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COMMENT

Computation of generalised spheroidal eigenfunctions and eigenvalues

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Abstract. Methods of solving the equation for generalised spheroidal eigenfunctions and eigenvalues are considered. An efficient variational method with Jacobi basis functions is worked out. Simple recurrence formulae are derived for analytical calculations of all matrix elements required to solve the variational problem. A fast algorithm for computing generalised spheroidal eigenvalues is proposed.

1. Introduction

Spheroidal harmonics have numerous applications in quantum mechanics, radiophysics and optics. The main results concerning the properties of these functions are contained in the monographs of Morse and Feshbach (1953), Meixner and Schäfke (1954), Flammer (1957) and Abramowitz and Stegun (1964). A good review of the classical and new results as well as applications of the spheroidal and Coulomb spheroidal harmonics are presented in a recent monograph of Komarov *et al* (1976).

In this paper we will consider generalised spheroidal (GS) eigenfunctions defined by the differential equation

$$\left(\mathscr{L}(t)+V(a,b;t)+\sum_{k=1}^{K}c_k t^k-\mathscr{E}\right)S^{(a,b)}(t)=0 \tag{1}$$

where

$$\mathscr{L}(t)\equiv(\mathrm{d}/\mathrm{d}\,t)(t^2-1)\mathrm{d}/\mathrm{d}\,t \qquad \text{and} \qquad V(a,b;t)\equiv[a^2/(1-t)+b^2/(1+t)]/2$$

$a>-1$ and $b>-1$ are real and $\{c_k\}$ are positive or negative real numbers.

This equation has singular points at $t=\pm1$ and we will search for the regular solutions which must be square integrable on the interval $-1\leqslant t\leqslant+1$. The regularity is a boundary condition which can be satisfied only for certain values of $\mathscr{E}$. The regular GS eigenfunction with n nodes will be denoted by $S_n^{(a,b)}(t)$ and the corresponding eigenvalue by $\mathscr{E}_n$.

Let us consider some important special cases of equation (1).

For $c_k=0$ and $a=b=m=0,1,\ldots$, the GS equation generates the associated Legendre polynomials $P_{n+m}^m(t)$.

For $c_2\neq0$ and $c_k=0$ for $k\neq2$, and $a=b=m$ the GS eigenfunctions become identical with spheroidal harmonics (Abramowitz and Stegun 1964).

For $c_2\neq0$, $c_1\neq0$ or $c_1=0$, and $c_k=0$ (for $k\neq1,2$), and $a=b>-1$, equation (1) defines the Coulomb spheroidal functions (Komarov *et al* 1976).

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For $c_k = 0$ and $a, b > -1$ the GS eigenfunctions take the form (Makarewicz 1988):

$$\mathscr{P}_n^{(a,b)}(t) = (1-t)^{a/2}(1+t)^{b/2}\tilde{P}_n^{(a,b)}(t) \tag{2}$$

where $\tilde{P}_n^{(a,b)}$ is the Jacobi polynomial, so the function $\mathscr{P}_n^{(a,b)}$ will be henceforth called the Jacobi function.

For $c_k \neq 0$ and $a \neq 0$ or (and) $b \neq 0$, equation (1) is known in the theory of molecular vibrational and rovibrational states (Wallace 1982, 1983, 1984, Sage 1985, Makarewicz and Pyka 1989). In this case $t = \cos\vartheta$, where ϑ is the vibrational coordinate describing the bending of molecular bonds. New applications of the GS equation in the theoretical rovibrational spectroscopy involve looking for effective methods of computation of the GS eigenfunctions and eigenvalues.

2. The variational method of solving the GS equation

Recently, the GS equation has been solved numerically by applying the Numerov method (Makarewicz and Pyka 1989). This method is efficient only if GS eigenfunctions with a small number of nodes n are required. For high n these functions quickly oscillate and the Numerov method becomes less accurate. Moreover, a large computer memory is required to store the eigenfunctions computed in a great number of grid points. The same applies to the relaxation method proposed recently for the computation of spheroidal harmonics (Caldwell 1988).

