Solution of Integral Equations by a Chebyshev Expansion

Method.

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A new spectral type method for solving the one dimensional quantum-mechanical Lippmann-Schwinger integral equation in configuration space is described. The radial interval is divided into partitions, not necessarily of equal length. Two independent local solutions of the integral equation are obtained in each interval via Clenshaw-Curtis quadrature in terms of Chebyshev Polynomials. The local solutions are then combined into a global solution by solving a matrix equation for the coefficients. This matrix is sparse and the equation is easily soluble. The method shows excellent numerical stability, as is demonstrated by several numerical examples.

I. INTRODUCTION.

In conjunction with Professor I. Koltracht and several students in the Mathematics Department of the University of Connecticut, we are in the process of developing a method for solving the one-dimensional Lippmann-Schwinger integral equations in configuration space, associated with the corresponding Schrödinger equation. At a later stage we hope to generalize the method to other types of integral equations, and attempt to increase the dimension of the number of variables. Our method is excellently suited for cases where either the potential has a long range with many oscillations occurring in the wave function, or for large systems of coupled equations in which some of the channel energies are positive and others negative. In both situations the conventional finite difference methods (Numerov, for example) experience difficulties because of the larger accumulation of roundoff errors, and because of linear independence problems in implementing the asymptotic boundary condi-
tions in the coupled channel case. A good physical application of our method is very likely the process of photoassociation in the collision of cold atoms, because of the very long range of the interaction between the atoms, and also because of the many excited configurations which participate and which lead to many coupled channels. Photoassociation is a relatively new field of study. It was recently reviewed by Julienne [2], and is observed experimentally at various laboratories, including the University of Connecticut [3]. The calculation of three-body reactions in coordinate space might furnish another example because of the large distances involved, especially if we are able to generalize our method to two dimensions, but this conjecture has not yet been examined.

The Chebyshev expansion method is "spectral", i.e., the accuracy increases faster than any inverse power of the number of mesh points employed. Our method is based on that of Greengard and Rokhlin [4], but differs [1] from it substantially in the manner in which the local solutions in each partition are combined into the global solution. We prefer to use Chebyshev polynomials for the expansion basis in each partition because these functions have excellent integral properties [5], and the node points can be obtained in terms of simple algebraic cosine expressions, rather than in terms of non-analytic expressions required for the zeros of Legendre Polynomials, for example.

II. THE ALGORITHM.

For the one-channel case our integral equation method (IEM) is as follows. The Schrödinger equation for the partial wave function $\psi(R)$

$$\left(-\frac{d^2}{R^2} + V_L(R) - k^2\right)\psi(R) = 0 \quad (1)$$

is first transformed into an equivalent integral equation

$$\psi(R) = F(R) + \int_0^T G_0(R, R')V_L(R')\psi(R') dR'. \quad (2)$$

In configuration space the Green’s function $G_0$ is semi-separable, i.e., it is given by the product of two independent solutions $F_0$ and $G_0$ of the Schrödinger equation, i.e., $G_0(R, R') \propto$
\( F_0(R_<) \times G_0(R_<) \). Here \( R_< \) (\( R_> \)) is the smaller (larger) of \( R \) and \( R' \), \( F_0 = \sin(kr) \), \( G_0 = \cos(kr) \), and \( F(R) \) is the driving function which is equal to \( F_0 \) in the uncoupled case, and the upper limit in the integral is \( T = R_{Max} \). Physicists would be tempted to use instead of \( F_0 \) and \( G_0 \) the \( L \)-dependent Riccati-Bessel functions \( F_L \) and \( G_L \), but because the spectral expansion technique is very robust, it allows us to place the \( L(L + 1)/R^2 \) term into the potential \( V_L \)

\[
V_L(R) = L(L + 1)/R^2 + V(R), \tag{3}
\]

without loss of accuracy [1].

