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ON DISCRETE SPECTRUM CALCULATIONS IN RADIATIVE TRANSFER

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Abstract—The discrete spectrum for each component problem in a Fourier decomposition of the equation of transfer is analyzed for the case of an Lth-order scattering law. The problem of determining the number of zeros of the dispersion function for each Fourier-component problem and the problem of computing all of these zeros are formulated and resolved in terms of Sturm sequences. Computational aspects of the numerical methods are discussed, and the developed algorithms are implemented to yield especially accurate numerical results for two test problems.

1. INTRODUCTION

Ambarzumian,[1] who used a method based on invariance principles, and Chandrasekhar,[2] who used a discrete ordinates method, have developed and reported, in two early works in the field of radiative transfer, formal solutions to the equation of transfer for the case of an Lth-order scattering law. Since the appearance of these two works, numerous methods for solving the equation of transfer have been developed and reported in the literature (see, for example, the survey edited by Lenoble[3]). We let $I(\tau, \mu, \varphi)$ denote the intensity and consider the equation of transfer[4] written as

$$\mu \frac{\partial}{\partial \tau} I(\tau, \mu, \varphi) + I(\tau, \mu, \varphi) = \frac{\varpi}{4\pi} \int_{-1}^{1} \int_{0}^{2\pi} p(\cos \Theta) I(\tau, \mu', \varphi')\, d\varphi'\, d\mu' \tag{1}$$

where τ is the optical variable, μ is the direction cosine measured from the positive τ axis, φ is the azimuthal angle and ϖ is the albedo for single scattering. In addition, we assume that the scattering law (phase function) can be represented by a finite Legendre expansion in terms of the cosine of the scattering angle Θ, i.e.

$$p(\cos \Theta) = \sum_{l=0}^{L} \beta_l P_l(\cos \Theta) \tag{2}$$

where $\beta_0 = 1$ and $|\beta_l| < 2l + 1$ for $l \geqslant 1$.

Equation (1) can be decomposed[2,5] into a set of azimuthally independent equations which can be written for $m = 0, 1, \ldots, L$ as

$$\mu \frac{\partial}{\partial \tau} I^m(\tau, \mu) + I^m(\tau, \mu) = \frac{\varpi}{2} \sum_{l=m}^{L} \beta_l P_l^m(\mu) \int_{-1}^{1} P_l^m(\mu') I^m(\tau, \mu')\, d\mu' \tag{3}$$

where we use the normalized associated Legendre functions

$$P_l^m(\mu) = \left[\frac{(l-m)!}{(l+m)!}\right]^{1/2} (1-\mu^2)^{m/2} \frac{d^m}{d\mu^m} P_l(\mu). \tag{4}$$

Among the methods reported in the literature for solving Eq. (3), the method of elementary solutions[6,7] and the F_N method[5,8–10] have one point in common: both require the determination of the discrete eigenvalues, i.e., the zeros of the dispersion function[11]

$$\Lambda^m(z) = 1 - z \int_{-1}^{1} \psi^m(\mu) \frac{d\mu}{z - \mu} \tag{5}$$

in the complex plane cut from -1 to 1 along the real axis. In Eq. (5) the characteristic function $\psi^m(\mu)$ is defined by

$$\psi^m(z) = \frac{\varpi}{2}(1-z^2)^{m/2} \sum_{l=m}^{L} \beta_l g_l^m(z) P_l^m(z) \tag{6}$$

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

$$(l^2 - m^2)^{1/2} g_{l-1}^m(z) - h_l z g_l^m(z) + [(l+1)^2 - m^2]^{1/2} g_{l+1}^m(z) = 0 \tag{7}$$

with

$$h_l = 2l + 1 - \varpi\beta_l \tag{8}$$

and the starting conditions $g_0^0(z) = 1$ and

$$g_m^m(z) = (2m-1)!![(2m)!]^{-1/2}, \quad m \geqslant 1. \tag{9}$$

The dispersion function can also be written as[11]

$$\Lambda^m(z) = 1 - \varpi z \sum_{l=m}^{L} \beta_l g_l^m(z) Q_l^m(z) \tag{10}$$

where

$$Q_l^m(z) = \frac{1}{2}\int_{-1}^{1} (1-\mu^2)^{m/2} P_l^m(\mu) \frac{\mathrm{d}\mu}{z-\mu}. \tag{11}$$