Here, we propose a variational method which is more effective, even if only a few isolated GS eigenfunctions or eigenvalues are required. The crucial point in the variational method is the choice of the basis functions into which the GS eigenfunctions can be expanded. In our problem the most convenient are Jacobi basis functions (JBF) $\mathscr{P}_n^{(\alpha,\beta)}$, mainly, due to to a simple calculation of the integrals needed for construction of the algebraic eigenvalue problem. These functions are parametrised by α and β which can be different from a and b in equation (1), respectively. $\mathscr{P}_n^{(\alpha,\beta)}$ are defined through the Jacobi polynomials (see equation (3)) which will be assumed to be *normalised* with the weight factor $\omega(t) = (1-t)^{\alpha}(1+t)^{\beta}$. This means that

$$\int_{-1}^{+1} \omega(t)\tilde{P}_n^{(\alpha,\beta)}(t)\tilde{P}_n^{(\alpha,\beta)}(t)\,\mathrm{d}t = \int_{-1}^{+1} \mathscr{P}_n^{(\alpha,\beta)}(t)\mathscr{P}_n^{(\alpha,\beta)}(t)\,\mathrm{d}t = 1.$$

The normalised $\tilde{P}_n^{(\alpha,\beta)}$ can be expressed by the *standard* Jacobi polynomials (Abramowitz and Stegun 1964) according to

$$\tilde{P}_n^{(\alpha,\beta)}(t) = \{2^{-\lambda}n!(2n+\lambda)\Gamma(n+\lambda)/[\Gamma(n+\alpha+1)\Gamma(n+\beta+1)]\}^{1/2}P_n^{(\alpha,\beta)}(t) \tag{3}$$

where $\lambda \equiv \alpha + \beta + 1$.

The GS eigenfunctions can be expanded into a series of the Jacobi functions:

$$S_n^{(a,b)}(t) = \sum_{i=0}^{N} a_i \mathscr{P}_i^{(\alpha,\beta)}(t) \tag{4}$$

and the coefficients a_i can be determined by applying the Rayleigh-Ritz variational method, from a set of algebraic secular equations:

$$(\mathbf{H} - \mathscr{E}\mathbf{1})\boldsymbol{a} = 0 \tag{5}$$

where

$$\mathbf{H} \equiv \mathbf{L} + (a^2 - \alpha^2)\mathbf{M}_{-1} + (b^2 - \beta^2)\mathbf{M}_{+1} + \sum_{k=1}^{K} c_k \mathbf{T}_k. \tag{6}$$

The matrix elements in equation (6) are defined as follows:

$$\begin{aligned} L(n, m) &\equiv \langle n\ (\mathscr{L} + V)\ m \rangle \qquad & T_k(n, m) &\equiv \langle n\ t^k\ m \rangle \\ M_s(n, m) &\equiv \tfrac{1}{2}\langle n\ (1 + st)^{-1}\ m \rangle \qquad & s &= \pm 1. \end{aligned} \tag{7}$$

The abbreviation $\langle n\, X\, m \rangle$ for an arbitrary operator $X(t)$ means

$$\langle nXm \rangle \equiv \int_{-1}^{+1} \mathscr{P}_n^{(\alpha,\beta)}(t) X(t) \mathscr{P}_m^{(\alpha,\beta)}(t)\, \mathrm{d}t.$$

Since the JBF fulfil

$$[\mathscr{L}(t) + V(\alpha, \beta; t) - \varepsilon_n(\alpha, \beta)]\mathscr{P}_n^{(\alpha,\beta)}(t) = 0 \tag{8}$$

where

$$\varepsilon_n(\alpha, \beta) = \nu(\nu + 1) \qquad \nu \equiv n + (\alpha + \beta)/2 \tag{9}$$

the integrals $L(n, m)$ can be immediately written as

$$L(n, m) = \varepsilon_n(\alpha, \beta)\delta_{n,m}.$$

The analytic recurrence formulae for the elements $T_k(n, m)$ and $M_s(n, m)$ are derived in appendix 1.

