , the first integral is approximately

$$\sum_{j=1}^{N} w_{j} [U(x_{i}, x_{j}) - U(x_{i}, x_{j})] \phi(x_{j})(x_{i} - x_{j})^{-1}, \qquad (9a)$$

where the j = i term is

$$-w_i\phi(x_i) \,\partial U(x_i\,,\,y)/\partial y \mid_{y=x_i}.$$
(9b)

As with nonsingular equations, this method will solve these linear equations by matrix inversion. In order that the matrix inversion be straightforward, the second integral of Eq. (8) should be accurately approximated by a sum in which  $\phi$  is evaluated at the same quadrature points  $\{x_i\}$  as those used in Eq. (9a) to approximate the first integral. To accomplish this, note that the quadrature abscissas are the zeros of some polynomial  $A_N(x)$  (for an N-point quadrature rule). That is,  $A_N(x_i) = 0$ . Thus,  $\phi$  is interpolated over the interval [-1, 1] as

$$\phi(y) = \sum_{j=1}^{N} \frac{A_N(y) \phi(x_j)}{(y - x_j) A_N'(x_j)}.$$
 (10)

(The reader is referred to Ref. [1].) Because the interval is [-1, 1], it is very convenient, though not necessary, to take  $A_N(y)$  to be the Legendre polynomial  $P_N(y)$ . It should be noted that Gaussian quadratures are convenient to use in this scheme. This is because the Gaussian quadrature points do not include the end points where  $\phi(y)$  is expected to be singular [2]. Methods have been presented which remove these endpoint singularities [3]. Thus, at the interior points, where  $\phi(y)$  is not singular, a polynomial approximation can be expected to work well.

Using Eq. (10), with  $A_N(y) = P_N(y)$ , the second integral becomes

$$\sum_{j=1}^{N} \frac{\phi(x_j)}{P_N'(x_j)} \int_{-1}^{1} P_N(y) (x_i - y)^{-1} (y - x_j)^{-1} dy.$$
(11)

Using the integral representation of the Legendre function of the second kind,

$$Q_N(x) = \frac{1}{2} \int_{-1}^{1} P_N(y)(x-y)_P^{-1} dy,$$

the second integral becomes

$$2 \sum_{j=1}^{N} \frac{\phi(x_j)}{P_N'(x_j)} \frac{[Q_N(x_i) - Q_N(x_j)]}{(x_i - x_j)}, \qquad (12a)$$

where the j = i term is

$$2\phi(x_i)[Q_N'(x_i)/P_N'(x_i)].$$
 (12b)

Thus, with Eqs. (9) and (12), the matrix equation for  $\phi$  is

$$\phi(x_i) = f(x_i) + \lambda \sum_{j=1}^N M_{ij} \phi(x_j), \qquad (13a)$$

where

$$M_{ij} = \left( w_j [U(x_i, x_j) - U(x_i, x_i)] + 2 \frac{U(x_i, x_i)}{P_n'(x_j)} [Q_N(x_i) - Q_N(x_j)] \right) (x_i - x_j)^{-1},$$
(13b)

the diagonal terms being given by Eqs. (9b) and (12b). The matrix elements are all finite and relatively simple to generate. Thus, a straightforward solution to Eq. (13a) can be achieved by matrix inversion. Values of the unknown function at points other than those in the abscissa set  $\{x_i\}$  can be found by inserting the values of  $\phi(x_i)$  from the solution of Eq. (13a) into Eq. (10).

To illustrate the accuracy of a numerical scheme, it is customary to solve an equation and compare the results to a known solution. An example of an equation of the type considered in this section is the Omnes equation [4], which arises in the theory of low-energy scattering processes involving the pion and nucleon in the initial or final state. The simplest form of the Omnes equation which contains the pole singularity is

$$\psi(z) = F(z) + \frac{1}{\pi} \int_{1}^{\infty} \frac{h^{*}(z')}{(z' - z - i\epsilon)} \,\psi(z') \,dz', \qquad (14)$$

where  $h(z) = \exp[i\delta(z)] \sin \delta(z)$ .

In general, since the kernel of Eq. (7) is singular, the homogeneous as well as the inhomogeneous equation has a nontrivial solution. Thus, the total solution is the

particular solution to the inhomogeneous equation added to a linear combination of the independent solutions to the homogeneous equations [2]. The inversion method presented here will only yield a solution to the inhomogeneous equation; that is, only a particular solution. However, for the Omnes equation, if the phase shift is zero at z = 1 in Eq. (14), the particular solution to Eq. (14) is the complete solution [2, 4]. This solution is (reproducing Eq. (2.11) of Ref. [4])

$$\psi(z) = \exp[i\delta(z)] \left( F(z) \cos \delta(z) + \frac{1}{\pi} P \int_{1}^{\infty} \frac{F(z') \sin \delta(z') \exp[-\rho(z')]}{(z'-z)} dz' \right), \quad (15)$$

where

$$\rho(z) = \frac{1}{\pi} P \int_{1}^{\infty} \frac{\delta(z')}{(z'-z)} dz'.$$
 (16)

To illustrate the approach of this paper, I solved the Omnes equation in the form of Eq. (14). Writing  $(z' - z - i\epsilon)^{-1} = (z' - z)_p^{-1} + i\pi\delta(z' - z)$ , and noting that  $1 - ih^*(z) = \exp[-i\delta(z)] \cos \delta(z)$ , Eq. (14) can be written as

$$G(z) = F(z) + \frac{1}{\pi} P \int_{1}^{\infty} \frac{\tan \delta(z')}{(z'-z)} G(z') dz', \qquad (17)$$

where  $G(z) \equiv \exp[-i\delta(z)] \cos \delta(z) \psi(z)$ . Using the transformations

z = 2/(1 + x), z' = 2/(1 + y),  $\phi(x) = G(z)/(1 + x),$  f(x) = F(z)/(1 + x)

Eq. (17) becomes

$$\phi(x) = f(x) + \frac{1}{\pi} P \int_{-1}^{1} \frac{\tan[2/(1+y)]}{(x-y)} \phi(y) \, dy. \tag{18}$$

I use a function F(z) = 0.5/z [5], and parametrize the phase shift by

$$\delta(z) = [(z-1)/z^2] \pi, \quad 1 \leq z \leq \infty,$$

or

$$\delta[2/(1+y)] = (1-y^2) \pi/4, \qquad -1 \leqslant y \leqslant 1.$$
(19)

With this parametrization, Eq. (15) is the complete solution to the Omnes equation.

