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NUMERICAL COMPUTATION OF THE EIGENVALUES FOR THE SPHEROIDAL WAVE EQUATION WITH ACCURATE ERROR ESTIMATION BY MATRIX METHOD*

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Abstract. A method to compute the eigenvalues of the spheroidal wave equations is proposed, as an application of a theorem on eigenvalues of certain classes of infinite matrices. The computation of its inverse problem (namely, solving another parameter c^2 for given eigenvalue λ) is likewise given. As a result, precise and explicit error estimates are obtained for the approximated eigenvalues.

Key words. spheroidal wave equation, eigenvalue, numerical computation, error estimate, infinite symmetric tridiagonal matrix

AMS subject classifications. 34L16

1. Introduction. The spheroidal wave equation

$$\frac{\mathrm{d}}{\mathrm{d}z}\left\{(1-z^2)\frac{\mathrm{d}w}{\mathrm{d}z}\right\}+\left(\lambda_{mn}-c^2z^2-\frac{m^2}{1-z^2}\right)w=0, \tag{1.1}$$

with m an integer and c real, is obtained when the Helmholtz equation is expressed in prolate spheroidal coordinates followed by separation of variables. In the oblate (spheroidal coordinates) case, c^2 is replaced by $(-c^2)$ in (1.1). In this paper, we assume $m \geq 0$ and the prolate case ($m < 0$ or the oblate case may be dealt with likewise). The eigenvalue problem of the spheroidal wave equation is to find λ_{mn} such that $w(z)$, the solution of (1.1), is regular in $[-1, 1]$. We call λ_{mn} an *eigenvalue* and $w(z)$ a *spheroidal wave function* denoted by $pe_n^m(z)$. As will be stated later, λ_{mn} is real. Eigenvalues sorted in an increasing order correspond to having $n = m, n = m + 1, \ldots$.

The spheroidal wave functions occur in the solution of equations involving separation of variables in spheroidal coordinates. The solution of the spheroidal wave equation plays a significant role in the study of light scattering problem in optics, atomic and molecular physics, and the like. Although there is abundant literature on this function, there are far fewer publications on the eigenvalues of the differential equation. The paper [4] applies an asymptotic iteration method to calculate the angular spheroidal eigenvalues, whereas [7] discusses different methods for the solution of the differential equation depending on the value of the parameter c^2.

In the present paper we propose a matrix method for determining the eigenvalues, which applies for all values of c^2, and we furthermore obtain an accurate estimate of the error of our approximation. In addition, our method also enables the solution of an inverse problem, i.e., the determination of c^2 corresponding to a given eigenvalue.

The expansion of $pe_n^m(z)$ by the associate Legendre functions gives

$$pe_n^m(z)=\sum_{k=0}^{\infty}A_{n,2k+s}^m\cdot P_{m+2k+s}^m(z), \tag{1.2}$$

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$$s = \mathrm{mod}(n-m, 2),$$

where $P^m_{m+2k+s}(z)$ is the associate Legendre function and $\mathrm{mod}(i,j)$ is the remainder when i is divided by j. $P^m_n(z)$ is of the form

$$P^m_n(z) = (1-z^2)^{m/2}\frac{\mathrm{d}^m P_n(z)}{\mathrm{d}z^m} \qquad (P_n(z): \text{ Legendre polynomial})$$

with orthogonality over [-1,1],

$$\int_{-1}^{1} P^m_l(z)P^m_k(z)\mathrm{d}z = 0 \ (l \neq k),$$
$$\int_{-1}^{1} \{P^m_n(z)\}^2\mathrm{d}z = \frac{2}{2n+1}\cdot\frac{(n+m)!}{(n-m)!}.$$

It is known that the substitution of (1.2) into (1.1) gives the following three-term recurrence relations [1, Chap 21, formula 21.7.3]. For convenience, let $A^m_{n,k}$ and λ_{mn} be simply rewritten as A_k and λ, respectively, in the sequel.