We avoid the occurrence of large non-sparse matrices by: a) Dividing the integration interval \([0, R_{Max}]\) into \( m \) partitions \([0, b_1], [b_1, b_2], \ldots [b_{m-1}, R_{Max}]\). The size of each partition can be arbitrary, but two or three partitions per local wave number is optimum. b) Solving the integral equation separately in each partition \( i \) for two functions \( Y \) and \( Z \)

\[
Y_i - \int_{b_{i-1}}^{b_i} G_0(R, R')V_L(R')Y_i(R')dR' = F(R), \quad b_{i-1} \leq R \leq b_i \tag{4}
\]

\[
Z_i - \int_{b_{i-1}}^{b_i} G_0(R, R')V_L(R')Z_i(R')dR' = G(R), \quad b_{i-1} \leq R \leq b_i. \tag{5}
\]

The method of solution for this step leads to small non-sparse matrices. It consists in expanding the unknown solutions into Chebyshev polynomials and making use of their convenient properties [4-6]. c) ”Stitching” together the separate solutions into the global one by means of the expressions, valid in each partition

\[
\psi(R) = A_iY_i(R) + B_iZ_i(R), \quad b_{i-1} \leq R \leq b_i. \tag{6}
\]

This ”stitching” procedure leads to a large but sparse matrix. It produces a seamless smooth continuation of the function \( \psi \) from one partition into the next, and is a consequence of the semi-separability of \( G \). As a consequence of this property the coefficients \( A \) and \( B \) obey [1] the matrix equation
where the $\alpha_j$ and $u$ are two-rowed columns

$$\alpha_j = \begin{pmatrix} A_j \\ B_j \end{pmatrix} ; \quad u = \begin{pmatrix} 1 \\ 0 \end{pmatrix} ; \quad 0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (8)$$

For the one-channel case the $M_{i,j}$ are $2 \times 2$ matrices whose elements are formed out of overlap integrals between combinations of the functions $Y, Z$, the potential $V$ and the functions $F$ and $G$. We call the matrix formed out of the blocks of the $M_{i,j}$s the "Big Matrix". It is sparse, and of dimension $2m \times 2m$, where $m$ is the number of partitions, while the matrices required to solve the equations for the $Y$ and $Z$ in each partition are of the dimension $n \times n$, where $n$ is the number of Chebyshev points in each partition. Following standard practice, that number is chosen to have the value $n = 16$. The end result of the whole calculation is the set of coefficients of the Chebyshev polynomials for the functions $Y$ and $Z$ in each partition, as well as the coefficients $A$ and $B$ for each partition. The calculations in one partition of the $Y, Z$, and the overlap integrals required for the construction of the $M_{i,j}$ can be performed independently of each other. Hence this part of the calculation can be carried out in a parallel computer architecture. Because of the simple structure of the "Big Matrix", the solution of Eq. (7) can be performed by simple pivoting, and does not require special big matrix techniques. The values of $\psi$ and its derivative $d\psi/dR$ can be obtained at any arbitrary point from the solution given by Eq. (6), because the values and the derivatives of Chebyshev functions are known analytically. At the end point $R_{Max} = T$ the expression for $d\psi/dR$ is especially simple.

When the Schrödinger Eq. is augmented to a system of coupled equations with $N$
channels, then each $F_0$ and the corresponding $Y$ is augmented into $N$ column vectors of length $N$, and similarly for the $G'$s and $Z'$s. The size of the block matrices $M_{ij}$ increases correspondingly to the dimension $2N \times 2N$, but the sparse structure of the "Big Matrix" remains the same. For the channels which are closed, the functions $F_0$ and $G_0$ are replaced by $\sinh(\kappa R)$ and $\exp(-\kappa R)$, respectively, where $\kappa$ is the imaginary part of the asymptotic wave number in the closed channel. Numerical experiments [7] for $L = 0$ show that the stability and high precision of the results is maintained in this case also, provided that a scaling procedure is introduced which reduces the numerical disparity between the two exponentials $\exp(\pm \kappa R)$ for large values of $\kappa R$. If in the positive energy channels the angular momentum $L \neq 0$, it is still advantageous to use for the channel Green functions the undistorted $G_0$ ones, even though one now has to solve the coupled integral equations as many times as there are open channels, each time with a different driving function $F$. The big matrix $M$ is the same in each case, the only change is in the vector $u$ on the right hand side of Eq. (7), and one can show [7] that the corresponding solutions are linearly independent asymptotically. In the next section several examples illustrate the numerical properties of our method.

