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Iterative Inverse Scattering Method Employing Gram–Schmidt Orthogonalization

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An inverse scattering method is tested which appears to work very well. It is an iterative procedure based on the distorted wave Born approximation. The resulting Fredholm equation of the first kind is solved by a projection method that requires the construction of an orthonormal set of basis functions from the set of kernel functions. This can be done by the spectral expansion method which entails matrix diagonalization or by Gram–Schmidt orthogonalization. The method is tested on a simple one-dimensional optical wave inverse scattering problem. Both orthonormalization methods lead to a rapidly convergent and stable iteration. The spectral expansion method gives somewhat better results, but the Gram–Schmidt orthogonalization method, which is the novel aspect of our approach, is much less time-consuming. We show how the projection method can be generalized to the case of acoustic wave scattering where the target must be characterized by more than a single independent function of position.

I. INTRODUCTION

In the direct scattering problem one seeks to calculate the scattering amplitude from a knowledge of the incident wave field and the properties of the scatterer. In the inverse scattering problem one seeks to determine the properties of the scatterer from a knowledge of the incident wave field and the scattering amplitude. The inverse problem is difficult because the relationship between the scattering amplitude and the scattering potential is nonlinear.

A solution to this problem for spherically symmetric potentials is provided by the Gel'fand–Levitan equation [1] and the analogous Regge–Newton equation [2, 3]. This approach requires knowledge of the scattering amplitude at all energies. An alternative approach is to linearize the relationship to be solved by introducing an estimate of the desired scattering potential and assuming that the difference between the potential and the estimate is small. The solution of the linearized relationship is then regarded as an improved estimate and the process is repeated. Iteration continues until the result for the scattering potential stabilizes.

For each iteration one must solve the direct scattering problem for the estimated scattering potential to provide input for the linearized relationship between the scattering amplitude and the scattering potential. This linearized relationship

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generally takes the form of a Fredholm equation of the first kind. Such an equation is regarded as ill-posed because ordinary methods of numerical solution tend to be unstable. Thus special methods of numerical solution are required.

As examples of recent iterative inverse scattering calculations we cite the work of A. G. Tijhuis [4], A. A. Ioannides and R. S. Mackintosh [5], and R. P. Hatcher and Y. M. Chen [6]. In the first two of these articles the ill-posed equation is solved by the method of linear least-squares inversion, also known as the selection method [7]. An alternative method used by Tijhuis is a smoothing procedure applied to the result of each iteration. Hatcher and Chen, on the other hand, use Tikhonov regularization [7] to solve their ill-posed equation. A survey of methods for dealing with the Fredholm equation of the first kind can be found in the paper of M. Z. Nashed [8].

Our purpose is to present a method for dealing with the inverse scattering problem which we believe to be new and which appears to be very practical. The method is simple in concept and appears to strike at the root of the problem. Our numerical tests show it to be effective and economical. The method consists in using the distorted wave Born approximation (DWBA) to linearize the relationship between the scattering amplitude and the scattering potential. The result is a Fredholm equation of the first kind for the scattering potential. This equation is solved by finding the linear combinations of the set of kernel functions that form an orthogonal set. This can be done by diagonalizing the overlap matrix (spectral expansion method) or by Gram–Schmidt orthogonalization. The ill-posedness of the Fredholm equation is overcome by weeding out the kernel functions which are not linearly independent of the set of retained functions.

The use of the spectral expansion method for the inverse problem is not new; see Ref. [9] and the papers cited therein. However, the use of Gram–Schmidt orthogonalization in this context does appear to be new, and it results in an algorithm which is much less time-consuming.

Our method for numerical solution of the Fredholm equation of the first kind is described in Section II. A simple one-dimensional optical wave inverse scattering problem is formulated in Section III. In Section III we also present the results of test calculations on that problem. Finally, in Section IV we show how our method can be generalized to deal with a more complicated class of inverse scattering problems where the integral equation has two unknown functions. This type of problem occurs in acoustic wave scattering and in electromagnetic wave scattering by magnetic or conducting targets. It also occurs in nuclear scattering where the scattering potential might have independent real and imaginary parts or independent central and spin-orbit parts.

II. Numerical Solution of the Fredholm Equation of the First Kind

The Fredholm equation of the first kind is encountered in many applications. In particular, many analyses of the inverse wave-scattering problem result in such an

integral equation. In any attempt at numerical solution this integral equation must be subjected to a discretization process that transforms it into a set of inhomogeneous linear algebraic equations. The process of improving the numerical accuracy increases the size of this set of simultaneous algebraic equations. The Fredholm equation of the first kind is regarded as ill-posed because this process of refining the discretization procedure often results in the determinant of the system becoming very small or even vanishing. There is nothing that insures the linear independence of the algebraic equations produced by the discretization process.