In Table I, the results of inverting the Omnes equation of Eq. (18) are compared with the appropriate analytic form. As can be seen, the technique yields accurate results. Using a 20-point quadrature rule, one can see that the numerical solution is within 0.003 % of the analytic value. A 40-point rule brings the inversion solution to within 0.0002 % of the analytic result. To illustrate that accurate results are obtained by this method at points other than those in the abscissa set, Table Ib presents values of  $\phi(x)$  at randomly chosen points not in  $\{x_i\}$ . Thus, this straightforward scheme appears to be very satisfactory for equations typified by Eq. (6).

TABLE	Ia
-------	----

Z	Calculated values	Analytic values	% Difference
	20 p	oints	
1.003	0.4188	0.4188	0.00069
2.166	0.1645	0.1645	0.0015
4.089	0.1315	0.1315	0.0012
7.884	0.1307	0.1307	0.00019
22.788	0.1380	0.1380	0.00043
291.061	0.1492	0.1492	0.0029
	40 p	oints	
1.001	0.4144	0.4144	0.000038
2.081	0.1703	0.1703	0.000075
3.869	0.1322	0.1322	0.000062
7.335	0.1304	0.1304	0.000010
20.429	0.1372	0.1372	0.000045
134.887	0.1508	0.1508	0.00019

Comparison of Solutio	n of	Omnes	Equation	with	Analytic	Form
-----------------------	------	-------	----------	------	----------	------

TABLE	Ъ
TADLL	10

Interpolation of Solution to Omnes Equation to Intermediate Points

x	Z	Calculated values	Analytic values	% Difference
	Us	ing 20-point solution	n	
0.99999	1.000	0.41364	0.41223	0.0034
0.80	1.111	0.43647	0.43646	0.00003
0.40	1.429	0.28826	0.28826	0.000004
0.20	2.500	0.14961	0.14961	0.000009
0.60	5.000	0.13001	0.13001	0.000004
-0.99999	$2  imes 10^5$	0.15106	0.15165	0.004
	Us	ing 40-point solution	n	
0.99999	1.000	0.41257	0.41220	0.0009
0.80	1.111	0.43646	0.43646	0.000003
0.40	1.429	0.28826	0.28826	0.00002
-0.20	2.500	0.14961	0.14961	0.00002
-0.60	5.000	0.13001	0.13001	0.00003
-0.99999	$2  imes 10^5$	0.15111	0.15113	0.0001

As mentioned before, the total solution to the general equation (6) also requires the solution to the homogeneous counterpart. When this interpolative approach is applied to the homogeneous form of Eq. (6), an algebraic system identical to Eq. (13) with  $f(x_i) = 0$  results. Thus, the solution of the homogeneous integral equation becomes the solution of a homogeneous set of algebraic equations

$$\phi(x_i) = \lambda \sum_{j=1}^N M_{ij} \phi(x_j), \qquad (20)$$

where  $M_{ij}$  is given by Eq. (13b).

To solve this set of algebraic equations, the idea is to normalize the unknown function so that, for example,  $\phi(x_N) = 1$ . That is, Eq. (20) is divided by  $\phi(x_N)$  and becomes

$$1 = \lambda M_{NN} + \lambda \sum_{j=1}^{N-1} M_{Nj} \psi_j, \qquad (21a)$$

$$\psi_i = \lambda M_{iN} + \lambda \sum_{j=1}^{N-1} M_{ij} \psi_j, \qquad (21b)$$

where  $\psi_i = \phi(x_i)/\phi(x_N)$ . The (N-1)-dimensional subset of equations in Eq. (21b) is solved by inversion, and Eq. (21a) serves as a consistency check on the solution.

To illustrate that the present approach is satisfactory for homogeneous equations, I solved the Milne equation for the radiative flux, which is given in a report by Bareiss and Neumann [6, Sect. IV]. This is a well-known problem arising in the theory of radiative transfer and neutron transport [7].

$$\left(1 - \frac{c}{2}z\log\frac{(1+z)}{(1-z)}\right)\psi(z) = \frac{c}{2}P\int_{-1}^{0}z'\psi(z')(z'-z)^{-1}dz'.$$
 (22)

To compare the results of inverting Eq. (22) by the present method with results obtained in Refs. [6, 7], I used a 20-point quadrature rule, and inverted the set of equations corresponding to Eq. (21b). I then used a Lagrange interpolation to obtain

TABLE IIa

Comparison of Radiative Flux as Found by Approach of This Paper, Method of Ref. [6], and Chandrasekhar Results

μ	Method of Ref. [6], 50 points	Method of this paper	Chandrasekhar results
0.05	0.4027	0.4031	0.4032
0.35	0.6154	0.6159	0.6159
0.65	0.8097	0.8102	0.8102
0.95	1.0000	1,0000	1.0000

### TABLE IIb

Check on Consistency of Solution of Eq. (21b) by Substitution of Solution into Eq. (21a)

$\lambda \sum_{j=1}^{N-1} M_{Nj}$	$1 - \lambda M_{NN}$	% Difference	
 1.14393	1.14402	0.008	

 $\psi(z)$  at the points reported in Refs. [6, 7]. The comparison is presented in Table IIa. As will be noted, the 20-point rule using the approach of this paper is closer to Chandrasekhar's results than the 50-point scheme used in Ref. [6]. As can be seen in Table IIb, the consistency of the calculation, suggested by Eq. (21a), is also quite good.

