

THE DISCRETE SPECTRUM IN AZIMUTHALLY DEPENDENT TRANSPORT THEORY

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Abstract

The discrete spectrum for each component of a Fourier decomposition of the azimuthally dependent transport equation is analyzed. For a non-multiplying medium described by an L^{th} -order scattering law, the problem of determining the zeros of the dispersion function for the m^{th} Fourier component is formulated in terms of Sturm sequences. In particular, a straightforward application of the Sturm-sequence property is used to compute the number of discrete eigenvalue pairs κ^m and to show that either $\kappa^m = \gamma^m$ or $\kappa^m = \gamma^m + 1$, where γ^m denotes the number of zeros of the Chandrasekhar polynomial $g_{L+1}^m(\xi)$ which are greater than unity. It is also shown how Sturm sequences can be used to construct effective algorithms to compute and to refine estimates of the discrete eigenvalues. Results are presented for a test problem.

Resumo

O espectro discreto associado a cada componente de uma decomposição de Fourier da equação de transporte com dependência azimutal é analisado. Para um meio não-multiplicador descrito por uma lei de espalhamento de ordem L , o problema da determinação dos zeros da função de dispersão para o m -ésimo componente de Fourier é formulado em termos de seqüências de Sturm. Em particular, uma aplicação direta da propriedade básica das seqüências de Sturm é utilizada para calcular o número de pares de autovalores discretos κ^m e mostrar que $\kappa^m = \gamma^m$ ou $\kappa^m = \gamma^m + 1$, onde γ^m denota o número de zeros do polinômio de Chandrasekhar $g_{L+1}^m(\xi)$ maiores que a unidade. A utilidade das seqüências de Sturm na construção de algoritmos efetivos para calcular e refinar estimativas dos autovalores discretos também é demonstrada. São apresentados resultados para um problema-teste.

1. Introduction

Formal solutions to azimuthally dependent transport models with L^{th} -order scattering laws have first been obtained by Ambarzumian [1] and Chandrasekhar [2], who employed respectively a method based on invariance principles and a discrete ordinates method. Since then, several other methods have been developed to solve the azimuthally dependent transport equation in the fields of neutron transport and radiative transfer (see, for example, the survey edited by Lenoble [3]).

The source-free, azimuthally dependent transport equation can be written as

$$\mu \frac{\partial}{\partial x} \psi(x, \mu, \varphi) + \psi(x, \mu, \varphi) = \frac{c}{4\pi} \int_{-1}^1 \int_0^{2\pi} f(\cos \Theta) \psi(x, \mu', \varphi') d\varphi' d\mu', \quad (1)$$

where x is the optical variable, μ is the direction cosine measured from the positive x axis, φ is the azimuthal angle and c is the mean number of secondary particles per collision. In addition, it is assumed that the scattering law can be represented by a finite Legendre expansion in terms of the cosine of the scattering angle Θ , i.e.

$$f(\cos \Theta) = \sum_{l=0}^L (2l+1) f_l P_l(\cos \Theta), \quad (2)$$

where $f_0 = 1$ and $|f_l| < 1$, $l \geq 1$.

Equation (1) can be decomposed [2,4] into a set of azimuthally independent equations which can be written for $m = 0, 1, \dots, L$ as

$$\mu \frac{\partial}{\partial x} \psi^m(x, \mu) + \psi^m(x, \mu) = \frac{c}{2} \sum_{l=m}^L \beta_l^m P_l^m(\mu) \int_{-1}^1 P_l^m(\mu') \psi^m(x, \mu') d\mu', \quad (3)$$

where the constants β_l^m are given by

$$\beta_l^m = \frac{(l-m)!}{(l+m)!} (2l+1) f_l \quad (4)$$

and the associated Legendre functions of the first kind $P_l^m(\mu)$ are defined by

$$P_l^m(\mu) = (1-\mu^2)^{m/2} \frac{d^m}{d\mu^m} P_l(\mu). \quad (5)$$

Among the methods reported in the literature for solving Eq. (3), the method of elementary solutions [5,6] and the F_N method [4,7-9] have one point in common: both require the determination of the discrete eigenvalues, i.e. the zeros of the dispersion function [10]