In addition, we can follow a procedure reported in Ref. 11 to show that the dispersion function can be written, for any $N \geqslant L$, as

$$\Lambda^m(z) = [(N+1)^2 - m^2]^{1/2} [Q_N^m(z) g_{N+1}^m(z) - Q_{N+1}^m(z) g_N^m(z)] \tag{12}$$

and

$$(1-z^2)^{m/2} P_N^m(z) \Lambda^m(z) = (1-z^2)^m g_N^m(z) - 2z\psi^m(z) Q_N^m(z). \tag{13}$$

Several properties of the dispersion function are useful for determining the discrete spectrum. In summary, the following results have been demonstrated for Lth-order scattering laws and sometimes, as in the work of Case,[12] also for infinite-order expansions of the scattering law:

(i) Since $\Lambda^m(z) = \Lambda^m(-z)$ the discrete eigenvalues appear in $\pm$ pairs;[5,13]
(ii) Since $\Lambda^m(z) = \overline{\Lambda^m(\bar{z})}$ the discrete eigenvalues appear in complex conjugate pairs;[5]
(iii) For $\varpi \leqslant 1$ the zeros of $\Lambda^m(z)$ are real and simple[12,13] except for the case $\varpi = 1$ and $m = 0$ for which $\Lambda^m(z)$ has a double zero at infinity;[14]
(iv) For $m = 0$, there are no zeros of $\Lambda^m(z)$ embedded in the continuum $[-1, 1]$ (Refs. 12, 15–17); the same is true for $m \geqslant 1$ if the endpoints ± 1 are excluded;[11]
(v) The number of discrete eigenvalue pairs is finite,[12] and for Lth-order scattering laws the number of pairs is $\leqslant L + 1 - m$ (Refs. 7 and 13).

The purpose of this paper is to show that the problem of determining the discrete eigenvalues for $\varpi \leqslant 1$ can be formulated in a convenient way in terms of Sturm sequences. In Sec. 2 a straightforward application of the Sturm-sequence property is used to determine the number of discrete eigenvalue pairs $\aleph^m$. In Sec. 3 Sturm sequences are used to construct effective algorithms for computing and refining discrete eigenvalue estimates, and especially accurate results for two test problems are presented in Sec. 4.

2. THE NUMBER OF DISCRETE EIGENVALUE PAIRS

A few papers[5,10,13,18] 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[19] has been employed to compute the number of discrete eigenvalue pairs $\aleph^m$.

During an implementation of the argument principle to compute $\aleph^m$ for all the Fourier components of a highly anisotropic ($L = 299$) problem for which $m = 0$ results are available,[10] 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 for $\aleph^m$ to be large for such problems (e.g., $\aleph^0 = 24$ for the $L = 299$ problem of Ref. 10 with $\varpi = 0.9$) 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 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 $\aleph^m$.

We consider here that $\varpi \leqslant 1$ and note from results (i), (iii) and (iv) of Sec. 1 that the discrete eigenvalues for $\varpi \leqslant 1$ are real numbers with magnitudes $\geqslant 1$ and appear in $\pm$ pairs. Thus if we let $\pm\nu_\alpha^m$, $\alpha = 1, 2, \ldots, \aleph^m$, denote the discrete eigenvalues, we can conclude from Eq. (12) that the condition $\Lambda^m(\pm\nu_\alpha^m) = 0$ implies that

$$g_{N+1}^m(\xi) = \frac{Q_{N+1}^m(\xi)}{Q_N^m(\xi)}\, g_N^m(\xi), \quad \xi \in \{\pm\nu_\alpha^m\} \text{ and } N \geqslant L. \tag{14}$$

Now if we use Eq. (7) for $l = m, m+1, \ldots, L$ and Eq. (14) for $N = L$, we find that the problem of determining the discrete eigenvalues for $\varpi \leqslant 1$ can be restated as the problem of determining those values of $\xi \in \mathscr{R}$ with magnitudes $\geqslant 1$ that satisfy the system

$$\mathbf{C}^m(\xi)\mathbf{g}^m(\xi) = \mathbf{0} \tag{15}$$

or, alternatively, $\det \mathbf{C}^m(\xi) = 0$. In Eq. (15), $\mathbf{C}^m(\xi)$ is a tridiagonal matrix of order $L + 1 - m$ given by