The solution of the eigenvalue problem (5) can be simplified by the appropriate choice of non-linear parameters α and β specifying the JBF. Let us first consider the case when the coefficients c_k in (1) are small. Then the operator $\mathscr{L}(t) + V(a, b; t)$ plays a dominant role in equation (1). Hence, $\mathscr{P}_n^{(a,b)}$ will be a good approximation of the eigenfunction $S_n^{(a,b)}$. This means that for small c_k the choice $\alpha = a$ and $\beta = b$ is reasonable.

It is important to notice that for $\alpha = a$ and $\beta = b$ the matrix $\mathbf{H}$ is simplified into $\mathbf{L} + \Sigma_k \mathbf{T}_k$ which has a banded structure because the elements $T_k(n, m)$ vanish if $m > n + k$ (see appendix 1). Thus in order to determine the eigenvalues $\mathscr{E}$ and eigenvectors $\boldsymbol{a}$ we must diagonalise the symmetric band matrix. For such matrices very effective algorithms (a tridiagonalisation or QR algorithm (Wilkinson and Reinsch 1971)) are available.

If the eigenvalues are required alone, they can also be found as zeros of the determinant $\det(\mathbf{H} - \mathscr{E}\mathbf{1})$. In appendix 2 we propose a fast algorithm based on the recursive computation of the determinant of the band matrix. This algorithm is preferable if an isolated eigenvalue corresponding to a GS eigenfunction with a given number of nodes must be determined.

When the c_k are large then the expansion of the eigenfunctions $S_n^{(a,b)}$ into the series of $\mathscr{P}_i^{(a,b)}$ is slowly convergent, so the dimension of the diagonalised matrix $\mathbf{H}$ is large. In this case it is better to optimise α and β to achieve the fast convergence of expansion (4). Such an optimisation can be performed in a very simple way, as will be shown in the next section.

3. Applications

The proposed JBF are universal, i.e. they can be applied in the whole range of the parameters a, b and c_k. In order to confirm this fact let us solve the usual spheroidal equation ($a = b = m$) for large values of $c_2 \neq 0$. In the standard method of computing the spheroidal harmonics the associated Legendre polynomials are used as basis functions. Let us note that they make a special case of the JBF, namely: $P_{n+m}^{m}(t) = \mathscr{P}_n^{(m,m)}(t)$. Thus, it is clear that the expansion of the spheroidal harmonics into these functions is ineffective for large c_2.

To find more appropriate basis functions, let us optimise the parameters α and β. For this purpose let us calculate the approximate eigenvalue $\tilde{\mathscr{E}}_n$ by using only one JBF. Since in the considered case $a = b$ then $\alpha = \beta$ and we obtain

$$\tilde{\mathscr{E}}_n(\alpha) = \varepsilon_n(\alpha) + 2(m^2 - \alpha^2) M_{-1}(n, n) + c_2 T_2(n, n) \tag{10}$$

where $M_{-1}(n, n)$ is defined in (A1.4) and $T_2(n, n)$ is given by

$$T_2(n, n) = [B_n^{(\alpha,\alpha)}]^2 + [B_{n+1}^{(\alpha,\alpha)}]^2$$

(see (A1.2) and (A1.3)). Taking into account that for large c_2, $\alpha \gg 1$, we obtain an approximate expression for $T_2(n, n)$:

$$T_2(n, n) \simeq T_2(\alpha) \equiv (n + \tfrac{1}{2})/\alpha + M(n)/4\alpha^2 \tag{11}$$

where

$$M(n) \equiv 3[1 + n^2/(n + \tfrac{1}{2})].$$

This leads to

$$\tilde{\mathscr{E}}_n(\alpha) \simeq (\alpha + n)(\alpha + n + 1) + (m^2 - \alpha^2)(n + \alpha + \tfrac{1}{2})/\alpha + c_2 T_2(\alpha).$$