$$\Lambda^m(z) = 1 - z \int_{-1}^1 \Psi^m(\mu) \frac{d\mu}{z-\mu} \quad (6)$$

in the complex plane cut from -1 to 1 along the real axis. In Eq. (6) the characteristic function $\Psi^m(\mu)$ is defined by

$$\Psi^m(z) = \frac{c}{2}(1-z^2)^{m/2} \sum_{l=m}^L \beta_l^m g_l^m(z) P_l^m(z), \quad (7)$$

where the Chandrasekhar polynomials $g_l^m(z)$, $l \geq m$, obey the three-term recursion relation

$$(1 - \delta_{l,m})(l+m)g_{l-1}^m(z) - h_l z g_l^m(z) + (l-m+1)g_{l+1}^m(z) = 0 \quad (8)$$

with

$$h_l = (2l+1)(1-cf_l) \quad (9)$$

and the starting condition

$$g_m^m(z) = (2m-1)!! \quad (10)$$

The dispersion function can also be written as [10]

$$\Lambda^m(z) = 1 - cz \sum_{l=m}^L \beta_l^m g_l^m(z) Q_l^m(z), \quad (11)$$

where

$$Q_l^m(z) = \frac{1}{2} \int_{-1}^1 (1-\mu^2)^{m/2} P_l^m(\mu) \frac{d\mu}{z-\mu}. \quad (12)$$

In addition, we can follow a procedure reported in Ref. 10 to show that the dispersion function can be written, for any $N \geq L$, as

$$\Lambda^m(z) = \frac{(N-m+1)!}{(N+m)!} [Q_N^m(z)g_{N+1}^m(z) - Q_{N+1}^m(z)g_N^m(z)] \quad (13)$$

and

$$(1-z^2)^{m/2} P_N^m(z) \Lambda^m(z) = (1-z^2)^m g_N^m(z) - 2z \Psi^m(z) Q_N^m(z). \quad (14)$$

Several properties of the dispersion function are useful for determining the discrete spectrum. In summary, the following results have been demonstrated for L^{th} -order scattering laws and sometimes, as in the work of Case [11], also for infinite-order expansions of the scattering law:

- (i) as $\Lambda^m(z) = \overline{\Lambda^m(-z)}$, the discrete eigenvalues appear in \pm pairs [4,12];
- (ii) as $\Lambda^m(z) = \overline{\Lambda^m(\bar{z})}$, the discrete eigenvalues appear in complex conjugate pairs [4];
- (iii) for $c \leq 1$ the zeros of $\Lambda^m(z)$ are real and simple [11,12], except the case $c = 1$ and $m = 0$ for which $\Lambda^m(z)$ has a double zero at infinity [13];
- (iv) for $m = 0$, there are no zeros of $\Lambda^m(z)$ embedded in the continuum $[-1, 1]$ (Refs. 11,14-16); the same is true for $m \geq 1$, if the endpoints ± 1 are excluded [10];

(v) the number of discrete eigenvalue pairs is finite [11]; for L^{th} -order scattering laws, the number of pairs is $\leq L - m + 1$ (Refs. 6 and 12).

The purpose of this paper is to show that the problem of determining the discrete eigenvalues for $c \leq 1$ can be formulated, in a convenient way, in terms of Sturm sequences. In Section 2, a straightforward application of the Sturm-sequence property will be used to determine the number of discrete eigenvalue pairs κ^m . In Section 3, Sturm sequences will be used to construct effective algorithms for computing and refining discrete eigenvalue estimates. Results will be presented in Section 4 for a test problem.

2. The Number of Discrete Eigenvalue Pairs

A few papers [4,9,12,17] have dealt with methods for computing the discrete eigenvalues for many-term ($L \gg 2$) scattering laws. In all of these references the argument principle [18] has been employed to compute the number of discrete eigenvalue pairs κ^m .