$$\mathbf{C}^m(\xi) = \begin{bmatrix} -\xi & \dfrac{\sqrt{2m+1}}{h_m} & & & & \\ \dfrac{\sqrt{2m+1}}{h_{m+1}} & -\xi & \dfrac{\sqrt{4m+4}}{h_{m+1}} & & & \\ & \dfrac{\sqrt{4m+4}}{h_{m+2}} & -\xi & \dfrac{\sqrt{6m+9}}{h_{m+2}} & & \\ & \ddots & & \ddots & \ddots & \\ & & & \dfrac{\sqrt{(L-1)^2-m^2}}{h_{L-1}} & -\xi & \dfrac{\sqrt{L^2-m^2}}{h_{L-1}} \\ & & & & \dfrac{\sqrt{L^2-m^2}}{h_L} & T^m(\xi) - \xi \end{bmatrix} \tag{16}$$

where

$$T^m(\xi) = \left(\frac{\sqrt{(L+1)^2 - m^2}}{h_L}\right)\left[\frac{Q_{L+1}^m(\xi)}{Q_L^m(\xi)}\right] \tag{17}$$

and $\mathbf{g}^m(\xi)$ is a vector of $L + 1 - m$ components given by

$$\mathbf{g}^m(\xi) = \begin{pmatrix} g_m^m(\xi) \\ g_{m+1}^m(\xi) \\ \vdots \\ g_L^m(\xi) \end{pmatrix}. \tag{18}$$

If we assume, for the moment, that $\varpi \neq 1$ when $m = 0$, it is clear from Eq. (8) that $h_l > 0$, $l \geqslant 0$. Consequently, the off-diagonal products of $\mathbf{C}^m(\xi)$, i.e. $C_{\alpha,\alpha+1}^m(\xi)C_{\alpha+1,\alpha}^m(\xi)$, are >0 for $\alpha = 1, 2, \ldots,$ and thus the problem formulated by Eq. (15) can be symmetrized by means of a similarity transformation with a diagonal matrix.[20] Following Wilkinson,[20] we let $S_l^m(\xi)$ denote the leading principal minor of order $l-m$ of $\mathbf{C}^m(\xi)$, define

$$S_m^m(\xi)=1, \tag{19a}$$

note that the first-order minor is

$$S_{m+1}^m(\xi)=-\xi \tag{19b}$$

and conclude that the higher-order principal minors satisfy the recursion relation

$$S_{l+1}^m(\xi)=[T^m(\xi)\delta_{l,L}-\xi]S_l^m(\xi)-\left(\frac{l-m}{h_{l-1}}\right)\left(\frac{l+m}{h_l}\right)S_{l-1}^m(\xi) \tag{19c}$$

for $l=m+1, m+2, \ldots, L$. 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 $S_m^m(\eta)$, $S_{m+1}^m(\eta), \ldots, S_{L+1}^m(\eta)$ obtained for any particular value of $\eta \geqslant 1$ is a Sturm sequence.[21] By the Sturm sequence property,[20,21] the number of sign agreements between consecutive elements of this sequence gives the number of zeros of $S_{L+1}^m(\xi)$ which are greater than η.

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

$$\lim_{\xi\to 1}\frac{Q_{L+1}^m(\xi)}{Q_L^m(\xi)}=\sqrt{\frac{L+1-m}{L+1+m}} \tag{20}$$

and thus $T^m(1)=(L+1-m)/h_L$, we compute the number of sign agreements between consecutive elements of the sequence $S_m^m(1)$, $S_{m+1}^m(1), \ldots, S_{L+1}^m(1)$, i.e. the number of zeros of $S_{L+1}^m(\xi)$ which are >1. Since these zeros are also the positive solutions (with magnitudes >1) to Eq. (15), their number gives the number of discrete eigenvalue pairs $\aleph^m$, except when $S_{L+1}^m(1)=0$ [referring to result (iv) of Sec. 1, we note that this can happen only for $m \geqslant 1$]. In this case, ± 1 are also eigenvalues and the number of discrete eigenvalue pairs $\aleph^m$ equals the number of zeros of $S_{L+1}^m(\xi)$ which are >1 plus one.

When $\varpi=1$, $h_0=0$ and the matrix $\mathbf{C}^m(\xi)$ becomes unbounded for $m=0$. Hence, the case $\varpi=1$ and $m=0$ requires special treatment. It can be shown that as $z\to\infty$ the dispersion function behaves, for $m=0$, as[22]

$$\Lambda^0(z)=\prod_{l=0}^{L}\left(\frac{h_l}{2l+1}\right)+\frac{a_2}{z^2}+\frac{a_4}{z^4}+\cdots, \tag{21}$$