From the condition $\mathrm{d}\tilde{\mathscr{E}}_n(\alpha)/\mathrm{d}\alpha = 0$ we determine the optimum value of α:

$$\alpha_0 \simeq c(1 - M(n)/c)^{1/2} \qquad c \equiv c_2^{1/2}. \tag{12}$$

For the ground state ($n = 0$) $\tilde{\mathscr{E}}_0(\alpha_0)$ is the best variational estimate of the exact eigenvalue $\mathscr{E}_0$. For higher states ($n \neq 0$) the variational principle is not valid because we use only one basis function which, in general, is not orthogonal to exact eigenfunctions of the lower states. However, the $\mathscr{E}_n(\alpha_0)$ are close to the exact eigenvalues $\mathscr{E}_n$.

In table 1 we present the eigenvalues of the spheroidal harmonics calculated for large c_2, by applying the JBF with α_0 determined from equation (12). We can see that for only one basis function the eigenvalues $\tilde{\mathscr{E}}(\alpha_0)$ calculated according to equation (10) are charged with a small error $\Delta\mathscr{E}_n$ of the order of 10^{-4} (or lower) for $c_2 = 10\,000$ and of 10^{-3} for $c_2 = 2500$. For the lowest states, ten basis functions give $\Delta\mathscr{E}_n \simeq 10^{-9}$ for $c_2 = 10\,000$ and $\Delta\mathscr{E}_n \simeq 10^{-7}$-$10^{-9}$ for $c_2 = 2500$. We proved that such accurate eigenvalues can be calculated with the Legendre basis of dimension $N \simeq 50$ for $c_2 = 10\,000$ and $N \simeq 35$ for $c_2 = 2500$. Thus, for large c_2, the computations of the spheroidal eigenfunctions and eigenvalues with the use of the JBF are several times faster than those using the standard Legendre basis functions. Naturally, the same refers to a more general case when other parameters c_k are large.

In order to illustrate the usefulness of the JBF for solving the GS equation, let us consider an example from the field of molecular spectroscopy. The Schrödinger equation for the wavefunctions describing a bending vibration in a triatomic molecule has a form of equation (1) and the quantum energy of this vibration is equal to

Table 1. Eigenvalues $[\mathscr{E}_{nm} - m(m+1)]/c$ of the spheroidal equation calculated by using the JBF with $\alpha = \alpha_0$ determined from (12). N is the dimension of the basis.

m	n	$N=1$	$N=5$	$N=10$	$N=15$
$c_2 = 2500$					
0	0	0.985 0	0.984 923 6	0.984 923 051	0.984 923 051
	1	2.965 0	2.964 615	2.964 611 20	2.964 611 166
	2	4.924 0	4.925 0	4.923 821 0	4.923 820 871
2	0	0.945 8	0.945 748 3	0.945 747 766	0.945 747 766
	1	2.927 5	2.927 142	2.927 138 107	2.927 138 078
	2	4.888 4	4.889 3	4.888 161	4.888 160 894
$c_2 = 10\,000$					
0	0	0.992 50	0.992 481 05	0.992 481 011	0.992 481 011
	1	2.982 50	2.982 404 8	2.982 404 567	2.982 404 567
	2	4.962 3	4.962 5	4.962 212 214	4.962 212 212
2	0	0.972 70	0.972 684 09	0.972 684 055	0.972 684 055
	1	2.963 11	2.963 020 3	2.963 019 987	2.963 019 987
	2	4.943 3	4.943 5	4.943 252 890	4.943 252 888

