

MOMENT METHODS FOR SOLVING SINGULAR INTEGRAL EQUATIONS
IN SCATTERING THEORY*

T. A. Osborn

Stanford Linear Accelerator Center
Stanford University, Stanford, California 94305

and

Department of Physics†
Brooklyn College of the City University of New York
Brooklyn, New York 11210

ABSTRACT

We study the use of moment methods for obtaining approximate numerical solutions to singular integral equations. With the techniques developed here we can obtain accurate solutions to these singular integral equations using matrices with dimensions smaller than 10×10 .

(Submitted for publication.)

*Work supported in part by the U. S. Atomic Energy Commission and the City University of New York Faculty Research Award Program.

†Permanent Address.

1. INTRODUCTION

It is our purpose here to develop a numerical method capable of solving singular multidimensional integral equations that arise in multichannel scattering theory. To this end we investigate the use of moment methods to obtain finite dimensional matrix representations of integral equations. We shall evaluate the utility of these moment methods by applying them to a simple model problem, namely the solution of the partial-wave one-dimensional Lippmann-Schwinger equation in momentum space. This choice of a model problem is motivated by the fact that the Lippmann-Schwinger equation shares some of the problems that occur in the solution of Faddeev's equations for the three-body problem. Specifically the integral equation is singular for positive energies and its domain of integration is infinite.

In our notation the Lippmann-Schwinger equation reads

$$t(p, p'; k^2 + i0) = v(p, p') - \frac{2}{\pi} \int_0^\infty \frac{v(p, p'') t(p'', p'; k^2 + i0)}{p''^2 - k^2 - i0} p''^2 dp'' \quad (1.1)$$

The potential in momentum space, after the partial wave reduction is $v(p, p')$, and $t(p, p'; k^2 + i0)$ is the t-matrix solution at an energy k^2 . The normalization here is such that the on-shell amplitude has the phase-shift representation given by,

$$t(k, k; k^2 + i0) = - \frac{e^{i\delta_\ell(k)}}{k} \sin \delta_\ell(k) \quad (1.2)$$

Let us now describe the general idea behind the moment method. These general aspects will be common to all of the various distinct formal realizations of the moment approach. In the following two sections we will develop two such distinct mathematical realizations. Consider an arbitrary one-dimension

integral equation

$$f(x) = g(x) + \int K(x, y) f(y) dy \quad (1.3)$$

with kernel $K(x, y)$, driving term $g(x)$ and solution $f(x)$. Let $\{h_i: i=1, N\}$ be a set of linearly independent functions such that there exists a linear combination of h_i which is a good approximation to f , that is

$$f(x) \approx \sum_{i=1}^N C_i g_i(x) \quad (1.4)$$

for some set of constants C_i . In the moment method one evaluates the moments

$$I_i(x) = \int K(x, y) g_i(y) dy \quad (1.5)$$

and from knowledge of these moments $I_i(x)$ one sets up a matrix equation to determine the expansion coefficients C_i . The resulting matrix will be N dimensional and the size of N needed for an accurate approximation to the exact f will be determined by the number of functions g_i necessary to reproduce the functional structure of f . One should contrast this with usual method of turning Eq. (1.3) into a matrix equation by using some quadrature rule to transform the integral into a finite sum, viz.

$$f(x_i) = g(x_i) + \sum_{j=1}^N K(x_i, x_j) f(x_j) \omega_j \quad i = 1, \dots, N. \quad (1.6)$$

where the ω_j are the weights and x_i are the abscissa of the quadrature rule. Here the size of the matrix, N , needed to obtain accurate solutions is controlled by the number of integration points, x_i , needed to do all the integrals

$$\int K(x, y) f(y) dy$$

accurately. In the moment method the problem of doing the integrals, which may be singular, is isolated from the problem of setting up a matrix equivalent

to the integral equation. It is for this reason that moment method is capable of much greater efficiency (smaller matrix size) and accuracy than a method based on Eq. (1.6).

2. AN EIGENFUNCTION EXPANSION

We shall now write down a moment method for Eq. (1.1) based on an eigenfunction choice for the expansion functions g_i . The eigenfunctions we choose are solutions of the operator equation

$$g_0(-\mu^2) v \phi_n = \lambda_n \phi_n \quad (2.1)$$

where $g_0(z) = (h_0 - z)^{-1}$ is the free Green's function for the free two-body Hamiltonian h_0 . Here the potential will be taken to be the square-well potential, which in momentum space has the form

$$v(p, p') = \frac{g a}{(2\pi)^2} \frac{1}{pp'} \left\{ j_0(a(p-p')) - j_0(a(p+p')) \right\} \quad (2.2)$$

The coupling constant g and the range a are defined by the coordinate space definition of the square-well potential, viz.

$$V(\vec{r}) = g \theta(a - |\vec{r}|) \quad (2.3)$$

These particular eigenfunctions were selected because they have a remarkably simple analytic form which is convenient for computation.