Let the integral equation be written in the form

$$b(\omega) = \int dx\, K(\omega, x)\, \phi(x). \tag{1}$$

The problem is to determine ϕ from a knowledge of the driving term b and the kernel K. In the inverse scattering problem we will be presented with a set of values $b_n \equiv b(\omega_n)$ $(n = 1, 2, \ldots, N)$ that is the result of a set of measurements. The kernel functions $K_n(x) \equiv K(\omega_n, x)$ express the dynamics of the scattering process by mapping the scattering potential ϕ onto the set of scattering amplitudes b_n. Our task is to determine ϕ from the finite set of equations

$$b_n = \int dx\, K_n(x)\, \phi(x), \qquad n = 1, 2, \ldots, N. \tag{2}$$

Such a finite set of equations can only determine some approximation to ϕ, and even that approximate solution will not be unique.

To discretize the equations we assume that $\phi(x)$ can be represented by the sum of N linearly independent functions:

$$\phi(x) = \sum_{n=1}^{N} f_n \chi_n(x). \tag{3}$$

Then Eq. (2) becomes

$$b_n = \sum_{m=1}^{N} K_{nm} f_m, \qquad n = 1, 2, \ldots, N \tag{4a}$$

$$K_{nm} = \int dx\, K(\omega_n, x)\, \chi_m(x). \tag{4b}$$

The solution to our problem then consists in inverting the matrix K. However, as N increases we often find that the determinant of K tends to become small, causing the inversion of K to become numerically unstable. It may also happen that the matrix K becomes increasingly ill-conditioned with increasing N.

One method for dealing with the ill-posed equation is called the selection method by Tikhonov and Arsenin [7]. In the selection method we replace N (=the number of equations) in Eqs. (2) and (4a) by $M > N$ (=the number of independent

functions χ_n) so that we have more equations than unknown coefficients f_m. Thus Eq. (42) is replaced by

$$b_n = \sum_{m=1}^{N} K_{nm} f_m, \qquad n = 1, 2, \ldots, N, N+1, \ldots, M. \tag{4a'}$$

The hope is that among the M equations there will be found N independent ones. The set of M equations is then solved by the method of least squares: the variational condition

$$\delta \sum_{n=1}^{M} \left| b_n - \sum_{m=1}^{N} K_{nm} f_m \right|^2 = 0 \tag{5}$$

is imposed. This results in

$$K^+ b = K^+ K f, \tag{6}$$

which is then solved by matrix inversion. The plus sign superscript denotes hermitian conjugation.

If the matrix K^+K is still ill-conditioned or nearly singular, then the still more complicated regularization method [7, 10] may be employed. In this method K^+K is replaced by another matrix $J(\beta)$ which is well-conditioned and which reduces the K^+K when $\beta \to 0$. For example, one might try

$$J(\beta) \equiv K^+ K + \beta I, \tag{7}$$

where I is the identity. Then the quantities

$$f(\beta) = J(\beta)^{-1} K^+ b \tag{8}$$

are found for a sequence of choices of the regularization parameter β, and an optimal value of β is determined by means of an error principle [11].

We employ a method for solving Eq. (2) which does not require matrix inversion and which circumvents the difficulties arising from the lack of strong linear independence of the kernel functions $K_n(x)$. Eq. (2) can be interpreted as giving the projections b_n of the vector ϕ in Hilbert space on a set of vectors $K_n^*(x)$ in that same space. Here the asterisk denotes complex conjugation. From this point of view it is a straightforward task to use this information to construct the projection $\hat{\phi}$ of ϕ onto the portion of Hilbert space spanned by the set K_n^* ($n = 1, 2, \ldots, N$).

To accomplish this task we construct an orthonormal basis $\chi_m(x)$ ($m = 1, 2, \ldots, N$) from the set of kernel functions:

$$\chi_m(x) = \sum_{n=1}^{N} A_{mn}^* K_n(x)^*, \qquad m = 1, 2, \ldots, N \tag{9a}$$

$$\langle \chi_m | \chi_n \rangle = \int dx\, \chi_m(x)^* \chi_n(x) = \delta_{mn}. \tag{9b}$$

Once the matrix A has been determined, the construction of the projection $\hat{\phi}$ of the solution ϕ follows directly. Multiplication of Eq. (2) by A_{mn} and summation on n gives

$$\sum_{n=1}^{N} A_{mn} b_n = \int dx\, \chi_m^*(x)\, \phi(x) = \langle \chi_m | \phi \rangle \tag{10}$$

by virtue of Eq. (9). It follows that

$$\begin{aligned} \hat{\phi}(x) &= \sum_{m=1}^{N} \chi_m(x) \langle \chi_m | \phi \rangle \\ &= \sum_{n=1}^{N} K_n(x)^* \sum_{m=1}^{N} A_{mn}^* \sum_{l=1}^{N} A_{ml} b_l. \end{aligned} \tag{11}$$

Thus the projection $\hat{\phi}$ of ϕ onto the subspace spanned by $K_n(x)^*$ $(n = 1, 2, \ldots, N)$ is expressed directly in terms of the elements of the orthonormalization matrix A. We will refer to this method as the projection method.