When $n-m$ is even

$$\begin{gathered}\beta_0 A_0 + \alpha_0 A_2 = \lambda A_0,\\ \gamma_{2k}A_{2k-2} + \beta_{2k}A_{2k} + \alpha_{2k}A_{2k+2} = \lambda A_{2k} \ (k=1,2,\ldots).\end{gathered} \tag{1.3}$$

When $n-m$ is odd

$$\begin{gathered}\beta_1 A_1 + \alpha_1 A_3 = \lambda A_1,\\ \gamma_{2k+1}A_{2k-1} + \beta_{2k+1}A_{2k+1} + \alpha_{2k+1}A_{2k+3} = \lambda A_{2k+1} \ (k=1,2,\ldots).\end{gathered}$$

The symbols α_k, β_k, and γ_k in the equations represent

$$\begin{aligned}\alpha_k &= \frac{(2m+k+2)(2m+k+1)}{(2m+2k+3)(2m+2k+5)}c^2 \sim \frac{c^2}{4} \ (k\to\infty),\\ \beta_k &= (m+k)(m+k+1) + \frac{2(m+k)(m+k+1)-2m^2-1}{(2m+2k-1)(2m+2k+3)}c^2\\ &\sim k^2 \ (k\to\infty), \text{ and}\\ \gamma_k &= \frac{k(k-1)}{(2m+2k-3)(2m+2k-1)}c^2 \sim \frac{c^2}{4} \ (k\to\infty),\end{aligned} \tag{1.4}$$

for $k = 0, 1, 2, \ldots$. Since the two cases are treated in the same way, only the former case will be discussed in this paper.

2. Behavior of expansion coefficients. In this section, we discuss the behavior of $\{A_{2k}\}$ $(k = 0, 1, 2, \ldots)$ of (1.3).

First, let us begin with the next inequality:

$$\sum_{k=0}^{\infty} A^2_{2k}\cdot K(m,2k) < \infty, \text{ where } K(m,a) = \frac{2}{2m+2a+1}\cdot\frac{(2m+a)!}{a!}. \tag{2.1}$$

This is easily shown as

$$\begin{aligned}\int_{-1}^{1}\{pe^m_n(z)\}^2\mathrm{d}z &= \int_{-1}^{1}\sum_{k=0}^{\infty}A^2_{2k}\{P^m_{m+2k}(z)\}^2\mathrm{d}z\\ &= \sum_{k=0}^{\infty}A^2_{2k}\cdot\frac{2}{2m+4k+1}\cdot\frac{(2m+2k)!}{(2k)!} < \infty.\end{aligned}$$

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Next, consider the recurrence relations with the same coefficients as (1.3), or

$$\begin{aligned} \beta_0 h_1 + \alpha_0 h_2 &= \lambda h_1, \\ \gamma_{2k} h_{k-1} + \beta_{2k} h_k + \alpha_{2k} h_{k+1} &= \lambda h_k \;\; (k = 2, 3, 4, \ldots). \end{aligned} \tag{2.2}$$

By [6, Theorem 2.3, case(a)], the existence of two independent solutions of (2.2) (say, $\{h_{k,1}\}, \{h_{k,2}\}$) is guaranteed with the behaviors

$$\frac{h_{k+1,1}}{h_{k,1}} = -\frac{16k^2}{c^2}[1 + o(1)], \; \frac{h_{k+1,2}}{h_{k,2}} = -\frac{c^2}{16k^2}[1 + o(1)] \to 0 \; (k \to \infty).$$

From (2.1), it is obvious that $\{A_{2k}\}$ $(k = 0, 1, 2, \ldots)$ shows the same behavior as $\{h_{k,2}\}$, the minimal solution of (2.2). Thus,

$$\frac{A_{2k+2}}{A_{2k}} = -\frac{c^2}{16k^2}[1 + o(1)] \; (k \to \infty). \tag{2.3}$$

3. (Ordinary) eigenvalue problem. In this section, a computation of eigenvalues is shown, along with its error estimate.