During an implementation of the argument principle to compute κ^m for all the Fourier components of a highly anisotropic ($L = 299$) problem for which $m = 0$ results are available [9], we found that argument principle calculations are subject to numerical limitations when applied to problems with highly anisotropic scattering laws. First, there is a tendency of κ^m to be large for such problems (e.g. $\kappa^0 = 24$ for the $L = 299$ problem of Ref. 9 with $c = 0.9$), which requires the use of very fine grids to follow the change of argument accurately. In addition to being computationally time consuming, calculations based on the argument principle give results which can be termed as ambiguous since there is no way to assure a priori that the selected grid is fine enough to avoid the loss of an eigenvalue pair during the calculation. Second, we have found that for relatively high Fourier components ($m > 20$) the computation of some functions involved in the argument principle calculation is subject to severe loss of accuracy. To make available an alternative to the argument principle method, we show that Sturm sequences can provide a simple and reliable way to compute the number of discrete eigenvalue pairs κ^m .

For ease of presentation, we restrict c here to $c \leq 1$, the range of interest for radiative transfer and radiation shielding applications. The case $c > 1$ concerning neutron transport in multiplying media requires a few modifications in the formulation that will be reported in a future work. It follows from results (i), (iii) and (iv) of the Introduction, that the discrete eigenvalues for $c \leq 1$ are real numbers with magnitudes ≥ 1 and appear in \pm pairs. Thus, if we let $\pm\nu_\alpha^m$, $\alpha = 1, 2, \dots, \kappa^m$, denote the discrete eigenvalues, we can conclude from Eq. (13) that the condition $\Lambda^m(\pm\nu_\alpha^m) = 0$ implies that

$$g_{N+1}^m(\xi) = \frac{Q_{N+1}^m(\xi)}{Q_N^m(\xi)} g_N^m(\xi), \quad \xi \in \{\pm\nu_\alpha^m\} \text{ and } N \geq L. \quad (15)$$

Now, if we use Eq. (8) for $l = m, m + 1, \dots, L$ and Eq. (15) for $N = L$, we find that the problem of determining the discrete eigenvalues for $c \leq 1$ can be restated as the problem of determining those values of $\xi \in \mathfrak{R}$ with magnitudes ≥ 1 that satisfy the system

for $l = m + 1, m + 2, \dots, L$. It follows that the zeros of $S_{l+1}^m(\xi)$ are strictly separated by the zeros of $S_l^m(\xi)$ and thus the sequence $S_m^m(\eta), S_{m+1}^m(\eta), \dots, S_{L+1}^m(\eta)$ obtained for any particular value of $\eta \in \mathfrak{R}$ is a Sturm sequence [20]. By the Sturm-sequence property [19,20], the number of sign agreements between consecutive elements of this sequence (excluding null elements) gives the number of zeros of $S_{L+1}^m(\xi)$ which are strictly greater than η .

Our method for computing the number of discrete eigenvalue pairs κ^m is very simple: we set $\eta = 1$ and, using the fact that

$$\lim_{\xi \rightarrow 1} \frac{Q_{L+1}^m(\xi)}{Q_L^m(\xi)} = 1 \quad (21)$$

and thus $R^m(1) = (L - m + 1)/h_L$, we compute the number of sign agreements between consecutive elements of the sequence $S_m^m(1), S_{m+1}^m(1), \dots, S_{L+1}^m(1)$, i.e. the number of zeros of $S_{L+1}^m(\xi)$ which are greater than 1. Since these zeros are also the positive solutions to Eq. (16), their number gives the number of discrete eigenvalue pairs κ^m , except when $S_{L+1}^m(1) = 0$ [referring to result (iv) of the Introduction, we note that this can happen only for $m \geq 1$]. In this case, ± 1 are also eigenvalues and the number of discrete eigenvalue pairs κ^m equals the number of zeros of $S_{L+1}^m(\xi)$ which are greater than 1 plus one.