One method of finding the matrix A is the spectral expansion method (SEM) described by R. L. Parker [9]. This method is also known as the singular value decomposition method. In this method one first evaluates the elements of the Gram (or overlap) matrix M:

$$M_{mn} = \langle K_m | K_n \rangle = \int dx\, K_m(x)^* K_n(x). \tag{12}$$

This is a hermitian matrix. Thus there exists a unitary transformation that diagonalizes the Gram matrix:

$$(U^+ M U)_{mn} = \Lambda_{mn} = \lambda_m \delta_{mn}. \tag{13}$$

The λ_m are the (real) eigenvalues of M, and the columns of U are the eigenvectors of M. One can easily verify that the elements

$$A_{nm} = \lambda_n^{-1/2} U_{mn} \tag{14}$$

form an orthonormalization matrix as defined by Eq. (9). Thus the solution of Eq. (2) can be achieved by diagonalizing the Gram matrix M.

Now it may happen that some of the eigenvalues λ_n turn out to be zero. Then in the decomposition of M

$$M = U \Lambda U^+ \tag{15}$$

the columns of U and the rows of U^+ associated with the zero eigenvalues in fact make no contribution to M. Thus they must be regarded as spurious. Zero eigenvalues occur when the members of the set of kernel functions are not all linearly

independent. Thus in the numerical diagonalization of M one may find that some of the eigenvalues λ_m are much smaller than the rest. The associated eigenvectors χ_m should be deleted from the sum for ϕ shown in Eq. (11). It is this step that overcomes the possible ill-posedness of the Fredholm equation.

The disadvantage of the SEM is that the numerical procedure for matrix diagonalization is much more time-consuming than that for matrix inversion. We consider an alternative method for the construction of the orthogonalization matrix A. This method is simply the application of Gram–Schmidt orthogonalization (GSO) to the set of kernel functions. To construct χ_n^* we simply subtract from the kernel function K_n its projection onto the space spanned by $K_1, K_2, \ldots, K_{n-1}$ and normalize the residue. Thus GSO requires the calculation of the overlaps M_{nm} defined in Eq. (12) followed by a simple sequence of multiplications, subtractions, square roots, and divisions. The computing time expenditure is comparable to that required for matrix inversion.

The projection method using GSO turns out to be essentially the application of an aspect of Engkog's method [12] for Fredholm equations of the second kind to Fredholm equations of the first kind.

If the norm of the residue of K_n following the subtraction of its projection onto the space spanned by $K_1, K_2, \ldots, K_{n-1}$ falls below some preassigned value, then K_n is removed from the set of kernel functions, reducing its membership by one. This eliminates those members of the set with inadequate linear independence and eliminates any ill-posedness that might be present.

III. Iterative DWBA Optical Wave Inverse Scattering Calculation

We tested the projection method by applying it to a simple one-dimensional optical wave inverse scattering problem. Consider wave propagation in one dimension:

$$\left[\frac{d^2}{dx^2} + k^2 n(x)^2\right] \psi(k, x) = 0. \tag{16}$$

We suppose that the index of refraction $n(x)$ is equal to 1 everywhere except in a layer $-L < x < L$. We pose the following inverse scattering problem. Suppose we irradiate this layer with beams of different wavenumbers k_n ($n = 1, 2, \ldots, N$). Then at each wavenumber k_n we have

$$\psi_n^{(+)}(x) = e^{ik_n x} - R(k_n)\, e^{-ik_n x}, \qquad x < -L \tag{17a}$$

$$= [1 - U(k_n)]\, e^{ik_n x}, \qquad x > L. \tag{17b}$$

Can we determine the index of refraction (IR) profile $n(x)^2$ from a knowledge of the values of the reflection amplitudes $R_n \equiv R(k_n)$ and transmission amplitudes $U_n \equiv U(k_n)$?