In 1995, the following theorem was proved by Ikebe et al.:
[9, Theorem 1] Given a non-compact complex symmetric tridiagonal matrix

$$T = \begin{bmatrix} d_1 & f_2 & & 0 \\ f_2 & d_2 & f_3 & \\ & f_3 & d_3 & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix} : D(T) \to \ell^2,$$

where $0 < |d_k| \to \infty$ $(k \to \infty)$, $0 < |f_k| <$ const $(k = 2, 3, \ldots)$, $D(T) = \{[u^{(1)}, u^{(2)}, \ldots]^T : [d_1 u^{(1)}, d_2 u^{(2)}, \ldots]^T \in \ell^2\}$. Let T have a simple eigenvalue $\lambda \neq 0$, and $0 \neq \chi = [\chi^{(1)}, \chi^{(2)}, \ldots]^T$ be an eigenvector corresponding to λ, and assume the existence of T^{-1}. Then

(i) Letting T_k $(k = 1, 2, \ldots)$ denote the k-th order principal submatrix of T, there is a sequence $\{\lambda_k\}$ of eigenvalues of T_k which converges to λ.

(ii) Letting $\chi^T \chi \neq 0$ and $f_{k+1}\chi^{(k+1)}/\chi^{(k)} \to 0$ $(k \to \infty)$, we have the following error estimate:

$$\lambda - \lambda_k = \frac{f_{k+1}\chi^{(k)}\chi^{(k+1)}}{\chi^T \chi}[1 + o(1)] \quad (k \to \infty).$$

In this theorem, ℓ^2 is the complex Hilbert space $\ell^2 \equiv \{[s_1, s_2, \ldots]^T : s_1, s_2, \ldots \in C, \sum_{i=1}^{\infty} |s_i|^2 < \infty\}$, $o(1)$ is a quantity converging to zero as $k \to \infty$, and T^{-1} exists if $z = 0$ is the only solution of $Tz = 0$. Also, an eigenvalue λ is said to be *simple* if and only if its corresponding eigenvector is unique (up to scalar multiplication) and also there are no corresponding generalized eigenvectors of rank 2. These definitions are retained throughout this paper.

This theorem is applicable to the computation of eigenvalues of the spheroidal wave equation.

THEOREM 3.1. *Given m and $c \neq 0$, $\lambda \neq 0$ is an eigenvalue of (1.1) if and only if λ is an eigenvalue of an infinite symmetric tridiagonal matrix T acting as a linear transformation from X into ℓ^2 defined below:*

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$$T = \begin{bmatrix} \beta_0 & \sqrt{\alpha_0}\sqrt{\gamma_2} & & 0 \\ \sqrt{\alpha_0}\sqrt{\gamma_2} & \beta_2 & \sqrt{\alpha_2}\sqrt{\gamma_4} & \\ & \sqrt{\alpha_2}\sqrt{\gamma_4} & \beta_4 & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}, \tag{3.1}$$

where $X = \{w \in \ell^2 : \mathrm{diag}[\beta_0, \beta_2, \ldots]w \in \ell^2\} \subset \ell^2$.

Moreover, if one lets an eigenvector of T *corresponding to* λ *be* $0 \neq y \equiv [y^{(1)}, y^{(2)}, \ldots]^T \in X$*, or*

$$Ty = \lambda y \tag{3.2}$$

holds, $y^{(i)}$ $(i = 1, 2, \ldots)$ *are expressed with a scalar* t $(\neq 0)$ *as*

$$y^{(i)} = t \cdot \Pi_{j=1}^{i-1} \frac{\sqrt{\alpha_{2j-2}}}{\sqrt{\gamma_{2j}}} A_{2i-2}. \tag{3.3}$$

Proof. (1.3) in matrix form, with its symmetrization, directly becomes an eigenvalue problem of T, namely, (3.2). What remains to be proved is $y \neq 0$ and $y \in X$.

$y = 0$ means $A_{2k} = 0$ $(k = 0, 1, 2, \ldots)$, which is the trivial solution of (1.1) (which we omit). In order to show $y \in X$ (or $\|y\|^2 = |\beta_0|^2|y^{(1)}|^2 + |\beta_2|^2|y^{(2)}|^2 + \cdots < \infty$), one only has to prove

$$R \equiv \lim_{k\to\infty} \sup \left|\frac{\beta_{2k}}{\beta_{2k-2}}\right| \cdot \left|\frac{y^{(k+1)}}{y^{(k)}}\right| < 1.$$

This holds since $\left|y^{(k+1)}/y^{(k)}\right| \to 0$ from (2.3) and $|\beta_{2k}/\beta_{2k-2}| \to 1$ from (1.4). □