It is not difficult to solve Eq. (2.1) explicitly for the ϕ_n . In its integral form Eq. (2.1) reads

$$\int_0^\infty \frac{v(p, p')}{p'^2 + \mu^2} \phi_n(p') p'^2 dp' = \lambda_n \phi_n(p) \quad (2.4)$$

If we define a Hilbert space, \mathcal{H}_μ , with respect to the inner product

$$(f, f) = \int_0^\infty |f(p)|^2 \frac{p^2 dp}{p^2 + \mu^2} \quad (2.5)$$

then the kernel of Eq. (2.4) generates a bounded self-adjoint operator on \mathcal{H}_μ and the ϕ_n are the corresponding orthonormal eigenfunctions. By exploiting the analytic properties of the kernel of Eq. (2.4) one can find the eigenfunctions and eigenvalues in closed form. These turn out to be

$$\lambda_n = \frac{g}{2(p_n^2 + \mu^2)} \quad (2.6)$$

$$\phi_n(p) = \gamma_n \frac{\cos ap + \mu a j_0(ap)}{p^2 - p_n^2} \quad (2.7)$$

where the p_n is the n th zero of the numerator in (2.7) and the normalization constant γ_n is

$$\gamma_n = \frac{2p_n}{\sqrt{\pi} \left[a + \frac{\mu}{p_n^2 + \mu^2} \right]^{1/2}} \quad (2.8)$$

Now let us employ the basis $\{\phi_n\}$ to obtain finite matrix approximations for the integral equation (1.1). Since the ϕ_n are a orthonormal basis let us use them to expand the arbitrary potential v appearing in Eq. (1.1),

$$v(p, p') = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_{ij} \phi_i(p) \phi_j(p') \quad (2.9)$$

where a_{ij} are given by

$$a_{ij} = \int_0^\infty \int_0^\infty \frac{\phi_i(p) v(p, p') \phi_j(p')}{(p^2 + \mu^2)(p'^2 + \mu^2)} p^2 dp p'^2 dp' \quad (2.10)$$

We can obtain an approximate v by truncating the double sum in Eq. (2.9) at some finite number of terms N . Defining

$$v^N(p, p') = \sum_{\substack{i=1 \\ j=1}}^N a_{ij} \phi_i(p) \phi_j(p') , \quad (2.11)$$

then our approximation is,

$$v^N(p, p') \approx v(p, p') .$$

With the eigenfunction method we are setting forth here this will be the only approximation used.

The next step is to solve the integral Eq. (1.1) exactly with the potential v^N . We denote this solution by t^N . A well known alternate form for the t -matrix in (1.1) is the operator equation

$$t^N(z) = v^N - v^N g(z) v^N \quad (2.12)$$

where $g(z) = (h_0 + v^N - z)^{-1}$ is the exact Green's function for any complex energy z . From this form and Eq. (2.11) it follows that t^N must have the form

$$t^N(p, p'; z) = \sum_{\substack{i=1 \\ j=1}}^N b_{ij}(z) \phi_i(p) \phi_j(p') \quad (2.13)$$

The problem now is reduced to finding the coefficients $b_{ij}(z)$. Substituting representations (2.13) and (2.11) into Eq. (1.1) gives

$$b_{ij}(z) = a_{ij} - \sum_{\ell=1}^N c_{i\ell}(z) b_{\ell j}(z) \quad (2.14)$$

where $c_{ij}(z)$ is given by

$$c_{ij}(z) = \sum_{\ell=1}^N a_{i\ell} \mathcal{G}_{\ell j}(z) \quad (2.15)$$

and

$$\mathcal{I}_{lj}(z) = \frac{2}{\pi} \int_0^\infty \frac{\phi_l(p) \phi_j(p) p^2 dp}{p^2 - z} \quad (2.16)$$