When $c = 1$, $h_0 = 0$ and the matrix $C^m(\xi)$ becomes unbounded for $m = 0$. Hence, the case $c = 1$ and $m = 0$ requires special treatment. It can be shown that, as $z \rightarrow \infty$, the dispersion function behaves, for $m = 0$, as [21]

$$\Lambda^0(z) = \prod_{l=0}^L (1 - cf_l) + \frac{a_2}{z^2} + \frac{a_4}{z^4} + \dots, \quad (22)$$

where a_2, a_4, \dots are constants. It is clear from Eq. (22) that $\Lambda^0(z)$ has a double zero at ∞ for $c = 1$. A simple modification of the above analysis makes it possible to find the number of pairs of bounded zeros of $\Lambda^0(\xi)$ for $c = 1$. Noting that $g_1^0(\xi) = 0$ [see Eq. (8) for $l = m = 0$], we can consider Eq. (8) for $l = 2, 3, \dots, L$ and Eq. (15) for $N = L$ to obtain the modified system for $c = 1$ and $m = 0$:

$$\widehat{C}^0(\xi) \widehat{g}^0(\xi) = 0, \quad (23)$$

where the tridiagonal $\widehat{C}^0(\xi)$ matrix of order $L - 1$ can be obtained by neglecting the first two rows and columns of $C^m(\xi)$ for $m = 0$ and the vector $\widehat{g}^0(\xi)$ by neglecting the first two components of $g^m(\xi)$ for $m = 0$. Following the procedure developed with the restriction that $c \neq 1$ when $m = 0$, we arrive at similar conclusions for $c = 1$ and $m = 0$, in regard to the relationship between the number of pairs of bounded discrete eigenvalues and the number of bounded zeros of $S_{L+1}^0(\xi)$ which are greater than 1.

It is interesting to note that if we arbitrarily set $R^m(\xi) = 0$ in the last diagonal element of the matrix $C^m(\xi)$ defined by Eq. (17), we reduce the problem formulated by Eq. (16) to an algebraic eigenvalue problem which has the zeros of $g_{L+1}^m(\xi)$ as eigenvalues. Since the Sturm sequence associated with this algebraic eigenvalue problem differs from

the Sturm sequence defined by Eqs. (20a) to (20c) only in the last element, the number of discrete eigenvalue pairs κ^m can be easily related to γ^m , the number of zeros of $g_{L+1}^m(\xi)$ which are greater than 1. In fact, it can be shown that, for $|S_{L+1}^m(1)| \geq R^m(1)|S_L^m(1)|$, we must have $\kappa^m = \gamma^m$, while for $|S_{L+1}^m(1)| < R^m(1)|S_L^m(1)|$ we can have $\kappa^m = \gamma^m$ if $S_L^m(1)S_{L+1}^m(1) < 0$ and $\kappa^m = \gamma^m + 1$ if $S_L^m(1)S_{L+1}^m(1) \geq 0$.

Finally we point out that, as was done in Ref. 9 for the Chandrasekhar polynomials [see Eq. (45) of Ref. 9], we could restate our problem in terms of a Sturm sequence involving only even $S_i^m(\xi)$; however, as the coefficients of the resulting three-term recursion relation for $S_{i-2}^m(\xi)$, $S_i^m(\xi)$ and $S_{i+2}^m(\xi)$ are more complicated than those of Eq. (20c), we believe that there is no advantage in adopting such a procedure here.

3. Computation of the Discrete Eigenvalues

Turning now to the problem of computing the discrete eigenvalues given the number of pairs κ^m , we first note that a method [4,21] based on a Wiener-Hopf factorization of the dispersion function $\Lambda^m(z)$ has provided explicit results for the discrete eigenvalues when $\kappa^m \leq 3$ and reduced the task of finding the discrete eigenvalues to one of solving a polynomial equation of order κ^m for the squares of the eigenvalues, in the general case. Since the explicit results for $\kappa^m \leq 3$ and the polynomial equations are given in terms of integrals that need to be evaluated numerically, the method has been used mainly for obtaining initial estimates of the discrete eigenvalues that can be refined subsequently by iterative techniques such as Newton's method. However, as discussed in Ref. 9, computational difficulties that arise from ill-conditioning of the polynomial equations have been observed in this method when κ^m is large, and so the method has not been used for problems with highly anisotropic scattering laws.