It therefore appears that an integral equation, the kernel of which contains a Cauchy singularity, can be inverted accurately, in a straightforward way, using a relatively small matrix.

## 3. KERNELS WITH FIXED POLES: THE LIPPMANN-SCHWINGER EQUATION

In this section the technique described for inverting linear equations with Cauchylike kernels is applied to equations with kernels containing a fixed pole. To illustrate the scheme for such a kernel a Lippmann–Schwinger equation will be used as an example.

The partial-wave Lippmann-Schwinger equation has the form

$$\psi_l(p^2, p'^2; k_0^2) = V_l(p^2, p'^2) - \frac{2}{\pi} \int_0^\infty \frac{V_l(p^2, k^2) \,\psi_l(k^2, p'^2; k_0^2)}{(k^2 - k_0^2 - i\epsilon)} \,k^2 \,dk, \quad (23)$$

where, in this form, the on-shell amplitude is related to the phase shift by

$$\psi_l(k_0^2, k_0^2; k_0^2) = -(1/k_0) \exp[i\delta_l(k_0^2)] \sin \delta_l(k_0^2).$$
(24)

As with Cauchy-like equations, the first step is to project out the principal-value integral in Eq. (23). Suppressing the angular momentum dependence, this yields

$$\psi(p^{2}, p'^{2}; k_{0}^{2}) = V(p^{2}, p'^{2}) - ik_{0}V(p^{2}, k_{0}^{2}) \psi(k_{0}^{2}, p'^{2}; k_{0}^{2})$$
$$- \frac{2}{\pi} \int_{0}^{\infty} \frac{V(p^{2}, k^{2}) \psi(k^{2}, p'^{2}; k_{0}^{2})}{(k^{2} - k_{0}^{2})_{P}} k^{2} dk.$$
(25)

Setting  $p^2 = k_0^2$  yields an equation for  $\psi(k_0^2, p'^2; k_0^2)$ . Inserting this into Eq. (25) yields the desired equation, containing only the principal-value integral.

$$\psi(p^{2}, p'^{2}; k_{0}^{2}) = V(p^{2}, p'^{2}) - ik_{0}V(p^{2}, k_{0}^{2}) V(k_{0}^{2}, p'^{2})[1 + ik_{0}V(k_{0}^{2}, k_{0}^{2})]^{-1} - \frac{2}{\pi} \int_{0}^{\infty} (V(p^{2}, k^{2}) - ik_{0}V(p^{2}, k_{0}^{2}) V(k_{0}^{2}, k^{2})[1 + ik_{0}V(k_{0}^{2}, k_{0}^{2})]^{-1}) + \psi(k^{2}, p'^{2}; k_{0}^{2}) = 0$$

$$\times \frac{\psi(k^2, p'^2; k_0^2)}{(k^2 - k_0^2)_P} k^2 dk.$$
<sup>(26)</sup>

It is now straightforward that one can proceed to use the technique of Section 2 to invert Eq. (26). First a transformation is made from  $(p, k, k_0)$  which  $\in [0, \infty]$  to variables (x, y, E) which  $\in [-1, 1]$ . Here,  $E = (k_0^2 - 1)/(k_0^2 + 1)$ . The subtraction of the smooth part of the kernel is now made at the fixed point  $y = E(k = k_0)$ , rather than at y = x (k = p) as in Section 2. Transformation to the (x, y, E) variables yields the matrix equation

$$\phi(x_i, x'; E) = f(x_i, x'; E) - \sum_{j=1}^{N} M_{ij}\phi(x_j, x'; E)$$
(27a)

with

$$M_{ij} = \left( w_j [U(x_i, x_j; E) - U(x_i, E; E)] + 2 \frac{U(x_i, E; E)}{P_N'(x_j)} [Q_N(x_j) - Q_N(E)] \right) (x_j - E)^{-1}.$$
 (27b)

U(x, y; E) results from the transformation of the bracketed terms in the integral of Eq. (26) and f(x, x'; E) comes from the transformation of the inhomogeneous term. As with Cauchy-like equations, all the elements of  $M_{ij}$  are finite, the differences being replaced by derivatives if the chosen value of E happens to equal one of the abscissa points.

To illustrate the viability of the proposed method in solving this type of equation, I consider the Lippmann-Schwinger equation with the Yamaguchi potential

$$V(p^2, p'^2) = \lambda(p^2 + \beta^2)^{-1} (p'^2 + \beta^2)^{-1}.$$
(28)

Osborn [8] has discussed the method of moments to solve the Lippmann-Schwinger equation, using this potential as an example. (Additional comments about the method of moments are presented in Appendix B.) Following Osborn,  $\lambda$  and  $\beta$  are chosen to be -8.110 and 1.444, respectively, so that the triplet *n-p* bound-state energy and scattering length are correctly given for this potential. This potential has the attractive feature that because it is separable, the kernel of Eq. (23) is degenerate. Thus, one can easily find the analytic solution. It is

$$\psi(p^2, p'^2; k_0^2) = (p^2 + \beta^2)^{-1} \left(p'^2 + \beta^2\right)^{-1} \left(1 + \frac{\lambda}{2\beta(\beta - ik_0)^2}\right)^{-1}.$$
 (29)