where $a_2, a_4, \ldots$ are constants. It is clear from Eq. (21) that $\Lambda^0(z)$ has a double zero at infinity for $\varpi=1$. A simple modification of the above analysis makes it possible to find the number of pairs of bounded zeros of $\Lambda^0(\xi)$ for $\varpi=1$. Noting that $g_1^0(\xi)=0$ [see Eq. (7) for $l=m=0$], we can consider Eq. (7) for $l=2, 3, \ldots, L$ and Eq. (14) for $N=L$ to obtain the modified system for $\varpi=1$ and $m=0$:

$$\hat{\mathbf{C}}^0(\xi)\hat{\mathbf{g}}^0(\xi)=\mathbf{0} \tag{22}$$

where the tridiagonal $\hat{\mathbf{C}}^0(\xi)$ matrix of order $L-1$ can be obtained by neglecting the first two rows and columns of $\mathbf{C}^m(\xi)$ for $m=0$ and the vector $\hat{\mathbf{g}}^0(\xi)$ by neglecting the first two components of $\mathbf{g}^m(\xi)$ for $m=0$. Following the procedure developed with the restriction that $\varpi \neq 1$ when $m=0$, we arrive at similar conclusions for $\varpi=1$ 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 >1.

It is interesting to note that if we arbitrarily set $T^m(\xi)=0$ in the last diagonal element of the matrix $\mathbf{C}^m(\xi)$ defined by Eq. (16), we reduce the problem formulated by Eq. (15) 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. (19) only in the last element, the number of discrete eigenvalue pairs $\aleph^m$ can be easily related to γ^m, the number of zeros of $g_{L+1}^m(\xi)$ which are >1. In fact, it can be shown that for $|S_{L+1}^m(1)| \geqslant T^m(1)|S_L^m(1)|$ we must have $\aleph^m=\gamma^m$, while for $|S_{L+1}^m(1)|<T^m(1)|S_L^m(1)|$ we can have $\aleph^m=\gamma^m$ if $S_L^m(1)S_{L+1}^m(1)<0$ and $\aleph^m=\gamma^m+1$ if $S_L^m(1)S_{L+1}^m(1)\geqslant 0$.

Finally, we point out that, as was done in Ref. 10 for the Chandrasekhar polynomials [see Eq. (45) of Ref. 10], we could restate our problem in terms of the squares of the eigenvalues; however, we believe 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 $\aleph^m$, we first note that a method[5,22] based on a Wiener–Hopf factorization of the dispersion function $\Lambda^m(z)$ has provided explicit results for the discrete eigenvalues when $\aleph^m \leqslant 3$. In addition, this explicit method has, for the general case, reduced the task of finding the discrete eigenvalues to one of solving a polynomial equation of order $\aleph^m$ for the squares of the eigenvalues. Since the explicit results for $\aleph^m \leqslant 3$ 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. 10, computational difficulties that arise from ill-conditioning of the polynomial equations have been observed in this method when $\aleph^m$ 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.[10] 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 $N \to \infty$. Indeed, by letting $N \to \infty$ in Eq. (13) and considering that[23]

$$\lim_{N\to\infty} \frac{Q_N^m(z)}{P_N^m(z)} = 0, \quad z \notin [-1, 1], \tag{23}$$

we conclude from Eq. (13) that

$$\Lambda^m(z) = \lim_{N\to\infty} (1 - z^2)^{m/2} \frac{g_N^m(z)}{P_N^m(z)}, \quad z \notin [-1, 1], \tag{24}$$

and thus the zeros of $g_N^m(z)$ outside $[-1, 1]$ approach the zeros of $\Lambda^m(z)$ outside $[-1, 1]$ as $N \to \infty$. It has been found that the larger the magnitude of a discrete eigenvalue, the faster the convergence of the corresponding P_N eigenvalue as N increases; however, when any of the discrete eigenvalues happens to be only slightly greater than 1 in magnitude very large values of N may be required to find a good estimate of such an eigenvalue. Alternatively, for $\varpi \leqslant 1$, a bisection calculation based on $\Lambda^m(\xi)$ has been used[10] to find initial estimates and to refine 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,[5,22] secant[24] and *regula falsi*[25] 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. (5) has been used sometimes,[5,18,25] but there are some disadvantages in this procedure: first, as the integrand of Eq. (5) can vary rapidly, especially near the endpoints ± 1, it is necessary to use a large number of quadrature points for integration, which sacrifices 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. (5) 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. (10) and some closely related expressions in which the function $Q_l^m(z)$ has been split into two terms.[5,10]