To get a linear relationship between R and U and the IR profile, we start with the well known two-potential formula [13]:

$$\frac{2i}{k_n}(R_n - R_n^{(0)}) = \langle \psi_n^{(0,+)*} | [n(x)^2 - n_0(x)^2] \psi_n^{(+)} \rangle \tag{18a}$$

$$\frac{2i}{k_n}(U_n - U_n^{(0)}) = \langle \psi_n^{(0,-)} | [n(x)^2 - n_0(x)^2] \psi_n^{(+)} \rangle \tag{18b}$$

where $\psi_n^{(0,+)}$ is the solution of Eq. (16) with k replaced by k_n, $n(x)$ replaced by $n_0(x)$, and which satisfies the asymptotic boundary condition contraints displayed in Eq. (17). $\psi_n^{(0,-)}$ is the same as $\psi_n^{(0,+)}$ except that its asymptotic behaviour is governed by

$$\psi_n^{(-)}(x) = [1 - V(k_n)]\, e^{ik_n x}, \qquad x < -L \tag{19a}$$

$$= e^{ik_n x} - W(k_n)\, e^{-ik_n x}, \qquad x > L. \tag{19b}$$

If the difference between $n(x)$ and $n_0(x)$ is small, then the wave field $\psi_n^{(+)}$ for the index of refraction $n(x)$ can be approximated by $\psi_n^{(0,+)}$, the wave field for $n_0(x)$. Then Eq. (18) becomes the distorted wave Born approximation (DWBA) and provides a Fredholm equation of the first kind for $n(x)^2 - n_0(x)^2$.

We employ this linear integral equation to calculate $n(x)^2$ in the following fashion. An iterative procedure is followed in which a first guess is made for n_0^2, the wave equation solved for the $\psi_n^{(0,\pm)}$, and the values of $R_n^{(0)}$ and $U_n^{(0)}$ determined. The first guess will be called the zeroth iterate. The integral equation is then used to calculate n^2 from the exact values of R_n and U_n. This result for n^2 is then used in place of n_0^2 and the process is repeated. Succcessive iterations are carried out until the result for n^2 stabilizes.

We have carried out a series of calculations using this DWBA iterative inverse scattering method. Three alternative methods of solving the integral equation were employed, and the results were compared. In the first two methods the equation was discretized by using a Fourier series to represent $n(x)^2$. In the first method the resulting algebraic equations were solved by matrix inversion. In the second method the equations were solved by the selection method. Finally, in the third method we used the projection method outlined above with Gram–Schmidt orthogonalization.

The results for a typical case are plotted in Figs. 1, 2, and 3. In that case we let $n(x)^2 = 10 + x$ in the interval $-2 < x < 2$. For the first guess we took $n_0(x)^2 = 10$. For $|x| > 2$ both n and n_0 equal unity. Four or five iterations sufficed to get a stable result. The spectrum of wavenumbers employed was chosen to be $k_n = 0.05 + (n-1)\,0.15$ for $n = 1, 2, \ldots, N$. We see that simple matrix inversion gives very poor results, the selection method gives fair results for large enough N, and that the projection method gives excellent results for small N.

On Table I we present some auxiliarly results relative to these calculations. Δ_1 and C_1 are the determinant and condition number of the matrix inverted in the

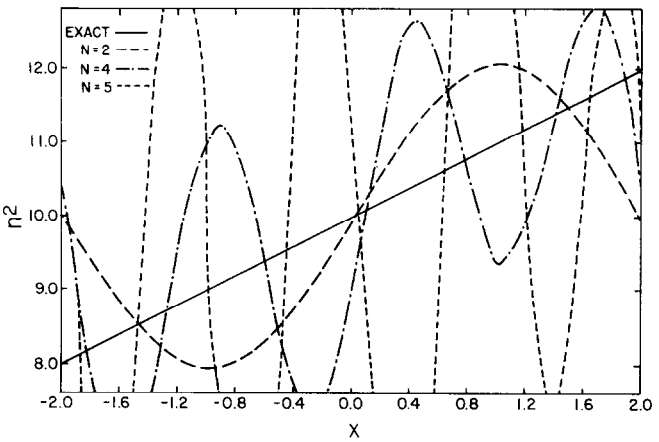

FIG. 1. Index of refraction calculated by means of the iterative DWBA inverse scattering method. The integral equations is discretized on a spectrum of N wavenumbers and solved by matrix inversion.

matrix inversion method. Δ_2 and C_2 are the corresponding values for the selection method. N and M have the definitions used in the text of this article. δ_i is the discrepancy

$$\delta_i = \sum_{n=1}^{N} \{(r_n - r_n^{(i)})^2 + (t_n - t_n^{(i)})^2\} \tag{20a}$$

where

$$r_n \equiv |R_n|^2, \tag{20b}$$

and

$$t_n \equiv |1 - U_n|^2. \tag{20c}$$

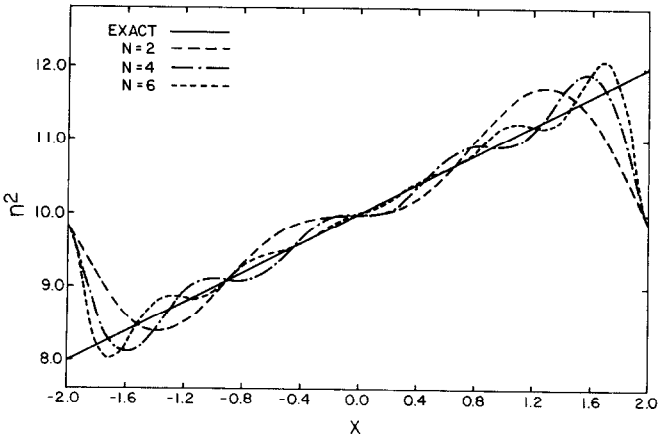

FIG. 2. Same as Fig. 1 except that the selection method is used to solve the integral equation.