THEOREM 3.2. *Let* $T^{(k)}$ *be the k-th principal submatrix of* T $(k = 1, 2, \ldots)$*. Then, one can choose each* $\lambda^{(k)}$*, an eigenvalue of* $T^{(k)}$*, such that* $\lambda^{(k)} \to \lambda$*. And the following error estimate is valid:*

$$\lambda - \lambda^{(k)} = \left(\frac{\Pi_{i=0}^{k-1}\alpha_{2i}}{\Pi_{i=1}^{k-1}\gamma_{2i}}\right) \cdot \frac{A_{2k-2}A_{2k}}{y^T y}[1 + o(1)]\ (k \to \infty). \tag{3.4}$$

Moreover, the rate of convergence is

$$\frac{\lambda - \lambda^{(k+1)}}{\lambda - \lambda^{(k)}} = \frac{\alpha_{2k}}{\gamma_{2k}} \cdot \frac{A_{2k+2}}{A_{2k-2}}[1 + o(1)] = \left(\frac{c^2}{16}\right)^2 \cdot \frac{1}{k^4}[1 + o(1)]\ (k \to \infty). \tag{3.5}$$

Proof. It only has to be shown that [9, Theorem 1] can be applied to the eigenvalue problem (3.2). To begin with, the existence of T^{-1} need not be verified since $T + \delta I$ is easily proved to have an inverse for appropriately taken δ. Since $\alpha_k \cdot \gamma_{k+2} > 0$ $(k = 0, 2, \cdots)$, T is real. So are λ and y (up to scalar multiplication). Therefore $y^T y \neq 0$, which should lead λ is simple. To prove this, take the contraposition, or 'λ is not simple $\Rightarrow y^T y = 0$'. First, y is uniquely determined up to scalar multiplication. Therefore, it suffices to show that when T has an eigenvector of rank two, $y^T y = 0$ holds. From the assumption, for given $y \neq 0$, there exists a vector v such that

$$0 \neq y = (T - \lambda I)\, v,\ \ (T - \lambda I)\, y = (T - \lambda I)^2\, v = 0.$$

$$\begin{aligned} \text{Thus,}\ \ y^T y &= \{(T - \lambda I)\, v\}^T (T - \lambda I)\, v \\ &= v^T (T - \lambda I)^2\, v \text{ (by the symmetry of } T) = 0. \end{aligned}$$

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What is left to show is $f_{k+1}x^{(k+1)}/x^{(k)} \to 0$ $(k \to \infty)$. This is, however, clear by (2.3). Hence, [9, Theorem 1] may apply the case of (3.2) and direct computation gives the error estimate (3.4) and rate of convergence (3.5). □

4. Inverse eigenvalue problem. In Section 3, the computation of λ (eigenvalue) was presented. In this section, its inverse case is discussed.

DEFINITION 4.1. *Given m and real λ, let any value of c^2 such that $w(z)$ of (1.1) is regular in* $[-1,1]$ *be called an* inverse eigenvalue.

Let us begin, as Section 3, with the prior result:

[8, Theorems 1.1 and 1.4] Given an infinite complex symmetric tridiagonal matrix

$$A = \begin{bmatrix} d_1 & f_2 & & 0 \\ f_2 & d_2 & f_3 & \\ & f_3 & d_3 & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix},$$

where $d_k \to 0, f_k \to 0$ $(k \to \infty)$, and $f_k \neq 0$ $(k = 2,3,\ldots)$, representing a compact operator in ℓ^2. Let A have a simple eigenvalue $\lambda \neq 0$, and $0 \neq \chi = [\chi^{(1)}, \chi^{(2)}, \ldots]^T \in \ell^2$ denote an eigenvector of A corresponding to λ. Under the stated assumptions, we have

(i) Letting A_k $(k = 1,2,\ldots)$ be the k-th order principal submatrix of A, and λ_k be an eigenvalue of A_k. Then, taking $\{\lambda_k\}$ properly, we have $\lambda_k \to \lambda$.