$E_n = B_e \mathscr{E}_n$, where $1/B_e$ is a moment of inertia characterising the bending motion (Makarewicz 1988, equations (4)-(9)). A typical potential energy function for this motion can be assumed to have the following general form:

$$U(t) = B_e \left\{ a^2/[2(1-t)] + b^2/[2(1+t)] + \sum_k c_k t^k \right\} \qquad t = \cos\vartheta. \tag{13}$$

In table 2 we present the calculated vibrational transition energies of the H_2O^+ molecule for which we assumed the potential energy function with four non-zero parameters: a^2, c_1, c_2 and c_3 ($b^2 = 0$ since the equilibrium configuration of H_2O^+ is linear). The values of these parameters have been determined by fitting the calculated transition energies to the observed ones.

We can see that the obtained results have a similar quality as those of Jungen *et al* (1980) who used a different vibrational coordinate and, consequently, a different form of the potential function adapted to linear molecules. Our potential function (13) is more general and can describe linear as well as non-linear molecules.

Table 2. Comparison of the observed and calculated transition energies $\Delta E_v \equiv E_{v+1} - E_v$ (in cm^{-1}) for the bending vibration of the H_2O^+ molecule. The values of the potential parameters (see equation (13)) are: $a^2 = 1572$, $c_1 = 108.7$, $c_2 = -256.6$ and $c_3 = -200.1$. The parameter $B_e = 33.655\ cm^{-1}$.

v	ΔE_v(obs) (Lew 1976)	ΔE_v(calc) (Jungen *et al* 1980)	ΔE_v(calc) (this work)
0	—	0.0	0.0
1	—	1682.2	1650.7
2	—	1808.4	1797.6
3	1893.7	1896.3	1893.5
4	1960.6	1961.7	1961.5
5	2009.6	2012.0	2012.1
6	2056.2	2051.4	2051.7
7	2082.0	2082.4	2084.5

To compute the GS eigenvalues we applied the JBF with $\alpha = a$, because the c_k are much smaller than a^2 (see table 2). Hence, the resulting matrix **H** had a banded structure and its eigenvalues were determined by the method presented in appendix 2. Only 15 basis functions $\mathscr{P}_i^{(a,0)}$ were sufficient to obtain the energy levels E_n with an accuracy of at least $10^{-4}\,\mathrm{cm}^{-1}$.

4. Summary

In this comment we have presented a generalisation of the spheroidal equation which is very important because of its applications in the theory of molecular vibrations.

A variational method of solving this equation was proposed. As the basis functions the JBF were chosen since they are very flexible and can be used in the whole range of the parameters specifying the GS equation. Fast algorithms needed for efficient computing of the GS eigenvalues were worked out. The usefulness and advantages of the presented method in the theory of molecular vibrations are illustrated.

Appendix 1

In order to calculate the matrix elements $T_k(n, m) \equiv \langle n t^k m\rangle$ we will use the recurrence relation for the normalised Jacobi polynomials which can be easily derived from an analogous relation for the standard Jacobi polynomials (Abramowitz and Stegun 1964):

$$B_{n+1}^{(\alpha,\beta)}\tilde{P}_{n+1}^{(\alpha,\beta)}(t) = [t - A_n^{(\alpha,\beta)}]\tilde{P}_n^{(\alpha,\beta)}(t) - B_n^{(\alpha,\beta)}\tilde{P}_{n-1}^{(\alpha,\beta)}(t) \tag{A1.1}$$

where

$$A_n^{(\alpha,\beta)} = (\beta^2 - \alpha^2)[(2n+\lambda)^2 - 1]^{-1} \qquad \lambda \equiv \alpha + \beta + 1$$

and

$$B_n^{(\alpha,\beta)} = 2\{n(n+\alpha)(n+\beta)(n+\lambda-1)/[(2n+\lambda-1)^2(2n+\lambda-2)(2n+\lambda)]\}^{1/2}.$$