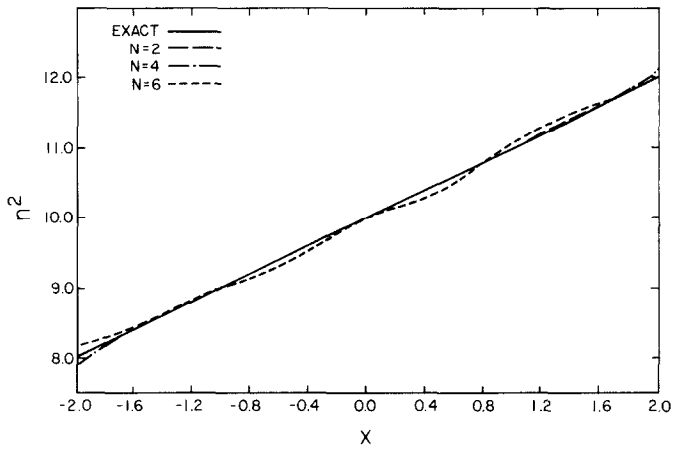

FIG. 3. Same as Fig. 1 except that the projection method using Gram–Schmidt orthogonalization is used to solve the integral equation.

It is a numerical measure of the quality of the inverse scattering calculation. r_n and t_n are the reflection and transmission probabilities calculated at wavenumber k_n from the IR profile $n(x)^2$ while $r_n^{(i)}$ and $t_n^{(i)}$ are the probabilities calculated from the IR profile provided by the inverse scattering calculation. δ_1 is the discrepancy for the matrix inversion method, δ_2 is for the selection method, and δ_3 is for the projection method. Finally, NF is the actual number of equations used in the projection method calculation after the linearly dependent equations have been weeded out from the 4N real equations originally given

The superiority of the projection method is apparent from the plots and the tabulated discrepancies. Note that for the matrix inversion method the condition number grows rapidly with increasing N. For the selection method, on the other

TABLE I

Parameters Relevant to the Calculations Displayed in Figs. 1, 2, and 3

N	M/NF	δ_1	δ_2	δ_3	Δ_1	Δ_2	C_1	C_2
2	5/4	$1.2E-5$	$6.7E-4$	$4.4E-10$	$8.9E-2$	$4.3E-5$	8.32	17.4
3	7/6	$2.5E-7$	$4.0E-3$	$1.8E-9$	$4.5E-3$	$9.3E-8$	20.2	21.3
4	9/7	$1.8E-4$	$5.0E-4$	$1.1E-9$	$1.8E-4$	$7.7E-11$	142	26.4
5	11/4	$4.2E-4$	$4.5E-3$	$6.0E-5$	$4.3E-6$	$5.9E-13$	478	24.8
6	13/5	$1.6E-0$	$8.7E-3$	$1.3E-4$	$1.3E-7$	$8.2E-16$	4901	26.5

Note. M is the number of members in the wavenumber spectrum and N is the dimension of the basis set used to represent the index of refraction profile. M is set equal to N in the matrix inversion method and projection method calculations. NF is the number of the original $4N$ kernel functions retained in the projection method calculation. δ_i is the discrepancy, Δ_i is the determinent, and C_i is the condition number where $i=1$ for the matrix inversion method, $i=2$ for the selection method, and $i=3$ for the projection method.

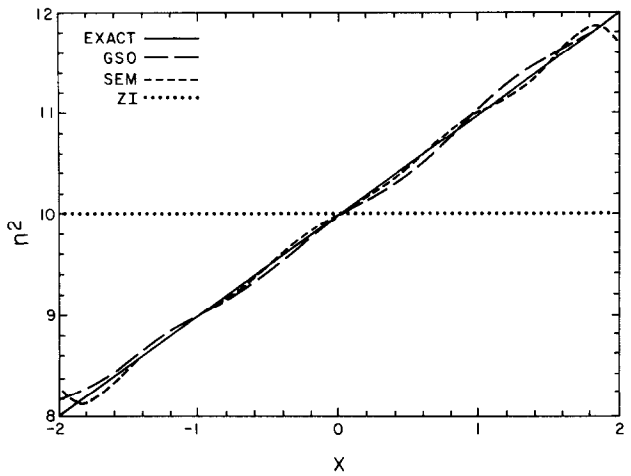

FIG. 4. Index of refraction profiles calculated by means of the iterative DWBA inverse scattering method using the projection method. SEM denotes that the spectral expansion method was usec while GSO denotes that Gram–Schmidt orthogonalization was used. ZI identifies the zeroth iterate or first guess. Four iterations were required. Each iteration consumed about 1.4 sec for the GSO and about 2.8 sec for the SEM. The wavenumber spectrum included six members.