(ii) Assuming that $\{\lambda_k\}$ is taken in the sense of (i), $\chi^T\chi \neq 0$, and $\chi^{(k+1)}/\chi^{(k)}$ is bounded for all sufficiently large k, we find the following estimate valid:

$$\lambda - \lambda_k = \frac{f_{k+1}\chi^{(k)}\chi^{(k+1)}}{\chi^T\chi}[1 + o(1)] \quad (k \to \infty).$$

By applying [8, Theorems 1.1 and 1.4], the inverse problem, namely, the computation of inverse eigenvalues c^2 is enabled. Beforehand, let us define new symbols a_k, b_k, r_k as

$$\alpha_k = a_k c^2,\ \beta_k = (m+k)(m+k+1) + b_k c^2,\ \gamma_k = r_k c^2, \tag{4.1}$$

and also g_k as

$$g_k = \lambda - (m+k)(m+k+1) \sim -k^2\ (k \to \infty). \tag{4.2}$$

Using (4.1) and (4.2), (1.3) is then rewritten as follows:

$$\begin{aligned} b_0 A_0 + a_0 A_2 &= \frac{g_0}{c^2} A_0, \\ r_{2k}A_{2k-2} + b_{2k}A_{2k} + a_{2k}A_{2k+2} &= \frac{g_{2k}}{c^2} A_{2k}\ (k = 1,2,3,\ldots). \end{aligned} \tag{4.3}$$

THEOREM 4.2. *Suppose $g_{2k} \neq 0$ $(k = 0,1,2,\ldots)$ for given m and real λ. Then, $c^2 \neq 0$ is an inverse eigenvalue of (1.1) if and only if $1/c^2$ is an eigenvalue of an infinite symmetric tridiagonal matrix A acting as a compact operator in ℓ^2, where*

$$A = \begin{bmatrix} b_0/g_0 & \sqrt{a_0 r_2}/\sqrt{g_0 g_2} & & 0 \\ \sqrt{a_0 r_2}/\sqrt{g_0 g_2} & b_2/g_2 & \sqrt{a_2 r_4}/\sqrt{g_2 g_4} & \\ & \sqrt{a_2 r_4}/\sqrt{g_2 g_4} & b_4/g_4 & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}. \tag{4.4}$$

Furthermore, if one lets an eigenvector of A corresponding to $1/c^2$ be $0 \neq x \equiv [x^{(1)}, x^{(2)}, \ldots]^T \in \ell^2$, i.e., if

$$Ax = \frac{1}{c^2}x \tag{4.5}$$

holds, then $x^{(i)}$ $(i = 1, 2, \ldots)$ can be expressed in the form

$$x^{(i)} = \tilde{t} \cdot \sqrt{g_{2i-2}}\, \Pi_{j=1}^{i-1} \frac{\sqrt{a_{2j-2}}}{\sqrt{r_{2j}}} A_{2i-2} \tag{4.6}$$

where $\tilde{t} \neq 0$ is a scalar.

Proof. (4.3) in matrix form, with its symmetrization, directly becomes an eigenvalue problem of A, namely, (4.5). Also, from (2.3) it holds that $x \in \ell^2$, since

$$\left|\frac{x^{(k+1)}}{x^{(k)}}\right| = \left|\frac{\sqrt{g_{2k}}}{\sqrt{g_{2k-2}}} \cdot \frac{\sqrt{a_{2k-2}}}{\sqrt{r_{2k}}}\right| \cdot \left|\frac{A_{2k}}{A_{2k-2}}\right| = \frac{c^2}{16k^2}[1 + o(1)] \;\to 0\; (k \to \infty). \;\square \tag{4.7}$$

THEOREM 4.3. *Let $A^{(k)}$ be the k-th principal submatrix of A $(k = 1, 2, \ldots)$. Then, assuming $x^T x \neq 0$, one can choose each $c^2_{(k)} = 1/\xi^{(k)}$, where $\xi^{(k)}$ represents one of the eigenvalues of $A^{(k)}$, such that $c^2_{(k)} \to c^2$. And the following error estimate is valid:*

$$\begin{aligned} c^2 - c^2_{(k)} &= \frac{-c^6 l_{m,k} A_{2k-2} A_{2k}}{x^T x}[1 + o(1)]\; (k \to \infty), \text{ where} \\ l_{m,k} &= \frac{(2m+1)^2(2m+2)}{(2m+4k-3)(2m+4k-1)(2m+4k+1)} \cdot {}_{2m+2k}\mathrm{C}_{2m+2}. \end{aligned} \tag{4.8}$$