It could be thought that Eq. (12) is a better expression from which to compute $\Lambda^m(z)$, since it is not subject to the accuracy limitations inherent in Eqs. (5) and (10). Unfortunately, there is one additional problem that affects Eq. (12) as well as Eq. (10): the lack of a method to compute $g_l^m(z)$, $l \geqslant m$, accurately for all z. As can be seen from Eq. (13), $g_N^m(z)$ is proportional to $Q_N^m(z)$ for $N \geqslant L$ when z is a discrete eigenvalue and approaches a constant times $P_N^m(z)$ as $N \to \infty$ when z is sufficiently far away from all discrete eigenvalues. Thus, following Gautschi,[26] we could use forward recursion of Eq. (7) to compute $g_N^m(z)$, $N \geqslant L$, when z is not near an eigenvalue and backward recursion when z is an eigenvalue. However, if we are planning to use Eq. (12) 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. (7) should be used to compute $g_N^m(z)$, $N \geqslant L$, accurately.

We now proceed to show, by making use of the basic property of Sturm sequences, that a bisection procedure used to find estimates for eigenvalues with magnitudes just greater than 1 and an iterative refinement of all eigenvalue estimates can be implemented without the need to compute $\Lambda^m(\xi)$. Since, as discussed in Sec. 2, the discrete eigenvalues appear in $\pm$ pairs and are real for $\varpi \leqslant 1$, 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. 10, 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. (19), hereafter denoted as the S^m sequence. In other words, suppose that the P_N method has provided ρ^m eigenvalue estimates and let $\nu_{\min}^m$ denote the smallest of these estimates. Then, the remaining $\aleph^m - \rho^m$ 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 find the eigenvalues of symmetric tridiagonal matrices and discussed in detail by Wilkinson.[20] Suppose, for example, that we wish to compute an estimate of ν_α^m, $\rho^m < \alpha \leqslant \aleph^m$, and we have found two points a_0^m and b_0^m in the interval $[1, \nu_{\min}^m)$ such that $b_0^m > a_0^m$, $s(a_0^m) \geqslant \alpha$ 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 bisection steps.

Having found the remaining $\aleph^m - \rho^m$ 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 $S_{L+1}^m(\xi)$, we have used the *regula falsi* method[27] (and also the bisection method) to refine the eigenvalue estimates.

In order to develop the required S^m sequence, it is clear that we first must be able to evaluate the function $T^m(\xi)$ defined by Eq. (17). We write

$$T^m(\xi) = (L + 1 - m)R^m(\xi)/h_L \tag{25}$$

and seek computational methods to evaluate

$$R^m(\xi) = \sqrt{\frac{L+1+m}{L+1-m}}\,\frac{Q_{L+1}^m(\xi)}{Q_L^m(\xi)}, \quad \xi \in (1, \infty). \tag{26}$$

Considering first of all $m = 0$, we have two ways of computing $R^0(\xi)$. For $\xi \in (1, 1+\epsilon)$, where $\epsilon = 10^{-6}$, we set $z = 1$ in the summation formula (No. 8.9.2 of Ref. 28)

$$(\xi - z)\sum_{l=0}^{\alpha}(2l+1)P_l^0(z)Q_l^0(\xi) = 1 - (\alpha+1)[P_{\alpha+1}^0(z)Q_\alpha^0(\xi) - P_\alpha^0(z)Q_{\alpha+1}^0(\xi)] \tag{27}$$

and use, for $\alpha = 0, 1, \ldots, L$,

$$Q_{\alpha+1}^0(\xi) = Q_\alpha^0(\xi) - \left(\frac{1}{\alpha+1}\right)\left[1 - (\xi - 1)\sum_{l=0}^{\alpha}(2l+1)Q_l^0(\xi)\right] \tag{28}$$

along with

$$Q_0^0(\xi) = -\tfrac{1}{2}\log\left(\frac{\xi-1}{\xi+1}\right) \tag{29}$$

to find $Q_{L+1}^0(\xi)$ and $Q_L^0(\xi)$ and subsequently $R^0(\xi)$. We note that since ξ can be very close to unity, which can lead to a loss of accuracy in the computation of the factor $\xi - 1$ required in Eqs. (28) and (29), we find it convenient, when ξ is close to unity, to work with the variable $v = \xi - 1$ or to introduce the change of variable[29]

$$\xi = (1 - \exp\{-u\})^{-1}. \tag{30}$$

For $\xi \in [1 + \epsilon, \infty)$ we use backward recursion to compute $R^0(\xi)$. Thus for some $M > L$ we take