Now, by multiplying both sides of equation (A1.1) by $\omega(t)\tilde{P}_m^{(\alpha,\beta)}(t)$ and integrating them over t, we obtain

$$\begin{aligned} &\langle n\, t\, n\rangle = A_n^{(\alpha,\beta)} \\ &\langle n\, t\, (n+1)\rangle = B_{n+1}^{(\alpha,\beta)} \\ &\langle n\, t\, (n+i)\rangle = 0 \qquad \text{for } i > 1. \end{aligned} \tag{A1.2}$$

The Jacobi functions $\mathscr{P}_n^{(\alpha,\beta)}$ form a complete set; hence for two arbitrary operators $X(t)$ and $Y(t)$ the equality

$$\langle n\, X(t)\, Y(t)\, m\rangle = \sum_p \langle n\, X(t)\, p\rangle\langle p\, Y(t)\, m\rangle$$

is satisfied, and using it for $X(t) = t$ and $Y(t) = t^k$ we obtain the following recurrence relation:

$$\begin{aligned} \langle n\, t^{k+1}\, (n+i)\rangle = {} & \langle n\, t\, (n-1)\rangle\langle (n-1)\, t^k\, (n+i)\rangle \\ & + \langle n\, t\, n\rangle\langle n\, t^k\, (n+i)\rangle + \langle n\, t\, (n+1)\rangle\langle (n+1)\, t^k\, (n+i)\rangle. \end{aligned} \tag{A1.3}$$

It can easily be proved that for $i > k$ the element $\langle n\, t^k\, (n+i)\rangle = 0$. Thus, for a given k we have $k+1$ equations of the form of (A1.3). Let us write these equations for $k = 1$:

$$\begin{pmatrix} \langle n\, t^2\, n\rangle \\ \langle n\, t^2\, (n+1)\rangle \\ \langle n\, t^2\, (n+2)\rangle \end{pmatrix} = \begin{pmatrix} \langle n\, t\, (n-1)\rangle & \langle n\, t\, n\rangle & \langle n\, t\, (n+1)\rangle \\ 0 & \langle n\, t\, (n+1)\rangle & \langle (n+1)\, t\, (n+1)\rangle \\ 0 & 0 & \langle (n+1)\, t\, (n+2)\rangle \end{pmatrix} \begin{pmatrix} \langle n\, t\, (n-1)\rangle \\ \langle n\, t\, n\rangle \\ \langle n\, t\, (n+1)\rangle \end{pmatrix}.$$

All elements occurring on the right-hand side of the above equation can be expressed by $A_m^{(\alpha,\beta)}$ and $B_m^{(\alpha,\beta)}$ with $m = n$, $n+1$ and $n+2$. Now, knowing $\langle n\, t^2\, m\rangle$ we can calculate $\langle n\, t^3\, m\rangle$, etc. In this way we can determine successively all elements for an arbitrary value of k.

In order to calculate the integrals $M_s(n, m)$ (see equation (7)) for $s = \pm 1$ let us consider equation (8). Since $\varepsilon_n(\alpha, \beta)$ is an eigenvalue corresponding to $\mathscr{P}_n^{(\alpha,\beta)}$ the relations

$$\partial\varepsilon_n(\alpha, \beta)/\partial\alpha = \partial\langle n\, (\mathscr{L} + V)\, n\rangle/\partial\alpha = \alpha < n\, (1-t)^{-1}\, n\rangle$$

and

$$\partial\varepsilon_n(\alpha, \beta)/\partial\beta = \partial\langle n\, (\mathscr{L} + V)\, n\rangle/\partial\beta = \beta\langle n\, (1+t)^{-1}\, n\rangle$$

hold. Thus, taking into account equation (9), we have

$$M_{-1}(n, n) = (2\nu+1)/(4\alpha) \qquad \text{and} \qquad M_{+1}(n, n) = (2\nu+1)/(4\beta). \tag{A1.4}$$