III. ACCUMULATION OF RONDOFF ERRORS.

This property is demonstrated by a numerical example for an uncoupled channel case with $L \neq 0$, but in which the only potential present is $L(L+1)/R^2$. In this case the solution is a Riccati-Bessel function $F_L(R) = kRj_L(kR)$. The numerical solution $\psi$ of Eq. (2) is proportional to $F_L$, and the constant of proportionality is obtained from the Wronskian of $\psi$ with $G_L$ at $R = R_{Max}$. The calculations are done in double precision on a IBM 3090 Mainframe machine. The functions $G_L$ and $F_L$ at $R_{Max}$ are obtained from the International Mathematical Scientific Library (IMSL). The error in the numerical solution $\psi$ is obtained by comparing it with the IMSL values of $F_L$ at many points in the interval $[0, R_{Max}]$, and the maximum of the absolute values of all these differences is denoted as "Error". This error is plotted in Fig. 1 as a function of $N$, the total number of integration points in
[0, R_{Max}]. For the IEM that number is equal to 16 times the number of partitions m, while for the Numerov method it is R_{Max} divided by the uniform mesh size. In this example with \( k = 1 \text{fm}^{-1}, R_{Max} = 50 \text{fm} \) and \( L = 6 \), one sees that the error rapidly drops as a function of N, and reaches a minimum (equal to machine accuracy in this case) at the point where the roundoff error overtakes the truncation error. Beyond that minimum the rise is a measure of the rapidity of accumulation of roundoff error. One sees from the figure that the Numerov error decreases much more slowly with N, and the accumulation of round-off error increases much faster. This is the reason why the best accuracy for the Numerov method is much worse. A variable step size improved Numerov method due to Raptis and Cash accumulates roundoff error more slowly than the Numerov method, but still does not reach the quality of the IEM.

A more taxing example with \( L = 8, k = 40 \text{fm}^{-1} \) and \( R_{Max} = 50 \) (not illustrated here) shows a similarly slow accumulation of the roundoff error for the IEM. In this case there are 580 nodes in the wave function, and the smallest error is one order of magnitude larger than machine accuracy \([1]\). The corresponding value of N is 12800, which corresponds to 800 partitions in the \([0, R_{Max}]\) interval, or 20 Chebyshev points per half wavelength. The corresponding number for best accuracy (\(~ 10^{-8}\)) of the Numerov method is 640 points per half wavelength, larger by a factor of 30. There results are summarized in the Table below.

### Maximum Accuracy of the Riccati-Bessel Function.

| \( k(\text{fm}^{-1}) \) | \( \lambda(\text{fm}) \) | \( 0 < R < 50 \) | IEM | Numerov |
|----------------|----------------|----------------|-----|---------|
| 1              | 6.3            | 8              | 50  | 1260    |
| 40             | 0.16           | 310            | 40  | 1280    |

**IV. IMPLEMENTATION OF BOUNDARY CONDITIONS.**

For the case of one channel the asymptotic boundary conditions \( \psi(R) \approx F_{L}(R) + \omega G_{L}(R) \) are easily obtained in both the IEM and the finite difference methods (FDM), by simple
normalization at the end point. However if there are two or more coupled channels, then
the various supposedly independent wave functions obtained in the FDM by starting the
solutions near the origin independently, can lose a large part of their independence near
the matching point, and the process of obtaining the appropriate linear combination which
satisfies the desired boundary condition loses accuracy. This is not the case for the IEM,
as will now be demonstrated for the case \( L = 0 \).