$$R_M(\xi) = \xi - (\xi^2 - 1)^{1/2} \tag{31}$$

and use

$$R_{l-1}(\xi) = l[(2l + 1)\xi - (l + 1)R_l(\xi)]^{-1} \tag{32}$$

for $l = M, M - 1, \ldots, L + 1$ to find $R_L(\xi)$. We then continue to increase M and repeat this calculation until a "converged" value $R_L^*(\xi)$ is obtained. The desired $R^0(\xi)$ is then identified by

$$R^0(\xi) = R_L^*(\xi). \tag{33}$$

Having found that we could obtain accurate results for $R^0(\xi)$, for $\xi \in (1, \infty)$ and for $0 \leqslant L \leqslant 1000$, we now use

$$R^\alpha(\xi) = \frac{L + \alpha - (L + 2 - \alpha)\xi R^{\alpha-1}(\xi)}{(L + \alpha)\xi - (L + 2 - \alpha)R^{\alpha-1}(\xi)} \tag{34}$$

for $\alpha = 1, 2, \ldots, m$ to obtain accurate results for the desired $R^m(\xi)$ for $\xi \in (1, \infty)$ and $1 \leqslant m \leqslant L \leqslant 1000$.

With the established numerical scheme we are able to use Eq. (25) to compute accurately the function $T^m(\xi)$, and so we use forward recursion, as described by Eqs. (19), to compute the required S^m sequence. It is worthwhile to mention that rescaling of the S^m-sequence calculation is usually required in order to avoid computer overflows and/or underflows during the refinement procedure.

4. NUMERICAL RESULTS

For our first numerical example, we use the scattering law introduced by Kaper, Shultis, and Veninga,[25] i.e.

$$p(\cos\Theta) = \frac{L + 1}{2^L}(1 + \cos\Theta)^L. \tag{35}$$

Table 1. The discrete eigenvalues for the KSV scattering law with $L = 59$.

$\varpi = 0.8783585$	$\varpi = 0.8115228$	$\varpi = 0.5678$
	$m = 0$	
1.091745459480726	1.055547311326692	1.000000000001147
1.463295282686077	1.340299700326329	1.091606657626732
2.460935156938731	2.050242473971546	1.367969626434857
5.351091071788712	3.783165533641392	1.912001500826044
	$m = 1$	
1.013490847758943	1.002003471942856	1.019807696402705
1.219686545145295	1.153855444893048	1.196648388280417
1.808093790081362	1.597621560783307	1.584496726525516
3.406447023693270	2.667560240371443	
	$m = 2$	
1.063991418783902	1.034163066112437	1.070993547938969
1.392493860675903	1.289122731342325	1.330387524558258
2.254575164875290	1.924450984271965	
	$m = 3$	
1.140132499173532	1.092195319895360	1.143346356987104
1.604513871227998	1.456176437134108	
	$m = 4$	
1.000000026175034	1.168724042905966	1.015898762767950
1.235765701352745		
	$m = 5$	
1.027401938072136	1.000000005561480	no eigenvalues

Table 2. The discrete eigenvalues for the cloud problem with $\varpi = 0.9$ and $m = 0$–7.