I compare the result of inverting Eq. (27a) with this analytic form setting  $p' = k_0$ . The transformation p = (1 - x)/(1 + x) takes the interval  $[0, \infty]$  to [-1, 1]. These

TABLE	ш
-------	---

Comparison of Solution to Lippmann-Schwinger Equation with Yamaguchi Potential to Analytic Solution

v	Calculated	Analytic
л	values	values
	$k_0{}^2 = 0.1$	
20 points		
0.9931	0.0067210.021557 <i>i</i>	0.006722-0.021556i
0.3737	0.4589–1.4720 <i>i</i>	0.4590-1.4719 <i>i</i>
-0.7463	0.8803-2.8236i	0.8805-2.8235i
0.9931	0.9401–3.0153 <i>i</i>	0.9403-3.0152 <i>i</i>
30 points		
0.9969	0.00304510.0097653 <i>i</i>	0.0030453-0.0097652i
0.3527	0.47038-1.50844 <i>i</i>	0.47041-1.50843 <i>i</i>
0,7678	0.88599–2.84125 <i>i</i>	0.88604–2.84121 <i>i</i>
-0.9969	0.94111–3.017998 <i>i</i>	0.94116–3.017959 <i>i</i>
	$k_0^2 = 10$	
20 points		
0.9931	-0.00194843-0.00029696 <i>i</i>	-0.00194839-0.00029694 <i>i</i>
0.3737	0.133043-0.020277 <i>i</i>	0.1330400.020276 <i>i</i>
-0.7463	0.2552140.038897 <i>i</i>	0.2552080.038895i
0.9931	-0.272543-0.041538 <i>i</i>	-0.272536-0.041536 <i>i</i>
30 points		
0.9960	-0.000882656-0.000134552 <i>i</i>	0.0008826500.000134519
0.3527	-0.136343-0.0207793 <i>i</i>	-0.136342-0.0207790 <i>i</i>
-0.7678	-0.256810-0.0391391 <i>i</i>	
0.9969	-0.272785 - 0.0415739i	-0.272783-0.0415733 <i>i</i>
	$k_0^2 = 0.22$	
	(E = -0.6361)	
20 points		
0.9931	0.000412360.01673687 <i>i</i>	-0.00041238-0.01673687 <i>i</i>
0.3737	-0.028157 - 1.142829i	-0.028156-1.142829 <i>i</i>
-0.6361	-0.052206-2.118930 <i>i</i>	-0.052204-2.118930 <i>i</i>
-0.9931	-0.057680-2.341118 <i>i</i>	0.057678-2.341118 <i>i</i>

comparative results at representative values of x are presented in Table III. As can be seen, a 20-point quadrature rule yields an accuracy to three decimal places. A 30point rule increases the accuracy to at least four decimal places. This indicates that this appraoch is a satisfactory one for solving equations with kernels containing fixed poles.

## 4. NONLINEAR EQUATIONS ARISING FROM DISPERSION RELATIONS

In this section, integral equations which result from dispersion relations for scattering amplitudes are studied. Such equations are of the form

Re 
$$F(s) = F_0(s) + \frac{1}{\pi} \int_a^\infty V(s, s') \operatorname{Im} F(s')(s' - s)_P^{-1} ds',$$
 (30)

where V(s, s') is specified by the type of subtraction made. The nonlinearity arises from the unitarity constraint

Im 
$$F(s) = \rho(s) |F(s)|^2$$
. (31)

The singularity of the kernel in Eq. (30) is again handled using the interpolative approach of this paper. Transforming the interval to [-1, 1] and then applying the interpolation to Eq. (30) yields

$$\alpha(x_i) = F_0(x_i) + \frac{1}{\pi} \sum_{j=1}^N C_{ij} \beta(x_j),$$
 (32)

where

$$F(s) \equiv \alpha(s) + i\beta(s), \qquad (33a)$$
  
$$s = -1 + 2a/x, \qquad a \neq 0,$$

$$=(1+x)/(1-x), \quad a=0,$$
 (33b)

and

$$C_{ij} = ([V_1(x_i, x_j) - V_1(x_i, x_i)] w_j + 2V_1(x_i, x_i)[Q_N(x_i) - Q_N(x_j)]/P_N'(x_j))(x_i - x_j)^{-1},$$
(33c)

where  $V_1(x_i, x_j) = V[s(x_i), s(x_j)]$  multiplied by a factor coming from transforming the range of integration.

Equation (31) can now be written as

$$\beta(x_i) = \rho(x_i)[\alpha^2(x_i) + \beta^2(x_i)].$$
(34)

Inserting Eq. (32) into Eq. (34) yields

$$\beta(x_i) = \rho(x_i) F_0^2(x_i) + \frac{2}{\pi} F_0(x_i) \rho(x_i) \sum_{j=1}^N C_{ij} \beta(x_j) + \rho(x_i) \frac{1}{\pi^2} \sum_{j,k=1}^N C_{ij} C_{ik} \beta(x_j) \beta(x_k) + \rho(x_i) \beta^2(x_i).$$
(35)

With

$$A_{ij} = \delta_{ij} - (2/\pi) F_0(x_i) \rho(x_i) C_{ij}$$
(36a)

and

$$V_{ijk} = \rho(x_i) [\delta_{ij} \delta_{ik} + (1/\pi^2) C_{ij} C_{ik}],$$
 (36b)

Eq. (35) can be rewritten as

$$\sum_{j} A_{ij}\beta_{j} = \rho(x_{i}) F_{0}^{2}(x_{i}) + \sum_{j,k} V_{ijk}\beta_{j}\beta_{k} .$$
(37)