For the eigenfunctions considered here one can exploit the fact that they are entire functions in p to use the residue method to evaluate (2.16). For $z = k^2 + i0$ one obtains for the moments \mathcal{I}_{nm} ,

$$\begin{aligned} \mathcal{I}_{nm}(k^2 + i0) &= \frac{\gamma_n \gamma_m}{(k^2 - p_n^2)(k^2 - p_m^2)} \left\{ \frac{\pi i}{2} e^{iak} (k - i\mu) [\cos ak + (\mu/k) \sin ak] \right\} \\ &+ \frac{\delta_{nm} \gamma_n \gamma_m}{(p_n^2 - k^2)} \frac{\pi}{4} \left[a + \frac{\mu + a\mu^2}{p_n^2} \right]. \end{aligned} \quad (2.17)$$

Our description of this method will be complete once we have obtained the expansion coefficients a_{ij} . We could use the definition Eq. (2.10) but this is tedious. A more convenient approach is to take advantage of the fact that the ϕ_n have identical zeroes with exception at $p = p_n$. So if we set $p = p_n$ and $p' = p_m$ in (2.9) then

$$v(p_n, p_m) = \sum_{\substack{i=1 \\ j=1}}^{\infty} a_{ij} \phi_i(p_n) \phi_j(p_m) \quad (2.18)$$

all the terms in this sum vanish except when $i=n$ and $j=m$, so we have

$$a_{ij} = \frac{v(p_i, p_j)}{\phi_i(p_i) \phi_j(p_j)} \quad (2.19)$$

Thus, for an arbitrary potential, we have a general scheme for calculating the matrices appearing in (2.14). All the moments \mathcal{I}_{nm} are given in a closed analytic form which is independent of the structure of the potential v . All the singular aspects of the original Lippmann-Schwinger Eq. (1.1) have been

absorbed in the calculation of the moments $\mathcal{I}_{nm}(k^2+i0)$. A further advantage, characteristic of the moment approach, is that the approximate solution is given in the analytic form, (2.13).

We have tested the convergence properties of this method by using this scheme to obtain the solution for the scattering problem where v is the Yamaguchi potential,

$$v(p, p') = \frac{\lambda}{(p^2 + \beta^2)(p'^2 + \beta^2)} \quad (2.20)$$

We have chosen λ and β to be such that this potential reproduces the N-P triplet boundstate energy and scattering length. The constants are $\beta = 1.444$ and $\lambda = -8.110$. The Yamaguchi potential scattering problem is a convenient test problem since Eq. (1.1) has a closed form solution given by

$$t(p, p'; k^2+i0) = \frac{\lambda}{(p^2 + \beta^2)(p'^2 + \beta^2) \left\{ 1 + \frac{\lambda}{2\beta(\beta - i\sqrt{k^2})^2} \right\}} \quad (2.21)$$

As expected we find that the approximate solutions of Eq. (1.1) given by Eq. (2.14) are completely insensitive to the scattering cut — i. e., solutions for positive energies are as accurate as solutions for negative energy.

We summarize the convergence properties of this method in the following table. We have examined the solutions $t^N(p, k; k^2+i0)$ at the points $p = p_n$ — the zeroes of our eigenfunctions. The percentage error between $t^N(p, k; k^2+i0)$ and the exact solution $t(p, k; k^2+i0)$ for the points $p = p_n$ turns out to be independent of n . Thus, it is instructive to plot this common percentage error against the

dimensionality, N , of the method. For $k=0.1$ we obtain the following results

Table 1

N	<u>percent error</u>
5	11.2
10	3.2
15	0.83
20	0.44
25	0.19
30	0.14
40	0.061

Our eigenfunctions ϕ_n have two free parameters — μ and a . We choose these so that v^N will approximate v accurately for small N . In the example above, $\mu=0.0535$ and $a=7.22$.

The results obtained here show that this method can give reliable solutions to the one-dimension Lippmann-Schwinger Eq. (1.1). However the number of points, 15 or greater, needed for an accurate solution suggested that this version of the moment method would not be able to cope with two-dimensional integral equations. One can not easily handle matrices of greater dimension than 100×100 on most computers. This implies that we need a solution method that utilizes 10 or fewer points for each dimension. A second drawback indicated by these results is that the rate of convergence as N increases is rather slow.

The underlying reason for these results is that all of the eigenfunctions, ϕ_n , are oscillatory. In order for a sum of them to reproduce a smooth function, like Eq. (2.20), one must sum many terms. If one specializes to the case where v is the same square-well potential as used to obtain the ϕ_n , then this

method becomes the unitary pole expansion¹ approach. A further useful observation is that since one has solved the Lippmann-Schwinger equation exactly with the potential v^N it follows that the result, t^N , is exactly unitary.