$m = 0$	$m = 1$	$m = 2$	$m = 3$
1.000389979100289	1.001153598613536	1.000111776800829	1.000476262313813
1.002932994823867	1.004548762454778	1.002216338699663	1.003295330516227
1.007484963089087	1.009865191302828	1.006396066982577	1.008098291491907
1.013879322803893	1.016987048883787	1.012436444996581	1.014721894445308
1.022052177311825	1.025874128647133	1.020254938712759	1.023103645265188
1.031988750345564	1.036525274139559	1.029826348735291	1.033227041363257
1.043709272679720	1.048971958733608	1.041161172098668	1.045109719296726
1.057261138191170	1.063271075343840	1.054298263973289	1.058794335814883
1.072717289782405	1.079503001150033	1.069301606090231	1.074346472153689
1.090178937015782	1.097780112342290	1.086259626931758	1.091859250559478
1.109775208698891	1.118242151269704	1.105288824858564	1.111448795665868
1.131670715243141	1.141068171766016	1.126536145353176	1.133262344084953
1.156074203314183	1.166481794346436	1.150188383140280	1.157482707254803
1.183252816544619	1.194773475636012	1.176479806702399	1.184341215157574
1.213551335402783	1.226317705822771	1.205711096159665	1.214127701485377
1.247430064829681	1.261624532898644	1.238272832948744	1.247218584555475
1.285516474694714	1.301392202246315	1.274691173942301	1.284099624271780
1.328721070560407	1.346646675776329	1.315699457326307	1.325433468857192
1.378439970833423	1.399007123290389	1.362368011279040	1.372140566731904
1.437038878132861	1.461337568135190	1.416385802062042	1.425539866248608
1.509302317538750	1.540086796804300	1.480761361607739	1.487547015267586
1.610657591350528	1.667874854173314	1.562729929706522	1.560727536639987
1.928954632196827	2.322719076780276	1.738846142025943	
4.282156025437291			
$m = 4$	$m = 5$	$m = 6$	$m = 7$
1.001120002487698	1.002072376601313	1.000300407429449	1.001056218094408
1.004667252515722	1.006363314799746	1.003355148922561	1.004947685306367
1.010126365584779	1.012510052987392	1.008403038238131	1.010749773559181
1.017372522812000	1.020419612500233	1.015263141243658	1.018332733507215
1.026359499964445	1.030059080701874	1.023868287196465	1.027648101955439
1.037080308169892	1.041432316668291	1.034198451851715	1.038689077456266
1.049559005859420	1.054569853913821	1.046267889033079	1.051478256361556
1.063843473937723	1.069525399130740	1.060115204782976	1.066062198095320
1.080002048419502	1.086375964303158	1.075799343344211	1.082509599110173
1.098130574417887	1.105220825911842	1.093406215207598	1.100911861259278
1.118347372150153	1.126184748131046	1.113042051020104	1.121383796069256
1.140802174225208	1.149423385628787	1.134841751575295	1.144069519024719
1.165676947330458	1.175129102452172	1.158969023981941	1.169146488813592
1.193201421605236	1.203540600582527	1.185630223256390	1.196835410331759
1.223659217042547	1.234957362846441	1.215078313668894	1.227412363212996
1.257418610747223	1.269758753746089	1.247641493638252	1.261225538999248
1.294945011395361	1.308441730923118	1.283732422729304	1.298729538670090
1.336849151477048	1.351663401172887	1.323895971876093	1.340527410001363
1.383942530602099	1.400315189262372	1.368868633174685	1.387445025002331
1.437289924147840	1.455613852935010	1.419665396704684	
1.498201754606247			

This scattering law, to which we hereafter refer as the KSV scattering law, has the advantage that it can be represented exactly with $L + 1$ terms in Eq. (2). A particularly concise way of generating the coefficients of Eq. (2) in the present case is to use $\beta_0 = 1$ and the recursion relation

$$\beta_l = \left(\frac{2l + 1}{2l - 1}\right)\left(\frac{L + 1 - l}{L + 1 + l}\right)\beta_{l-1} \tag{36}$$

for $l = 1, 2, \ldots, L$. We note that the recursion relation expressed by Eq. (36) can be easily derived from a result given in Ref. 30 (see formula 7.127).

Having used the methods of Secs. 2 and 3 for the KSV scattering law with $L = 59$, we list in Table 1 the discrete eigenvalues, which we believe to be correct to within ± 1 in the last figure shown, for three selected values of ϖ.

As a second application, we consider the challenging *cloud problem* solved, for the case $m = 0$, in Ref. 10. The scattering law for this cloud problem is defined with $L = 299$, and we note that the coefficients β_l, $l = 0, 1, \ldots, L$, have been tabulated in Ref. 10. We have again used the methods of Secs. 2 and 3 to enumerate and to compute the discrete eigenvalues for all Fourier components, $m = 0, 1, 2, \ldots, L$, for the considered cloud problem with $\varpi = 0.9$ and $\varpi = 1$. The methods proved to be very stable from a computational point-of-view, and so we report in Tables 2–4 our results, thought to be correct to within ± 1 in the last figure shown, for the case $\varpi = 0.9$.

Table 3. The discrete eigenvalues for the cloud problem with $\varpi = 0.9$ and $m = 8$–15.