A simple and effective method to compute initial estimates for the discrete eigenvalues has been proposed to overcome these difficulties [9]. The method is based on the fact that the spherical harmonics (P_N) eigenvalues outside $[-1, 1]$ approach the "exact" discrete eigenvalues outside $[-1, 1]$ as $N \rightarrow \infty$. Indeed, by letting $N \rightarrow \infty$ in Eq. (14) and considering that [22]

$$\lim_{N \rightarrow \infty} \frac{Q_N^m(z)}{P_N^m(z)} = 0, \quad z \notin [-1, 1], \quad (24)$$

we conclude from Eq. (14) that

$$\Lambda^m(z) = \lim_{N \rightarrow \infty} (1 - z^2)^{m/2} \frac{g_N^m(z)}{P_N^m(z)}, \quad z \notin [-1, 1], \quad (25)$$

and thus the zeros of $g_N^m(z)$ outside $[-1, 1]$ approach the zeros of $\Lambda^m(z)$ outside $[-1, 1]$ as $N \rightarrow \infty$. It has been found that the larger the magnitude of a discrete eigenvalue is, the faster the convergence of the corresponding P_N eigenvalue is, as N increases; however, when any of the discrete eigenvalues happens to be only slightly > 1 in magnitude very large values of N may be required to find a good estimate of such an eigenvalue. Alternatively,

for $c \leq 1$, a bisection calculation based on $\Lambda^m(\xi)$ has been used [9] to compute initial estimates of those zeros of $\Lambda^m(\xi)$ that are very close to ± 1 .

Once initial estimates of all the discrete eigenvalues are computed, they can be refined, if necessary, by iterative techniques; some works have reported experiences with Newton's [4,21], secant [23] and *regula falsi* [24] methods. All of these methods plus the above mentioned bisection technique rely on accurate calculations of the dispersion function (and its derivative, if Newton's method is applied). Consequently, efficient and accurate methods for computing the dispersion function have been sought. Evaluation of $\Lambda^m(z)$ by numerical integration of Eq. (6) has been used sometimes [4,17,24], but there are some disadvantages in this procedure: first, as the integrand of Eq. (6) can vary quite rapidly, especially near the endpoints ± 1 , it is necessary to use a large number of quadrature points for integration, which sacrifices the computational efficiency (computer time); second, even when sufficient care is taken to define the integration rule, the maximum degree of precision normally available in a computer (16 decimal digits for double precision in short-word computers) may not be sufficient to evaluate the right-hand side of Eq. (6) accurately, as the dispersion function can be very small in magnitude (for example, 10^{-50}) even relatively far from zeros, especially for large m . This second point is also a limiting factor for the expression given by Eq. (11) and some closely related expressions in which the function $Q_l^m(z)$ has been split into two terms [4,9].

It could be thought that Eq. (13) is a better expression from which to compute $\Lambda^m(z)$, since it is not subject to the accuracy limitations inherent in Eqs. (6) and (11). Unfortunately, there is one additional problem that affects Eq. (13) as well as Eq. (11): the lack of a method to compute $g_l^m(z)$, $l \geq m$, accurately for all z . As can be seen from Eq. (14), $g_N^m(z)$ is proportional to $Q_N^m(z)$ for $N \geq L$ when z is a discrete eigenvalue and approaches a constant times $P_N^m(z)$ as $N \rightarrow \infty$ when z is sufficiently far away from all discrete eigenvalues. Thus, following Gautschi [25], we could use forward recursion of Eq. (8) to compute $g_N^m(z)$, $N \geq L$, when z is not near an eigenvalue and backward recursion when z is an eigenvalue. However, if we are planning to use Eq. (13) to refine estimates of the discrete eigenvalues, z in general will be very close to (although not exactly) an eigenvalue so that it is not clear in which direction the recursion relation given by Eq. (8) should be used to compute $g_N^m(z)$, $N \geq L$, accurately.

We now proceed to show, for $c \leq 1$, that the bisection procedure used to find estimates for eigenvalues with magnitudes just > 1 and the iterative refinement of all eigenvalue estimates can be carried out independently of computations of $\Lambda^m(\xi)$, by making use of Sturm sequences and their basic property. Since, as discussed in Section 2, the discrete eigenvalues appear in \pm pairs and are real for $c \leq 1$, we limit our discussion here to the computation of positive discrete eigenvalues.