In order to illustrate the usefulness of the proposed approach to this type of problem, I considered the problem introduced by Blankenbecler *et al.* [9] with which they tested the validity of approximating the left-hand cut in potential scattering by the contribution from the Born term. The equation involved is

$$F(s) = -2g/(1+4s) + \frac{1}{\pi} \int_0^\infty \frac{\mathrm{Im} \, F(s')}{(s'-s-i\epsilon)} \, ds' \tag{38a}$$

with

Im 
$$F(s) = s^{1/2} |F(s)|^2$$
. (38b)

This equation has the solution

$$F(s) = \frac{-2g}{(1+4s)} \left( 1 + \frac{2g(1+4s)}{\pi} \int_0^\infty \frac{(s')^{1/2} \, ds'}{(1+4s')^2 \, (s'-s-i\epsilon)} \right)^{-1}.$$
 (39)

To solve Eqs. (38), the transformation from  $s \in [0, \infty]$  to  $x \in [-1, 1]$  was made (see Eq. (33b)). The functions

$$a(x) \equiv \alpha[s(x)]/(1-x) \quad \text{and} \quad b(x) \equiv \beta[s(x)]/(1-x) \quad (40)$$

arise naturally from the transformation. A nonlinear algebraic system of equations for  $b(x_i)$ , which evolve from Eq. (37), was solved, and  $a(x_i)$  was generated from  $b(x_i)$  according to Eq. (32).

In Table IV, the numerical solutions to these functions are compared to the appropriate analytic values with g = 1. As can be seen, the numerical and analytic solutions are within 1.6% of each other when 20 quadrature points are used. This difference is reduced to 0.74% or less by increasing the number of quadrature points to 40. Even though these errors are very small it should be noted that the largest differences do occur at s = 0, where F(s) has a square root branch point. The small size of the errors does indicate, however, that this interpolation scheme is a viable one for nonlinear equations as well.

The solutions presented in Table IV were obtained using a program, available on the Stanford computing system, called NS01A. The algorithm uses the method of steepest descent to get near a solution. The program then switches to a Newton method to home in on the solution. This makes for very rapid convergence. This approach is documented in Technical Report AERE-R.5947, Harwell, England, November 1968.

x	a(x)	Analytic value	% Difference	<i>b</i> ( <i>x</i> )	Analytic value	% Difference	5
			20-Point-quadi	ature rule			
0.993	-0.4965	-0.4987	0.45	0.0289	0.0292	0.91	290.06
0.746	-0.4618	-0.4618	0.0083	0.1587	0.1587	0.019	6.88
0.007	-0.4290	-0.4290	0.0073	0.2418	0.2418	0.021	1.17
-0.374	-0.4596	-0.4596	0.0028	0.2573	0.2573	0.0081	.46
-0.993	-0.6672	-0.6619	0.80	0.5241	0.5158	1.6	.003
			40-Point quadi	ature rule			
0.998	0.4985	-0.4997	0.24	0.0148	0.0148	0.48	1133.89
0.825	-0.4718	-0.4718	0.0022	0.1364	0.1364	0.0045	10.40
0.342	-0.4317	-0.4317	0.00087	0.2210	0.2210	0.0024	2.04
-0.268	-0.4475	-0.4475	0.00084	0.2562	0.2562	0.0025	.58
-0.998	0.6679	-0.6654	0.37	0.2651	0.2632	0.74	0.001

TA	BL	Æ	IV
- 1 4 1			

Results at Selected Points for Dispersion Integral Equation of Blankenbecler et al.

## APPENDIX A: INTERPOLATIVE APPROACH APPLIED TO LINEAR INTEGRAL EQUATIONS WITH INFINITE OR SEMI-INFINITE LIMITS

In the body of this paper, all integrals were transformed to the interval [-1, 1], including equations in which the parameters ranged over the interval  $[a, \infty]$ . The range [-1, 1] is found to be very convenient for this approach since the integral

$$\int_{-1}^{1} \frac{\phi(y)}{(x-y)_P} \, dy$$

is easily evaluated when  $\phi(y)$  is interpolated over the Legendre polynomials. Considerable information about the second Legendre functions  $Q_N(x)$  is readily available. Equations involving the interval  $[-\infty, \infty]$  were not considered because there is no simple transformation which will take

$$\int_{-\infty}^{\infty} f(x')(x'-x)_P^{-1} dx' \to \int_{-1}^{1} f(y') T(y')(y'-y)_P^{-1} dy',$$

where T(y') is defined from dx' = T(y') dy'.

However, it may be possible to deal directly with semi-infinite or infinite intervals using the interpolative approach of this paper.

In this appendix, I consider equations of the form

$$\phi(x) = f(x) + \lambda \int_a^\infty \frac{U(x, y)}{(x - y)_P} \phi(y) \, dy \qquad (a \text{ finite}) \tag{A1}$$

and

$$\phi(x) = f(x) + \lambda \int_{-\infty}^{\infty} \frac{U(x, y)}{(x - y)_P} \phi(y) \, dy. \tag{A2}$$

In Eq. (A1) there is no loss of generality in taking a = 0, and this will be done henceforth. For integrals over the range  $[0, \infty]$ , the most natural quadrature to use is one over the Laguerre polynomials. This rule approximates an integral as

$$\int_0^\infty \exp[-x] f(x) \, dx \simeq \sum_{j=1}^N w_j f(x_j),\tag{A3}$$

where  $x_i$  is a zero of the Nth Laguerre polynomial.