$m = 8$	$m = 9$	$m = 10$	$m = 11$
1.002132339938634	1.000027437419281	1.000821130664178	1.001904468706302
1.006827468095151	1.003498628696048	1.005130436297479	1.007005699783873
1.013374555759685	1.008969987530013	1.011354377580926	1.013963471619675
1.021680019126139	1.016251691377068	1.019358753922739	1.022679004654549
1.031710589137234	1.025274985023264	1.029093157255540	1.033118349080497
1.043471538560993	1.036021157966385	1.040552180860370	1.045285838805675
1.056994101877314	1.048504518930511	1.053758990625113	1.059212750695516
1.072330348885676	1.062764509772019	1.068758301705021	1.074952838405016
1.089558857271397	1.078862557853792	1.085620969786781	1.092582491112014
1.108777774656722	1.096882795156472	1.104436724126241	1.112198805921483
1.130112492270336	1.116931172420344	1.125321234400075	1.133923926373632
1.153715156260448	1.139140890730823	1.148414789289055	1.157908206952960
1.179777190959969	1.163675725704861	1.173894027262453	1.184334968752226
1.208531271816884	1.190738412454895	1.201971783068786	1.213436311180691
1.240278124846740	1.220583546220196	1.232919459682506	1.245496283338074
1.275395233415470	1.253527447558321	1.267077052447685	1.280877505592311
1.314377548778322	1.289979731733468	1.304885209189289	
1.357893362524082	1.330481527518500		
$m = 12$	$m = 13$	$m = 14$	$m = 15$
1.003247165741183	1.000163170981848	1.001185938607807	1.002447008154250
1.009107295607765	1.004826826449371	1.006626201396009	1.008631308649636
1.016782659295061	1.011421794203924	1.013936688843537	1.016641222946213
1.026198778862466	1.019800881098146	1.023006887581295	1.026393736416021
1.037336742986784	1.029909735494897	1.033800209739118	1.037865567856717
1.050210357206299	1.041740420877021	1.046319232696027	1.051067591047232
1.064856238489530	1.055314732765262	1.060591493041455	1.066036250670179
1.081337123539542	1.070678040633498	1.076671240496160	1.082830539228964
1.099733934382855	1.087898261297708	1.094630543035628	1.101529442361119
1.120152199502264	1.107063400730110	1.114565054464650	1.122231947192457
1.142719666306533	1.128284295433462	1.136590729548459	1.145063698848036
1.167597276056413	1.151699009012264	1.160851518207487	1.170174543999502
1.194979651557818	1.177472380798614	1.187525095473716	1.197750340350737
1.225108803168451	1.205812961618084	1.216826508397167	
1.258286110896357	1.236973492405995		

Table 4. The discrete eigenvalues for the cloud problem with $\varpi = 0.9$ and $m = 16$–299.

$m = 16$	$m = 17$	$m = 18$	$m = 19$
1.003927202502307	1.005611079058116	1.001035866989380	1.002382232900363
1.010832054388393	1.013217080777625	1.007487588530618	1.009545762576835
1.019527658054946	1.022588089444052	1.015778984648288	1.018510462685335
1.029953577267715	1.033680905467539	1.025815804840559	1.029206236974888
1.042098674092698	1.046493470733173	1.037569741382572	1.041615421526792
1.055980180497388	1.061052580926555	1.051046351456067	1.055754289982214
1.071643269814672	1.077407845572837	1.066281266397076	1.071662261468931
1.089150893823824	1.095629899584672	1.083328776407054	1.089400674738072
1.108588529303737	1.115807208981510	1.102263296065786	1.109049765584623
1.130062421538230	1.138051478696484	1.123181089097136	1.130708481274928
1.153700775265870	1.162500434297218	1.146198772981937	
1.179664571585585			
$m = 20$	$m = 21$	$m = 22$	$m = 23$
1.003922137544877	1.005643398874659	1.000152392824666	1.001521655119800
1.011778047031088	1.014176314628730	1.007537180433021	1.009595459245190
1.021405367357474	1.024458181553947	1.016734558774208	1.019447868801839
1.032753367949149	1.036451751987533	1.027663266316458	1.031016261411271
1.045813907514059	1.050161613106285	1.040299319293542	1.044290560048354
1.060611717856731	1.065617502431105	1.054655036972556	1.059290353515943
1.077193031597558	1.082870374720546	1.070766802715633	1.076057633575474
1.095622829448330	1.101990608801886	1.088691067289518	
1.115985258356963			
$m = 24$	$m = 25$	$m = 26$	$m = 27$
1.003065048470729	1.004772526145614	1.006638008871783	1.008653517212453
1.011811849884141	1.014179654455716	1.016693447280858	1.019348581409128
1.022308972983460	1.025314574293119	1.028460439804122	1.031742738139702
1.034512822677810	1.038149769840295	1.041923565675444	
1.048422856274098	1.052693177218516		
1.064065378214677			
$m = 28$	$m = 29$	$m = 30$	$m = 31 - 299$
1.001208097161088	1.002860337739749	1.004656331018524	no eigenvalues
1.010813196303162	1.013112023912043		
1.022140751212102			

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