The rate of convergence is thus derived:

$$\frac{c^2 - c^2_{(k+1)}}{c^2 - c^2_{(k)}} = \left(\frac{c}{4}\right)^4 \cdot \frac{1}{k^4}\,[1 + o(1)]\; (k \to \infty). \tag{4.9}$$

Proof. Let us prove a few conditions to apply [8, Theorems 1.1 and 1.4] to (4.5). $x^{(k+1)}/x^{(k)}$ is bounded for all sufficiently large k, since $|x^{(k+1)}/x^{(k)}| \to 0$ $(k \to \infty)$ from (4.7). Also, from the assumption $x^T x \neq 0$, it is derived that the eigenvalue $1/c^2$ of A is simple, in the same way as the proof of Theorem 3.2.

Direct computation leads to the error estimate (4.8) and rate of convergence (4.9). $\square$

LEMMA 4.4. *[8, Theorems 1.1 and 1.4] is applied also when $g_{2k} = 0$ for some non-negative integer k in (4.3).*

Proof. When $k = 0$, or $g_0 = \lambda - m(m+1) = 0$, the first line of (4.3) yields $A_0 = -\frac{a_0}{b_0}A_2$. Substituting this into the second line of (4.3) gives

$$\left(b_2 - \frac{a_0 r_2}{b_0}\right) A_2 + a_2 A_4 = \frac{g_2}{c^2} A_2.$$

With this and the subsequent equations, one can reformulate them into the matrix eigenvalue problem by the same procedure.

When k is non-zero, $A_{2k} = -\frac{1}{b_{2k}}(r_{2k}A_{2k-2} + a_{2k}A_{2k+2}) = 0$ holds. Substituting this into $(k-1)$-th and $(k+1)$-th equations yields

$$\begin{aligned} r_{2k-2}A_{2k-4} + \left(b_{2k-2} - \frac{a_{2k-2}r_{2k}}{b_{2k}}\right) A_{2k-2} - \frac{a_{2k-2}a_{2k}}{b_{2k}} A_{2k+2} &= \frac{g_{2k-2}}{c^2} A_{2k-2}, \\ -\frac{r_{2k}r_{2k+2}}{b_{2k}} A_{2k-2} + \left(b_{2k+2} - \frac{a_{2k}r_{2k+2}}{b_{2k}}\right) A_{2k+2} + a_{2k+2}A_{2k+4} &= \frac{g_{2k+2}}{c^2} A_{2k+2}. \end{aligned}$$

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Likewise, [8, Theorems 1.1 and 1.4] applies to the new set of equations. □

5. Geometrical properties of λ–c^2 graph. The λ-c^2 graph, created by the proposed method, is shown in Fig. 5.1 (for $m = 0$). The graph above λ-axis is the prolate output, while the graph below is the oblate case.

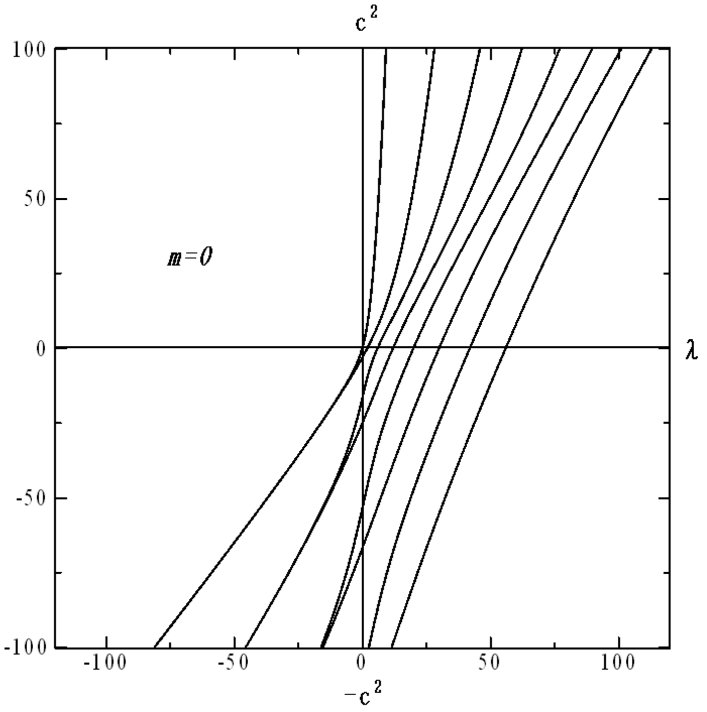

FIG. 5.1. *λ-c^2 graph (prolate and oblate cases combined for $m = 0$)*

The following two geometrical properties are proved regarding λ-c^2 graph.