hand, the condition number is stable but the determinant diminishes rapidly with increasing N. Some diminution of quality is seen in the projection method for sufficiently large N. Our interpretation of this is that it is a reflection of the lack of uniqueness of the solution.

In a second series of calculations we compare projection method inverse scattering calculations using the spectral expansion method (SEM) with calculations using Gram–Schmidt orthogonalization (GSO). These are shown in Figs. 4, 5, and 6. The

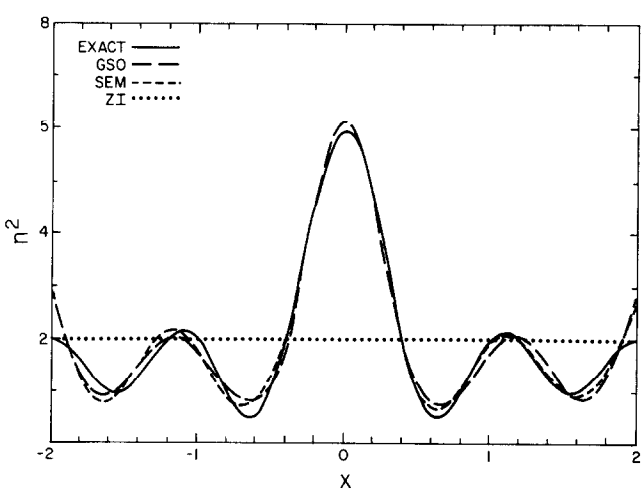

FIG. 5. Same as Fig. 4 except that each GSO iteration consumed about 2 sec, each SEM iteration consumed about 5.5 sec, and the wavenumber spectrum included eight members.

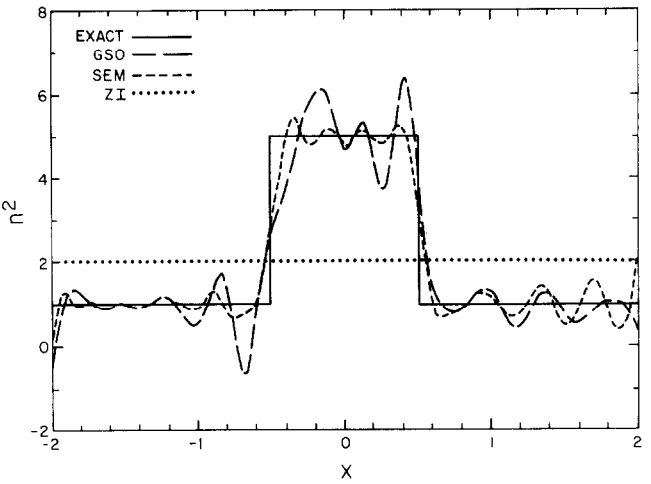

FIG. 6. Same as Fig. 4 except that six iterations were required, each GSO iteration consumed about 10 sec, each SEM iteration consumed about 90 sec, and the wave number spectrum included 24 members.

case shown in Fig. 4 is the same as was used in the first three figures. For the cases displayed in Figs. 4 and 5 the SEM and GSO give results of comparable quality. For the case displayed in Fig. 6 the SEM gives somewhat better results than the GSO method. The case shown in Fig. 5 was calculated with a spectrum of eight wavenumbers, $k_n = 0.3n$ $(n = 1, 2,..., 8)$, while the case shown in Fig. 6 was calculated with a spectrum of 24 wavenumbers, $k_n = 0.25n$ $(n = 1, 2,..., 24)$. Increasing the membership of the spectrum generally improves the quality of the result at the cost of a greater expenditure of computing time. However, one does reach a point of diminishing returns.

For the cases shown in Figs. 4 and 5 there was stabilization after four iterations while for the case shown in Fig. 6 six iterations were required. For the case shown in Fig. 4 we had $N = 6$ and the GSO required about 1.4 sec per iteration while the SEM required 2.8 sec per iteration. For the case shown in Fig. 5 we had $N = 8$ and the GSO required 2 sec per iteration while SEM required 5.5 sec per iteration. For the case shown in Fig. 6, on the other hand, we had $N = 24$ and the GSO required about 10 sec per iteration while the SEM required 90 sec per iteration. We can see that as we address more demanding inverse scattering problems, the difference between GSO and SEM in computer time expenditure becomes more significant.