Similarly, an integral over the range  $[-\infty, \infty]$  is approximated by a Hermite quadrature rule as

$$\int_{-\infty}^{\infty} \exp[-x^2] f(x) \, dx \simeq \sum_{j=1}^{N} w_j f(x_j) \tag{A4}$$

with  $x_j$  a zero of the Nth Hermite polynomial. It is generally agreed that it is essential for the exponential factors to appear explicitly in the integrand of Eqs. (A3) and (A4) [10]. Otherwise, unless the function g(x) falls off at least as rapidly as the exponential, one obtains very poor results by approximating the integrals involving infinite limits as

$$\int_{0}^{\infty} g(x) \, dx = \int_{0}^{\infty} \exp[-x](\exp[x] g(x)) \, dx \simeq \sum_{j=1}^{N} w_j \exp[x_j] g(x_j) \tag{A5}$$

or

$$\int_{-\infty}^{\infty} g(x) \, dx = \int_{-\infty}^{\infty} \exp[-x^2](\exp[x^2] g(x)) \, dx \simeq \sum_{j=1}^{N} w_j \exp[x_j^2] g(x_j).$$
(A6)

The failure of such approximations is due to the fact that the exponential factor multiplying g(y) in the approximate sum weights the contribution from the large  $x_j$ 's much too heavily [10]. Thus, in order that one be able to apply an interpolative approach to Eq. (A1) directly, without first transforming to [-1, 1], or be able to apply such a scheme to Eq. (A2) at all, it is required that one have

$$U(x, y) = \exp[-y] V(x, y)$$
 for Eq. (A1),  
=  $\exp[-y^2] V(x, y)$  for Eq. (A2), (A7)

with V(x, y) a well-behaved function. If the above condition is satisfied, one can then proceed. Writing the integral equations in subtracted form,

$$\phi(x) = f(x) + \lambda \int_0^\infty \frac{[V(x, y) - V(x, x)]}{(x - y)_p} \exp[-y] \phi(y) \, dy$$
$$+ \lambda V(x, x) \int_0^\infty \frac{\exp[-y] \phi(y)}{(x - y)_p} \, dy$$
(A8)

and

$$\phi(x) = f(x) + \lambda \int_{-\infty}^{\infty} \frac{[V(x, y) - V(x, x)]}{(x - y)_P} \exp[-y^2] \phi(y) \, dy + \lambda V(x, x) \int_{-\infty}^{\infty} \frac{\exp[-y^2] \phi(y)}{(x - y)_P} \, dy.$$
(A9)

The first integral in Eq. (A8) will now be well approximated by a sum over Laguerre quadratures, and the first integral of Eq. (A9) is well approximated by a Hermite quadrature rule (since V(x, y) is assumed to be well behaved). Then, as suggested by the approach outlined in the body of the paper,  $\phi(y)$  in the second integral of each equation must be interpolated as in Eq. (10) using a Laguerre and a Hermite polynomial, respectively.

Consider

$$I_L(x) = \int_0^\infty \frac{\exp[-y] \phi(y)}{(x-y)_P} \, dy.$$
 (A10)

As in Eq. (10),  $\phi$  is written

$$\phi(y) = \sum_{j=1}^{N} \frac{\phi(x_j) L_N(y)}{(y - x_j) L_N'(x_j)}.$$
 (A11)

Defining

$$\Lambda_N(x) \equiv \int_0^\infty \frac{\exp[-y] L_N(y)}{(x-y)_P} \, dy, \tag{A12}$$

it is straightforward to show that

$$I_L(x_i) = \sum_{j=1}^{N} \frac{\phi(x_j)}{L_{N'}(x_j)} \frac{[\Lambda_N(x_i) - \Lambda_N(x_j)]}{(x_i - x_j)}.$$
 (A13)

All that is required now is to study the properties of  $\Lambda_N(x)$  so that  $\Lambda_N(x_i)$  and  $\Lambda_N'(x_i)$  (for the j = i term) can be generated.

The Laguerre polynomials satisfy

$$NL_N(x) = (2N - 1 - x) L_{N-1}(x) - (N - 1) L_{N-2}(x), \qquad N \ge 2.$$
(A14)

From this, using the orthogonality relation

$$\int_{0}^{\infty} \exp[-y] L_{N-1}(y) \, dy = 0, \qquad N \ge 2, \tag{A15}$$

it is easy to show that  $\Lambda_N(x)$  satisfies the same recurrence relation, Eq. (A14). Thus, noting that

$$\Lambda_0(x) = \exp[-x] Ei(x), \qquad \Lambda_1(x) = 1 + (1-x) \Lambda_0(x), \tag{A16}$$

581/26/3-2

 $\Lambda_N(x)$  can be generated from Eq. (A14). From the recurrence relation

$$xL_{N}'(x) = N[L_{N}(x) - L_{N-1}(x)]$$
(A17)

one can generate

$$\Lambda_{N}'(x) = (1/x) L_{N}(0) - \Lambda_{N}(x) + (N/x)([\Lambda_{N}(x) - \Lambda_{N-1}(x)] - [\Lambda_{N}(0) - \Lambda_{N-1}(0)])$$
(A18)

and all the needed properties of  $\Lambda_N(x)$  are well defined.

To apply this scheme to Eq. (A9), one seeks to interpolate  $\phi(y)$  over Hermite polynomials in the second integral. Define

$$I_{H}(x) \equiv \int_{-\infty}^{\infty} \frac{\exp[-y^{2}] \phi(y)}{(x-y)_{P}} dy.$$
 (A19)

As expected, one writes

$$\phi(y) = \sum_{j=1}^{N} \frac{\phi(x_j) H_N(y)}{H_N'(x_j)(y - x_j)}$$
(A20)

and  $I_H(x_i)$  becomes

$$I_{H}(x_{i}) = \sum_{j=1}^{N} \frac{\phi(x_{j})}{H_{N}'(x_{j})} \frac{[\eta_{N}(x_{i}) - \eta_{N}(x_{j})]}{(x_{i} - x_{j})},$$
(A21)

where I have defined

$$\eta_N(x) \equiv P \int_{-\infty}^{\infty} \frac{\exp[-y^2] H_N(y)}{(x-y)} \, dy.$$
 (A22)

As with the Laguerre interpolation, all that is needed to completely define this system is a detailing of the properties of  $\eta_N(x)$ .