The non-diagonal elements $M_s(n, m)$ can be calculated by applying the Cristoffel-Darboux relation (Abramowitz and Stegun 1964) which for the normalised Jacobi polynomials has the form

$$\sum_k^n \tilde{P}_k^{(\alpha,\beta)}(t)\tilde{P}_k^{(\alpha,\beta)}(s) = B_{n+1}^{(\alpha,\beta)}(t-s)^{-1}[\tilde{P}_{n+1}^{(\alpha,\beta)}(t)\tilde{P}_n^{(\alpha,\beta)}(s) - \tilde{P}_n^{(\alpha,\beta)}(t)\tilde{P}_{n+1}^{(\alpha,\beta)}(s)]. \tag{A1.5}$$

Let us multiply both sides of equation (A1.5) by $\omega(t)\tilde{P}_m^{(\alpha,\beta)}(t)$ and integrate them over the variable t. We obtain

$$-sB_{n+1}^{(\alpha,\beta)}[M_s(m, n+1)\tilde{P}_n^{(\alpha,\beta)}(s) - M_s(m, n)\tilde{P}_{n+1}^{(\alpha,\beta)}(s)] = \begin{cases} \tilde{P}_m^{(\alpha,\beta)} & \text{for } m \leqslant n \\ 0 & \text{for } m > n. \end{cases}$$

This equation, for $m > n$, gives

$$M_s(m, n+1) = -sM_s(m, n)R_n^{(\alpha,\beta)}(s) \tag{A1.6}$$

where

$$R_n^{(\alpha,\beta)}(s) \equiv \tilde{P}_{n+1}^{(\alpha,\beta)}(s)/\tilde{P}_n^{(\alpha,\beta)}(s).$$

Taking the values of the Jacobi polynomials at the point $s = \mp 1$ we obtain

$$R_n^{(\alpha,\beta)}(-1) = \{(2n+\lambda+2)(n+\lambda)(n+\alpha+1)/[(2n+\lambda)(n+1)(n+\beta+1)]\}^{1/2} \tag{A1.7}$$

and

$$R_n^{(\alpha,\beta)}(+1) = -[(n+\beta+1)/(n+\alpha+1)]R_n^{(\alpha,\beta)}(-1).$$

Finally, in order to reach the numerically stable recursion we rewrite (A1.6) to the following form:

$$M_s(n, n-k) = -sM_s(n, n+1-k)/R_n^{(\alpha,\beta)}(s). \tag{A1.8}$$

From this relation we can generate all non-diagonal elements by substituting $k = 1, 2, \ldots, n$ into (A1.8).

Appendix 2

The eigenvalues of a symmetric band matrix, for example, a heptadiagonal matrix:

$$\mathbf{H} = \begin{bmatrix} A_1 & B_2 & C_3 & D_4 & 0 & 0 & \dots & 0 \\ B_2 & A_2 & B_3 & C_4 & D_5 & 0 & \dots & 0 \\ C_3 & B_3 & A_3 & B_4 & C_5 & D_6 & \dots & 0 \\ \vdots & & & & & & & \\ 0 & & & 0 & D_N & C_N & B_N & A_N \end{bmatrix}$$

can be calculated as zeros of the determinant $\Delta(\mathscr{E}) = \det(\mathbf{H} - \mathscr{E}\mathbf{1})$. The standard method of finding the zeros of $\Delta(\mathscr{E})$ of a tridiagonal matrix is based on a bisection algorithm (Wilkinson and Reinsch 1971). In this algorithm a sequence of leading principal minors $\Delta_k(\mathscr{E}')(k = 1, 2, \dots, N)$ for a trial value $\mathscr{E}'$ must be computed. However, the method in which the values of $W_k(\mathscr{E}') \equiv \Delta_k(\mathscr{E}')/\Delta_{k-1}(\mathscr{E}')$ are computed is simpler and stable numerically. For a tridiagonal matrix, the W_k are generated from the recursion which is started from

$$W_1 = \tilde{A}_1$$

and then is continued from $k = 1$ to $N - 1$:

$$W_{k+1} = \tilde{A}_{k+1} - B_{k+1}^2 / W_k \qquad \text{where} \qquad \tilde{A}_k \equiv A_k - \mathscr{E}'.$$