The case shown in Fig. 6 has additional interest as an example of a case where the spatial extent of the true target is less than that of the zeroth iterate model target. Of course, the method cannot converge to the correct IR distribution if the extension of the zeroth iterate model target is too small.

IV. Projection Method for the Inverse Scattering of Acoustic Waves

In the optical wave scattering example discussed in the previous section, the target was characterized by a single function of position, the index of refraction $n(x)$. In other cases more than one function of position is required to represent the scattering inhomogeneity. Consider the equation for an acoustic wave field:

$$\nabla \cdot \rho^{-1} \nabla \psi + \omega^2 K^{-1} \psi = 0, \tag{21}$$

where ρ is the density, K is the bulk modulus, and ω is 2π times the frequency. Acoustic wave scattering will be produced by inhomogeneities in ρ or in K or in both. Thus we might take K_0 and ρ_0 to be the constant background values of K and ρ and write Eq. (21) in the form

$$(\nabla^2 + k^2)\,\psi = k^2 \left(1 - \frac{K_0}{\rho_0}\frac{\rho}{K}\right)\psi + \rho^{-1} \nabla \rho \cdot \nabla \psi \tag{22a}$$

$$k^2 \equiv \omega^2 \rho_0 / K_0. \tag{22b}$$

To provide a simple example, we consider the one-dimensional case of acoustic scattering. Then Eq. (22) becomes

$$\left(\frac{d^2}{dx^2} + k^2\right)\psi(x) = k^2 P(x)\,\psi(x) + Q(x)\frac{d}{dx}\psi(x) \tag{23a}$$

$$P(X) \equiv 1 - \frac{K_0}{\rho_0}\frac{\rho(x)}{K(x)} \tag{23b}$$

$$Q(x) \equiv \frac{d}{dx} \ln \rho(x). \tag{23c}$$

Then in place of Eq. (18a) for the reflection amplitudes we would have in the DWBA

$$-2ik_n(R_n - R_n^{(0)}) = \left\langle \psi_n^{(0,+)*} \middle| \left[k_n^2(P - P^{(0)}) + (Q - Q^{(0)})\frac{d}{dx}\right]\psi_n^{(0,+)} \right\rangle. \tag{24}$$

Thus if we were seeking to determine the scattering "potentials" $P(x)$ and $Q(x)$ from a series of measurements of the reflection amplitude R_n, we would be required to solve the set of equations

$$b_n = \int dx\, \{K_n(x)\,\phi(x) + L_n(x)\,\zeta(x)\}, \qquad n = 1, 2, \ldots, N \tag{25a}$$

where

$$\phi(x) \equiv P(x) - P^{(0)}(x) \tag{25b}$$

$$\zeta(x) = Q(x) - Q^{(0)}(x) \tag{25c}$$

$$b_n \equiv -i2k_n(R_n - R_n^{(0)}) \tag{25d}$$

$$K_n(x) \equiv k_n^2 \psi_n^{(0,+)}(x)^2 \tag{25e}$$

$$L_n(x) \equiv \psi_n^{(0,+)}(x) \frac{d}{dx} \psi_n^{(0,+)}(x). \tag{25f}$$

Let us rewrite Eq. (25a) to read

$$b_n = \langle K_n^* | \phi \rangle + \langle L_n^* | \zeta \rangle, \qquad n = 1, 2, \ldots, N. \tag{26}$$

Clearly, the best we can hope for is the projection $\hat{\phi}$ of ϕ onto the space spanned by the K_n^*'s and the projection $\hat{\zeta}$ of ζ onto the space spanned by the L_n^*'s. These will be

$$\hat{\phi}(x) = \sum_{n=1}^{N} \chi_n(x) \langle \chi_n | \phi \rangle \tag{27}$$

$$\hat{\zeta}(x) = \sum_{n=1}^{N} \xi_n(x) \langle \xi_n | \zeta \rangle \tag{28}$$

where the χ's provide an orthogonal basis for the space spanned by the K_n^*'s and the ξ_n's provide an orthogonal basis for the space spanned by the L_n^*'s. Thus we will have

$$\chi_n(x) = \sum_{m=1}^{N} A_{nm}^* K_m^*(x), \qquad \langle \chi_n | \chi_m \rangle = \delta_{nm} \tag{29}$$

$$\xi_n(x) = \sum_{m=1}^{N} B_{nm}^* L_m^*(x), \qquad \langle \xi_n | \xi_m \rangle = \delta_{nm} \tag{30}$$

where the orthogonalization matrices A and B are to be determined by the spectral expansion method or by Gram–Schmidt orthogonalization.