3. THE INDEPENDENT FUNCTION APPROACH

The slow convergence of our eigenfunction approach was due to the fact that the basis eigenfunctions do not have a functional behavior similar to the solution of the integral equation. We shall amend this difficulty by deliberately constructing a basis set that mimics the solution for typical potential problems. The method we now present is an adaptation of the one used by Kim² on the bound-state three-body problem. Let us select the functions g_i , in Eq. (1.4), to be

$$g_i(p) = \frac{1}{p^2 + \beta^2} \left(\frac{p^2}{p^2 + \beta^2} \right)^{i-1} \quad i=1, \dots, N \quad (3.1)$$

These functions all fall off asymptotically like $1/p^2$ and a linear combination of these g_i can reproduce the structural detail of the solution for small p . In the Lippmann-Schwinger equations we deal with, it can be proved³ that they are only functions of p^2 and not p .

Given the functions g_i we could construct a sequence of orthonormal functions and proceed as in Section 2. However it is somewhat simpler to work directly in terms of the g_i in order to obtain a finite matrix equation. Here our principal approximation is to assume that the solution can be written as a finite linear sum of the $g_i(p)$, viz.

$$t^N(p, p'; k^2 + i0) = \sum_{i=1}^N C_i(p', k^2 + i0) g_i(p) \quad (3.2)$$

Now we substitute this form in (1.1) and solve for t^N . We proceed by developing a quadrature rule for the integral in (1.1) that has no error when t^N has the

form given in (3.2). This quadrature rule is defined relative to a set of integration points $\{p_i; i=1, N\}$. The construction of this quadrature rule is determined by calculating the moments,

$$\frac{2}{\pi} \int_0^{\infty} \frac{v(p_i, p) g_j(p) p^2 dp}{p^2 - k^2 - i0} = I_j(p_i, k^2 + i0) \quad , \quad (3.3)$$

and requiring that the associated weights give an exact result for any function of the form (3.2). That is

$$I_j(p_i, k^2 + i0) = \sum_{\ell=1}^N W_{i\ell}(k^2 + i0) f_j(p_\ell) \quad (3.4)$$

For fixed i this is a linear system for the N -dimensional vector $W_{i\ell}$.

The real and imaginary parts of $(p^2 - k^2 - i0)^{-1}$ behave quite differently so we shall treat each part individually. The imaginary part of $(p^2 - k^2 - i0)^{-1}$ becomes proportional to a delta function for positive k^2 . For this reason we let require one of the quadrature points in $\{p_i; i=1, N\}$, say p_N , to be equal to k . We now use the delta function property to determine the weights $\text{Im } W_{i\ell}(k^2 + i0)$. We obtain

$$\text{Im } W_{i\ell}(k^2 + i0) = \delta_{\ell N} v(p_i, k) \quad (3.5)$$

Now let us examine the real part of $(p^2 - k^2 - i0)^{-1}$ in the moment Eq. (3.3).

First let us simplify the problem by the following definitions. Let

$$\tilde{W}_{i\ell}(k^2 + i0) = \frac{W_{i\ell}(k^2 + i0)}{p_\ell^2 + \beta^2} \quad , \quad (3.6)$$

and

$$\chi_\ell = \frac{p_\ell^2}{p_\ell^2 + \beta^2} \quad , \quad \ell=1, \dots, N \quad . \quad (3.7)$$

With this notation Eq. (3.4) now has the structure

$$\begin{pmatrix} \text{Re } I_1 \\ \text{Re } I_2 \\ \text{Re } I_3 \\ \vdots \\ \text{Re } I_N \end{pmatrix} = \begin{pmatrix} 1 & 1 & \dots & 1 \\ \chi_1 & \chi_2 & \dots & \chi_N \\ \chi_1^2 & \chi_2^2 & \dots & \chi_N^2 \\ \vdots & \vdots & \vdots & \vdots \\ \chi_1^{N-1} & \chi_2^{N-1} & \dots & \chi_N^{N-1} \end{pmatrix} \begin{pmatrix} \text{Re } \tilde{W}_{i1} \\ \text{Re } \tilde{W}_{i2} \\ \text{Re } \tilde{W}_{i3} \\ \vdots \\ \text{Re } \tilde{W}_{iN} \end{pmatrix} \quad (3.8)$$

The matrix, in this linear system is the Vandermonde matrix. This is known to be ill-conditioned, but by using the special algorithms developed by Björck and Pereyra⁴ one may reliably solve Eq. (3.8) for the $\text{Re } \tilde{W}$'s and so obtain $\text{Re } W$ via (3.6).