We assume that initial estimates for the positive zeros of $\Lambda^m(\xi)$ that are sufficiently far from 1 have been found, as in Ref. 9, by computing P_N eigenvalues with two different values of N , say N_1 and N_2 , and accepting as valid estimates those eigenvalues that do not differ by more than a specified amount when N is changed from N_1 to N_2 . The remaining estimates can be conveniently computed from a bisection procedure applied to the Sturm

sequence defined by Eqs. (20a) to (20c), hereafter denoted as the S^m sequence. In other words, suppose that the P_N method has provided ρ^m eigenvalue estimates and let ν_{\min}^m denote the smallest of these estimates. Then, the remaining $\kappa^m - \rho^m$ estimates are to be computed by bisection in the reduced interval $[1, \nu_{\min}^m]$. The manner by which bisection is applied to the S^m sequence is entirely analogous to the bisection procedure used to calculate the eigenvalues of symmetric tridiagonal matrices and discussed extensively in the book by Wilkinson [19].

Suppose, for example, that we wish to compute an estimate of ν_α^m , $\rho^m < \alpha \leq \kappa^m$, and we have found two points a_0^m and b_0^m in the interval $[1, \nu_{\min}^m]$ such that $b_0^m > a_0^m$, $s(a_0^m) \geq \alpha$ and $s(b_0^m) < \alpha$, where $s(\eta)$ denotes the number of sign agreements between consecutive elements of the S^m sequence, evaluated at η . Then, $a_0^m < \nu_\alpha^m < b_0^m$ and we can locate ν_α^m in the interval (a_n^m, b_n^m) of size $(b_0^m - a_0^m)/2^n$ in n iterative steps by repeating the following procedure for $k = 1, 2, \dots, n$:

- (i) let $c_k^m = \frac{1}{2}(a_{k-1}^m + b_{k-1}^m)$ and compute $s(c_k^m)$;
- (ii) if $s(c_k^m) \geq \alpha$, take $a_k^m = c_k^m$ and $b_k^m = b_{k-1}^m$, otherwise take $a_k^m = a_{k-1}^m$ and $b_k^m = c_k^m$.

As a matter of fact, we have used in our computer program a bisection scheme that calculates estimates for $\nu_\alpha^m - 1$ instead of ν_α^m . This is a particularly convenient procedure, in the event that ν_α^m happens to be very close to 1.

Having found the remaining $\kappa^m - \rho^m$ estimates by bisection, we now discuss our method of refining all the discrete eigenvalue estimates. Instead of looking at the condition $\Lambda^m(\nu_\alpha^m) = 0$ to refine the estimate of ν_α^m , we prefer to use the condition that the last element of the S^m sequence evaluated at ν_α^m should be zero, i.e. $S_{L+1}^m(\nu_\alpha^m) = 0$. To avoid computing derivatives of $S_{L+1}^m(\nu_\alpha^m)$, we elected to use the *regula falsi* method [26] for refining the eigenvalue estimates. Denoting as $\nu_{\alpha,0}^m$ the estimate of ν_α^m provided by either the P_N method or the bisection procedure, we find the two initial values $\nu_{\alpha,1}^m$ and $\nu_{\alpha,2}^m$ required to start the *regula falsi* iterative scheme by computing $\nu_{\alpha,0}^m(1 \pm 10^{-k})$ for $k = 15, 14, \dots$, until a value K such that

$$S_{L+1}^m[\nu_{\alpha,0}^m(1 + 10^{-K})] S_{L+1}^m[\nu_{\alpha,0}^m(1 - 10^{-K})] < 0 \quad (26)$$

is reached. We then take $\nu_{\alpha,1}^m = \nu_{\alpha,0}^m(1 - 10^{-K})$ and $\nu_{\alpha,2}^m = \nu_{\alpha,0}^m(1 + 10^{-K})$, compute, for $i=2,3,\dots$, the sequence of *regula falsi* approximations to ν_α^m ,

$$\nu_{\alpha,i+1}^m = \nu_{\alpha,i}^m - \frac{\nu_{\alpha,i}^m - \nu_{\alpha,i-1}^m}{S_{L+1}^m(\nu_{\alpha,i}^m) - S_{L+1}^m(\nu_{\alpha,i-1}^m)} S_{L+1}^m(\nu_{\alpha,i}^m), \quad (27)$$