Since the Hermite polynomials satisfy

$$H_{N+1}(x) = 2xH_N(x) - 2NH_{N-1}(x), \qquad N \ge 1,$$
 (A23)

one can easily show, using the orthogonality condition

$$\int_{-\infty}^{\infty} \exp[-y^2] H_N(y) \, dy = 0, \qquad N \ge 1, \tag{A24}$$

that  $\eta_N(x)$  satisfies the same recurrence relation as  $H_N(x)$ . Thus,  $\eta_N(x)$  can be generated by first evaluating

$$\eta_0(x) = \int_{-\infty}^{\infty} \frac{\exp[-y^2]}{(x-y)_P} dy$$
 and  $\eta_1(x) = 2[x\eta_0(x) - \pi^{1/2}].$  (A25)

Using

$$H_{N}'(y) = 2NH_{N-1}(y),$$
 (A26)

it can easily be shown that

$$\eta_{N'}(x) = \eta_{N+1}(x). \tag{A27}$$

So all the necessary properties of  $\eta_N(x)$  are known. Thus, if the kernel of Eq. (A1) or Eq. (A2) satisfies the conditions of Eq. (A7), one can also apply an interpolative approach directly to integral equations with parameters that run over a semi-infinite or an infinite range.

APPENDIX B: Other Techniques Applied to Integral Equations with Poles

In an earlier paper by Ickovic and myself [11] integral equations that had weakly singular kernels were considered. A weakly singular kernel is defined by

$$\lim_{z \to z'} K(z, z') = \infty, \qquad \lim_{z \to z'} (z - z') K(z, z') = 0.$$
(B1)

The method presented in Ref. [11] is outlined briefly at this point. Beginning with the equation

$$\psi(x) = \psi_0(x) + \lambda \int_a^b K(x, x') \, \psi(x') \, dx', \tag{B2}$$

the interval [a, b] was broken into small segments. If  $x_i$  is a quadrature point the integral was written

$$\int_{a}^{b} K(x, x') \psi(x') dx' = \sum_{j} \int_{\theta_{j}}^{\theta_{j+1}} K(x, x') \psi(x') dx',$$
(B3)

where  $\theta_j$  is the midpoint between  $x_{j-1}$  and  $x_j$ .  $\psi(x')$  is then approximated in each segment  $[\theta_j, \theta_{j+1}]$  by the constant  $\psi(x_j)$ . Thus, Eq. (B3) becomes

$$\psi(x_i) = \psi_0(x_i) + \lambda \sum_{j} \psi(x_j) \int_{\theta_j}^{\theta_{j+1}} K(x_i, x') \, dx'.$$
(B4)

The integrated kernel is no longer infinite and matrix inversion can be applied.

In Ref. [11], we compared this approach with two other techniques which also handle weakly singular equations successfully. A scheme introduced by Ullman [12] treats the equation as if the kernel were nonsingular, as in Eq. (2). However, the singular (diagonal) term is replaced by

$$\psi(x_i) \int_{z_i - w_i/2}^{z_i + w_i/2} K(x_i, x') \, dx', \tag{B5}$$

which is no longer infinite. Thus, the integral equation can be inverted.

The other successful approach considered in Ref. [11] was a well-known subtraction technique used by Schlitt [13] (referred to here as the Schlitt method) to solve the

weakly singular equation used as an example in Ref. [11]. In this approach, Eq. (B1) is written

$$\psi(z) = \psi_0(z) + \lambda \int_a^b K(z, z') [\psi(z') - \psi(z)] dz' + \lambda \psi(z) \int_a^b K(z, z') dz'.$$
 (B6)

Assuming  $\psi(z')$  has a Taylor series expansion around z' = z, the first integrand is no longer infinite, and so the first integral can be approximated by a quadrature sum. The second integral is evaluated analytically, the integrated kernel being finite for all z, since the singularity is weak.

I have investigated the possibility that these approaches might be applicable to equations with pole singularities. First, I attempted to solve an equation with a Cauchy singularity using the Cohen–Ickovic technique outlined in Eqs. (B3) and (B4). Applying this to the Omnes equation, I found very poor agreement with the analytic values. The results were incorrect by about 50% on the average, and by as much as 200% at some points. I found that the Ullman scheme, applied to the Omnes equation, yielded highly inaccurate results also, with the same errors obtained with the Cohen–Ickovic approach.

A simple investigation, approximating a known integral containing a pole

$$\int_{-1}^{1} \frac{y^{M}}{(x-y)_{P}} \, dy$$

by a Cohen-Ickovic or Ullman sum, indicates that the inaccuracies are due to the failure of both of these methods near the end points  $(\pm 1)$ .

The Schlitt method faired considerably better. This method yielded results which were in reasonable agreement with the analytic values. However, the results were not as accurate as the interpolative approach of this paper. To evaluate the derivative  $\partial \psi / \partial x$  arising from the diagonal term in the approximation of the first integral of Eq. (B6), I used the Legendre polynomial interpolation of Eq. (10). In Table V, a

TABLE V

Comparison of Solution of Omnes Equation Using Schlitt and Interpolative Methods with Analytic Form

Z	Interpolative method	Analytic values	% Difference	Schlitt method	% Difference
		20-Point q	uadrature		
1.003	0.4188	0.4188	0.00069	0.4258	1.67
2.166	0.1645	0.1645	0.0015	0.1608	2.25
4.089	0.1315	0.1315	0.0012	0.1276	2.96
7.884	0.1307	0.1307	0.00019	0.1272	2.66
22.788	0.1380	0.1380	0.00043	0.1355	1.79
291.061	0.1492	0.1492	0.0029	0.1490	0.16

comparison of these Schlitt results, the interpolative approach, and the analytic values is made. As can be seen, the interpolative method is preferable.