In this example we have two channels, both with the same positive energy
\( E = k^2 fm^{-2} \), and all potentials (coupling as well as diagonal) are of exponential form
\( V_0 \exp(-r/a) \), with the same decay parameter \( a \) and the same magnitude of the strength \( V_0 \).
For the single channel \( L = 0 \) case there exists an analytic solution given in terms of Bessel
functions \( J_\nu(y) \) of imaginary index \( \nu = \pm 2iak \), and argument \( y = 2a\sqrt{-V_0} \exp(-r/2a) \),
which can be generalized to the coupled channel case when the energies in all the channels
are equal. In our example \( |V_0| = 5/\sqrt{2} fm^{-2} \) and \( a = 4 fm \). Channel 1 is the incident
channel, with \( V_0 > 0 \), and \( \psi_1(R) \approx F_0(R) + w_1G_0(R) \), while in channel 2 \( V_0 < 0 \) and
\( \psi_2(R) \approx w_2G_0(R) \). The value of \( R_{Max} \) is 180 \( fm \) and 140 \( fm \), respectively, in the IEM and
Numerov calculations, again carried out in double precision on the IBM mainframe. For
each value of the wave number \( k \) the number of points in each method of calculation is
varied until the combined error in \( w_1 \) and \( w_2 \) is a minimum, and this minimum error is
displayed on the vertical axis in Fig. 2. The reason why the Numerov error (open circles)
increases as \( k \) decreases is because of the lack of independence of the two solutions. This is
shown either by an analytical argument, valid in this exponential case, or can seen from
the fact that the Numerov error for \( w \) in the uncoupled channels is much less dependent on
\( k \). The latter is shown by the lines with squares or triangles, labeled ”Attr.” and ”Rep.”,
respectively. The error in the IEM is even more independent on \( k \), and is also much smaller
since the boundary conditions are automatically built into the Green’s functions.

The case with the same exponential potentials in which however the energy in the second
channel is negative has also been examined. Since an analytical solution does not exist in
this case, the accuracy of the solution has to be inferred from the stability of the values of
$w_1$ and $w_2$. For the IEM the values of both $w_1$ and $w_2$ are stable to 13 sign figures, while for the Numerov method the value of $w_2$ is correct to less than 4 significant figures for $kR_{Max} > 25$, while $w_1$ is correct to about 7.

V. SUMMARY AND CONCLUSIONS.

We have demonstrated a method for solving the Lippmann-Schwinger integral equation in configuration space which is linear in the number of the integration points, and which is numerically very stable. The stability of the IEM method is due to two factors: 1. The solution of integral equations lead to a smaller accumulation of roundoff errors than the finite difference methods of solving a differential equation, and 2), The IEM is a spectral method, which has an inherently higher accuracy than finite difference methods.

Furthermore the IEM is easy to implement: a) The boundary conditions on the channel wave functions are automatically incorporated through the Green’s functions; b) The size of each partition $b_{i-1} - b_i$ can be assigned independently of the sizes of the other partitions; c) The overlap integrals required for the construction of matrix elements can be obtained with the Gauss-Legendre quadrature because the functions in the integrand, being given in terms of Chebyshev expansions, can be calculated easily for any given sets of points, no interpolation being required. The Curtis-Clenshaw (C-C) quadrature \[\text{[5]}\] is also a good option (see Table 2 in Ref. \[1\]) because the wave functions and potentials are already known at the appropriate Chebyshev points, and certainly exceeds the efficiency of equidistant point methods.

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**B. Figures**

Fig. 1 Accumulation of roundoff errors for a Riccati-Bessel function, as a function of the number of integration steps N.

Fig. 2. Accuracy of the R-matrix elements for two channels
coupled by exponential potentials, as a function of the wave number.