For band matrices wider than tridiagonal the bisection algorithm can be efficiently applied if W_k can be computed recursively. For a pentadiagonal matrix we derived such a recursion which is started from

$$W_0 = \infty$$

$$W_1 = \tilde{A}_1 \qquad Z_1 = B_2/\tilde{A}_1$$

$$W_2 = \tilde{A}_2 - B_2 Z_1$$

and then is continued from $k = 1$ to $N - 2$:

$$X_k = (\tilde{A}_{k+1} - C_{k+1}^2/W_{k-1})/W_k$$

$$Y_{k+1} = (B_{k+2}Z_k - C_{k+2}X_k)/W_{k+1}$$

$$Z_{k+1} = (B_{k+2} - C_{k+2}Z_k)/W_{k+1}$$

$$W_{k+2} = \tilde{A}_{k+2} - B_{k+2}Z_{k+1} + C_{k+2}Y_{k+1}.$$

For a heptadiagonal matrix the recursion is started from

$$W_{-1} = \infty$$

$$W_0 = \infty \qquad Z_0 = 1 \qquad V_0 = \tilde{A}_1 \qquad R_0 = 1 \qquad P_0 = B_2$$

$$W_1 = \tilde{A}_1 \qquad Z_1 = B_2/\tilde{A}_1 \qquad V_1 = \tilde{A}_2/\tilde{A}_1$$

$$W_2 = \tilde{A}_2 - B_2 Z_1 \qquad Z_2 = (B_3 - C_3 Z_1)/W_2 \qquad Y_2 = (B_3 Z_1 - C_3 V_1)/W_2$$

$$W_3 = \tilde{A}_3 - B_3 Z_2 + C_3 Y_2$$

and then is continued from $k=1$ to $N-3$:

$$L_{k-1}=(\tilde{A}_{k+1}-D_{k+1}^2/W_{k-2})/W_{k-1}$$

$$M_k=(B_{k+2}R_{k-1}-D_{k+2}L_{k-1})/W_k$$

$$N_k=(B_{k+2}Z_{k-1}-D_{k+2}P_{k-1})/W_k$$

$$P_k=(B_{k+2}-D_{k+2}R_{k-1})/W_k$$

$$Q_k=(C_{k+2}Z_{k-1}-D_{k+2}V_{k-1})/W_k$$

$$R_k=(C_{k+2}-D_{k+2}Z_{k-1})/W_k$$

$$S_{k+1}=(\tilde{A}_{k+2}Z_k-C_{k+2}P_k+D_{k+2}N_k)/W_{k+1}$$

$$T_{k+1}(\tilde{A}_{k+2}V_k-B_{k+2}P_k+D_{k+2}M_k)/W_{k+1}$$

$$V_{k+1}=(\tilde{A}_{k+2}-C_{k+2}R_k+D_{k+2}Q_k)/W_{k+1}$$

$$X_{k+2}=(B_{k+3}Y_{k+1}-C_{k+3}S_{k+1}+D_{k+3}T_{k+1})/W_{k+2}$$

$$Y_{k+2}=(B_{k+3}Z_{k+1}-C_{k+3}V_{k+1}+D_{k+3}S_{k+1})/W_{k+2}$$

$$Z_{k+2}=(B_{k+3}-C_{k+3}Z_{k+1}+D_{k+3}Y_{k+1})/W_{k+2}$$

$$W_{k+3}=\tilde{A}_{k+3}-B_{k+3}Z_{k+2}+C_{k+3}Y_{k+2}-D_{k+3}X_{k+2}.$$

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