As a final note, I discuss the method of moments used by Osborn in Ref. [8] for equations with fixed poles. As with the approach of this paper, it is an interpolative scheme, which can be applied to equations with Cauchy singularities as well as those with fixed poles.

Briefly, the method involves writing the unknown function  $\psi(x)$  as

$$\psi(x) \simeq \sum_{i=1}^{N} C_i g_i(x). \tag{B7}$$

Inserting this back into the integral equation yields an integral of the form

$$\int_{a}^{b} \frac{U(x, y) g_{i}(y)}{(x - y - i\epsilon)} dy$$
(B8)

for a Cauchy pole, or

$$\int_{a}^{b} \frac{U(p^{2}, k^{2}) g_{i}(k^{2})}{(k^{2} - k_{0}^{2} - i\epsilon)} dk^{2}$$
(B9)

for a fixed pole. Such an integral is called the *i*th moment of the kernel.

There are a few drawbacks to this approach, however. Often the moments cannot be evaluated analytically (and thus take appreciable computer time for accurate numerical evaluation). If the unknown function  $\psi$  has rapid variations, or singularities, the function set  $\{g_i\}$  will only be able to reproduce such behavior if the functions have some relation to the original unknown function  $\psi(x)$ . For the Lippmann–Schwinger equation with the Yamaguchi potential, Osborn suggests that one use the solutions to the homogeneous equation for the functions  $g_i$ . The Yamaguchi potential is separable and thus the solutions to the homogeneous equation are easy to find. For moregeneral equations, finding the homogeneous solutions involves considerable calculation, if the solutions can be found at all. For these reasons, the method of moments may not be satisfactory.

### ACKNOWLEDGMENTS

I am grateful to Mr. Jeffery Schmidt for his contribution to the work on the Cohen-Ickovic and Ullman schemes applied to the equations of Section 2. Mr. Nicholas Copping was very helpful with some of the computer work involved, and I thank him for that. I also acknowledge useful discussions with Dr. David Gregorich. I am especially grateful to Professor D. W. Schlitt for offering his unsolicited help concerning Ref. [6]. I appreciated useful conversations with Professor R. Ginowski and Mr. W. Coughran of the Computer Sciences Department of Stanford University concerning the material in Appendix A. I also want to thank two unknown reviewers for this journal for helpful comments they made about an earlier version of this work. Finally, I wish to express my appreciation for support I received from Associated Western Universities, Inc. Part of this work was completed while I was visiting the Stanford Linear Accelerator Center, and I thank the people at that installation for their hospitality, particularly Dr. Y. S. Tsai.

### References

- K. ATKINSON, Numer. Math. 19 (1972), 248–259; K. ATKINSON, SIAM Num. Anal. 9 (1972), 284–299; J. A. DE SANTO AND O. SHISHA, J. Computational Physics 15 (1974), 286–292; D. B. HUNTER, Numer. Math. 19 (1972), 419–424.
- N. I. MUSKHELISHVILI, "Singular Integral Equations," Chap. 6, (Noordhoff-Groningen, Holland, 1946; F. TRICOMI, "Integral Equations," p. 194, Interscience, New York, 1957.
- S. KRENK, Quart. Appl. Math. 33 (1975), 225-232; F. ERGODAN AND G. D. GUPTA, Quart. Appl. Math. 30 (1972), 525-534; F. ERGODAN, SIAM J. Appl. Math. 17 (1969), 1041-1059.
- R. OMNES, Nuovo Cimento 8 (1958), 316–326. (I am indebted to Professor A. Pagnamenta for bringing this article to my attention.) See also I. J. R. AITCHISON AND P. R. GRAVES-MORRIS, Nucl. Phys. B14 (1969), 683–698.
- 5. G. F. CHEW AND F. E. LOW, Phys. Rev. 101 (1956), 1579-1587.
- 6. E. H. BAREISS AND C. P. NEUMANN, ANL Report 6988 (1965), p. 36, and references therein. (I want to thank Professor D. W. Schlitt for informing me of the existence of this report.)
- 7. S. CHANDRASEKHAR, "Radiative Transfer," Dover, New York, 1960.
- T. OSBORN, Nucl. Phys. A 211 (1973), 211–220, and private communication; F. J. YNDURAIN, The moment problem and applications in Padé Approximants, in "Proceedings of the University of Kent Summer School (P. R. Graves-Morris, Ed.), p. 45, Institute of Physics, London, 1972.
- 9. R. BLANKENBECLER, M. GOLDBERGER, N. KHURI, AND S. TREIMAN, Ann. Phys. (N.Y.) 10 (1960), 62–93.
- 10. W. COUGHRAN, (Computer Science Department, Stanford University), private communication.
- 11. H. COHEN AND J. ICKOVIC, J. Computational Physics 16 (1974), 371-382.
- 12. R. ULLMAN, J. Chem. Phys. 40 (1964), 2193-2201; R. ULLMAN AND N. ULLMAN, J. Mathematical Phys. 7 (1966), 1743-1748.
- 13. D. W. SCHLITT, J. Mathematical Phys. 9 (1968), 436–439; L. KANTOROVICH AND V. I. KRYLOV, "Approximate Methods of Higher Analysis," pp. 101–102, Interscience, New York, 1958.