Now let us multiply Eq. (26) by either A_{ln} or B_{ln}, sum on n, and use either Eq. (29) or Eq. (30). The results are

$$\sum_n A_{ln} b_n \equiv v_l = \langle \chi_l | \phi \rangle + \langle \tau_l | \zeta \rangle \tag{31}$$

$$\sum_n B_{ln} b_n \equiv w_l = \langle \sigma_l | \phi \rangle + \langle \xi_l | \zeta \rangle \tag{32}$$

where

$$\tau_1(x) \equiv \sum_n A_{ln}^* L_n^*(x) \tag{33}$$

$$\sigma_l(x) \equiv \sum_n B_{ln}^* K_n^*(x). \tag{34}$$

We next expand the functions τ_l and σ_l in terms of our orthogonal basis sets:

$$\tau_l(x) = \sum_m \xi_m(x) \langle \xi_m | \tau_l \rangle = \sum_m C_{lm} \xi_m(x) \tag{35}$$

$$\sigma_l(x) = \sum_m \chi_m(x) \langle \chi_m | \sigma_l \rangle = \sum_m D_{lm} \chi_m(x). \tag{36}$$

Substitution into Eqs. (31) and (32) gives

$$v_m = \langle \chi_m | \phi \rangle + \sum_{l=1}^{N} C_{ml}^* \langle \xi_l | \zeta \rangle \tag{37}$$

$$w_m = \langle \xi_m | \zeta \rangle + \sum_{l=1}^{N} D_{ml}^* \langle \chi_l | \phi \rangle. \tag{38}$$

This provides us with $2N$ linear algebraic equations for the N amplitudes $\langle \xi_m | \phi \rangle$ and the N amplitudes $\langle \xi_m | | \zeta \rangle$ needed in the expansions of Eqs. (27) and (28).

By substituting Eqs. (37) and (38) into each other we can decouple the equations for the amplitudes $\langle \chi_m | \phi \rangle$ from the equations for the amplitudes $\langle \xi_m | \zeta \rangle$. The result is

$$x_m = \langle \chi_m | \phi \rangle - \sum_{n=1}^{N} E_{mn} \langle \chi_n | \phi \rangle \tag{39}$$

$$y_m = \langle \xi_m | \zeta \rangle - \sum_{n=1} F_{mn} \langle \xi_n | \zeta \rangle \tag{40}$$

where

$$x_m \equiv v_m - \sum_{l=1}^{N} C_{ml}^* w_l \tag{41}$$

$$y_m \equiv w_m - \sum_{l=1}^{N} D_{ml}^* v_l \tag{42}$$

$$E_{mn} \equiv \sum_{l=1}^{N} C_{ml}^* D_{ln} \tag{43}$$

$$F_{mn} \equiv \sum_{l=1}^{N} D_{ml}^* C_{ln} \tag{44}$$

and

$$C_{ml} \equiv \langle \xi_l | \tau_m \rangle = \sum_n \sum_r B_{ln} A^*_{mr} \langle L_r | L_n \rangle \tag{45}$$

$$D_{ml} \equiv \langle \chi_l | \sigma_m \rangle = \sum_n \sum_r A_{ln} B^*_{mr} \langle K_r | K_n \rangle. \tag{46}$$

Thus the projection method for acoustic wave inverse scattering requires two steps. First, the orthonormalization matrices A and B must be determined. Second, the N equations represented by Eq. (39) must be solved for the N amplitudes $\langle \chi_m | \phi \rangle$, and the N equations represented by Eq. (40) must be solved for the N amplitudes $\langle \xi_m | \zeta \rangle$.

Appendix

Let us outline here in a compact manner the iterative DWBA inverse scattering method tested in this paper.

1. A choice is made for the model index of refraction $n_0(x)$ and $\psi_n^{(0,\pm)}$, $R_n^{(0)}$, and $U_n^{(0)}$ are calculated by solving Eq. (16) and using the boundary conditions displayed in Eqs. (17) and (19).

2. The distorted wave Born approximation is used to provide a linear integral equation relating the observed scattering amplitudes R_n and U_n to the unknown index of refraction $n(x)$. This is Eq. (18) with $\psi_n^{(+)}$ replaced by $\psi_n^{(0,+)}$. The $\psi_n^{(0,\pm)}$, $R_n^{(0)}$, and $U_n^{(0)}$ in Eq. (18) come from step 1. The equation is solved for $n(x)$ using the spectral expansion method (SEM) or Gram–Schmidt orthogonalization (GSO).

3. Return to step 1 using $n(x)$ calculated in step 2 in place of $n_0(x)$. Keep repeating the process until the result for $n(x)$ stabilizes, i.e., is unaffected by subsequent iterations.

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