followed by $\nu_{\alpha,i}^m = \nu_{\alpha,i-1}^m$ if $S_{L+1}^m(\nu_{\alpha,i+1}^m) S_{L+1}^m(\nu_{\alpha,i}^m) > 0$, and stop the iteration when either both of the conditions [26]

$$|\nu_{\alpha,i+1}^m - \nu_{\alpha,i}^m| \geq |\nu_{\alpha,i}^m - \nu_{\alpha,i-1}^m| \quad \text{and} \quad |\nu_{\alpha,i}^m - \nu_{\alpha,i-1}^m| < \delta, \quad (28a)$$

where δ is a tolerance slightly greater than the machine precision, are satisfied or

$$S_{L+1}^m(\nu_{\sigma, i+1}^m) = 0. \quad (28b)$$

Finally, it is worthwhile to mention that rescaling of the S^m -sequence calculation is usually required for large eigenvalues, in order to avoid the occurrence of overflows during the refinement procedure.

4. Numerical Results

For our numerical example, we have used the scattering law introduced by Kaper, Shultis and Veninga [24], *i.e.*

$$f(\cos \Theta) = \frac{L+1}{2^L} (1 + \cos \Theta)^L, \quad (29)$$

hereafter denoted as the KSV scattering law. The KSV scattering law has the advantage that it can be represented exactly with $L+1$ terms in Eq. (2).

A scheme based on a three-term recursion relation in the two-dimensional space (L, l) was used in Ref. 24 to compute the coefficients f_l , $l = 0, 1, \dots, L$, of the KSV scattering law. We have found however that these coefficients can be computed in a much simpler way by using the starting value $f_0 = 1$ and

$$f_l = \left(\frac{L-l+1}{L+l+1} \right) f_{l-1} \quad (30)$$

for $l = 1, 2, \dots, L$.

Table 1 shows the number of discrete eigenvalue pairs κ^m computed according to the methods of Section 2 for a few values of c and $L = 59$. Table 2 shows the positive discrete eigenvalues for three selected values of c and $L = 59$, which resulted from our application of the methods presented in Section 3. We believe that the results of Table 2 are accurate to within ± 1 in the last figure shown.

Table 1. The number of discrete eigenvalue pairs κ^m for the KSV scattering law with $L = 59$.

m	$c = 0.2$	$c = 0.4$	$c = 0.6$	$c = 0.8$	$c = 1.0$
0	2	3	4	4	5
1	1	2	3	4	4
2	1	2	2	3	3
3	0	1	2	2	3
4	0	0	1	1	2
5	0	0	0	0	1
6 - 59	0	0	0	0	0

Table 2. The discrete eigenvalues for the KSV scattering law with $L = 59$.

m	$c = 0.5678$	$c = 0.8115228$	$c = 0.8783585$
0	1.912001500826044	3.783165533641392	5.351091071788712
	1.367969626434857	2.050242473971546	2.460935156938731
	1.091606657626732	1.340299700326329	1.463295282686077
	1.000000000001147	1.055547311326692	1.091745459480726
1	1.584496726525516	2.667560240371443	3.406447023693270
	1.196648388280417	1.597621560783307	1.808093790081362
	1.019807696402705	1.153855444893048	1.219686545145295
	-	1.002003471942856	1.013490847758943
2	1.330387524558258	1.924450984271965	2.254575164875290
	1.070993547938969	1.289122731342325	1.392493860675903
	-	1.034163066112437	1.063991418783902
3	1.143346356987104	1.456176437134108	1.604513871227998
	-	1.092195319895360	1.140132499173532
4	1.015898762767950	1.168724042905966	1.235765701352745
	-	-	1.000000026175034
5	-	1.000000005561480	1.027401938072136

Finally, we should like to mention that we have successfully used the methods of Sections 2 and 3 to compute the discrete eigenvalues for all the Fourier components of the challenging $L = 299$ problem described in Ref. 9. In addition to being efficient, the methods proved to be very stable computationally speaking.

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