Thus in this version of the moment technique the integral term in Eq. (1.1) becomes

$$\frac{2}{\pi} \int_0^\infty \frac{v(p_i, p) t^N(p, p'; k^2 + i0) p^2 dp}{p^2 - k^2 - i0} = \sum_{\ell=1}^N W_{i\ell}(k^2 + i0) t^N(p_\ell, p'; k^2 + i0) \quad (3.9)$$

The related matrix equation for the vector $t^N(p_\ell, p'; k^2 + i0)$ is

$$\sum_{\ell=1}^N \left\{ \delta_{i\ell} + W_{i\ell}(k^2 + i0) \right\} t^N(p_\ell, p'; k^2 + i0) = v(p_i, p') \quad (3.10)$$

Given the solution $t^N(p_\ell, p'; k^2 + i0)$ one may obtain the expansion constants, $C_i(p'; k^2 + i0)$, by inverting (3.2). This inversion will involve the transposed Vandermonde problem. Once the C_i are known then one has an analytic representation of the approximate solution.

Now that we have completed the formal description of this method, let us summarize our numerical experience with this approach. For this method

there is no point in choosing the Yamaguchi potential as a test problem. For a Yamaguchi potential the approximation (3.2) is exact with $N=1$, and our method provides an exact solution. Thus this choice does not test the validity or convergence of the expansion (3.2). The potential we have selected to test this method is the Yukawa potential

$$v(p, p') = \frac{\lambda}{2pp'} Q_0 \left(\frac{\mu^2 + p^2 + p'^2}{2pp'} \right) . \quad (3.11)$$

Here Q is the Legendre function of the second kind. The value of the parameters are taken to be

$$\begin{aligned} \mu &= 0.633 F^{-1} \\ \lambda &= -1.58 \end{aligned} \quad (3.12)$$

These values reproduce the N-P triplet scattering length and binding energy. We shall relate the accuracy of our method by calculating the half-off-shell extension function defined by

$$f(p; k) = \frac{t(p, k; k)}{t(k, k; k)} . \quad (3.13)$$

This is convenient since f is known⁵ to be a real function and depends only on one variable p . We do not have an exact solution for this problem so we have calculated f independently by using the nonsingular Kowalski-Noyes integral equation⁶ for f with a high order (32 point) Gaussian method. However, the errors are so small in the independent function method when one contrasts with the f from the Kowalski-Noyes approach, frequently most of the difference is due to error in the Kowalski-Noyes solution. It thus seems more reasonable to take a high order (here $N=13$) solution of Eq. (3.10) as representing a reference solution which is near to exact.

In the following table, we list the differences between the solutions of Eq. (3.10) with $k=0.1$ for various N and our reference solution. Our notation is defined

Table 2

p	Reference Solution	Δ_5	Δ_7
0.0	1.001620	-0.000109	+0.000011
1.0	0.672624	+0.007127	+0.000755
2.0	0.321474	+0.001283	+0.000078
3.0	0.173898	+0.000014	+0.000089
4.0	0.106189	-0.000020	-0.000006
5.0	0.070838	+0.000033	-0.000021

by

$$\Delta_N(p) = f_{\text{reference}}(p) - f_N(p) \quad (3.14)$$

where $f_N(p)$ is the f function determined from Eq. (3.2) after the expansion coefficients C_i are obtained from solution, t^N of (3.10). The content of Table 2 may be roughly summarized by noting that for $N=5$ the maximum error is about 1%; for $N=7$ the maximum error reduces to 0.1%. These results demonstrate that the moment method can provide the solution of singular integral equations with fewer than 10 points and is rapidly convergent as the number of points (or terms in (3.2)) is increased.

We conclude that the moment method used here leads to remarkably accurate results for one-dimension singular integral equations with matrix sizes smaller than 10×10 . This method seems to be powerful enough to solve the two-dimensional integral equations occurring in multichannel scattering theory.

ACKNOWLEDGEMENT

The author would like to thank D. Brayshaw for suggesting the use of the eigenfunctions, ϕ_n , employed in the method described in Section 2.

REFERENCES

1. E. Harms, Phys. Rev. C1, 1667 (1970).
2. Y. E. Kim, J. Math. Phys. 10, 1491 (1969).
3. D. D. Brayshaw, Phys. Rev. 167, 1505 (1967).
4. A. Björck and V. Pereyra, Math. Comp. 24, 893 (1970).
G. Galimberti and V. Pereyra, Math. Comp. 24, 357 (1970).
5. T. A. Osborn, Nucl. Phys. A138, 305 (1969).
6. K. L. Kowalski, Phys. Rev. Letters 15, 798 (1965).
H. P. Noyes, Phys. Rev. Letters 15, 538 (1965).