REMARK 5.1. *In the prolate case, $\lambda \geq m(m+1)$ holds.*

Proof. Suppose the contrary, or $\lambda < m(m+1)$, and let the contradition be derived. Since $g_{2k} = \lambda - (m+2k)(m+2k+1) < 0$ $(k = 0, 1, 2, \ldots)$, the eigenvalue problem

$$Ux_1 = -\frac{1}{c^2}x_1, \text{ where}$$

$$U = \begin{bmatrix} \frac{b_0}{-g_0} & \frac{\sqrt{a_0}\sqrt{r_2}}{\sqrt{-g_0}\sqrt{-g_2}} & & 0 \\ \frac{\sqrt{a_0}\sqrt{r_2}}{\sqrt{-g_0}\sqrt{-g_2}} & \frac{b_2}{-g_2} & \frac{\sqrt{a_2}\sqrt{r_4}}{\sqrt{-g_2}\sqrt{-g_4}} & \\ & \frac{\sqrt{a_2}\sqrt{r_4}}{\sqrt{-g_2}\sqrt{-g_4}} & \frac{b_4}{-g_4} & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix} \text{ and} \tag{5.1}$$

$$x_1 = \left[\sqrt{-g_0}A_0, \frac{\sqrt{a_0}}{\sqrt{r_2}}(\sqrt{-g_2}A_2), \frac{\sqrt{a_2}}{\sqrt{r_4}}\frac{\sqrt{a_0}}{\sqrt{r_2}}(\sqrt{-g_4}A_4), \ldots\right]^T$$

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are both real, is obtained. U is found to be decomposed into $U = S^T S$, where

$$S = \begin{bmatrix} 0 & & & 0 \\ e_2 & e_3 & & \\ & e_4 & e_5 & \\ 0 & & \ddots & \ddots \end{bmatrix}, \text{ with}$$

$$e_k = \frac{1}{\sqrt{-g_{P_k}}} \cdot \sqrt{\frac{(k-1)(2m+k-1)}{(2m+2k-3)(2m+2k-1)}} \; (k = 2, 3, \ldots) \text{ and}$$
$$P_k = k - 2 + \mathrm{mod}(k, 2).$$

This shows that U is positive definite (refer to Appendix A for a detailed proof), leading to a contradiction (since the eigenvalues of U are assumed $-1/c^2 < 0$). ☐

REMARK 5.2. *Given m, we have $dc^2/d\lambda \neq 0$.*

Proof. The next equation is obtained by applying [11, Corollary 1],

$$\left(\frac{\mathrm{d}c^2}{\mathrm{d}\lambda}\right) \cdot (x^T x) = c^2 \cdot (y^T y),$$

with x and y respectively defined in (4.6) and (3.3). Since $y^T y \neq 0$ (y is non-zero and real), the proposition obviously holds. ☐

6. Numerical experiments. Some experiments were conducted to show the validity of the error estimates presented in (3.4) and (4.8). The computations were executed on Dell Dimension XPS (Pentium 4 CPU 3.00GHz, 1GB RAM), using double precision floating-point arithmetic by Intel Visual Fortran Compiler (version 8). For computing eigenvalues of symmetric tridiagonal matrices, we used the FORTRAN subroutine COMQR in EISPACK [12].

EXPERIMENT 6.1. *Computation of eigenvalues λ, given m and c.* We first computed an eigenvalue of a sufficiently large order principal submatrix of (3.1) and regarded it as the true value λ. Then, for each k, we computed all the eigenvalues of $T^{(k)}$ and chose the closest to λ to be $\lambda^{(k)}$. The values of $y^{(k)}$ $(k = 1, 2, \ldots)$ were obtained by backward-substitution by (1.3), initiating $y^{(K)} = 0$ for sufficiently large K, and $y^{(K-1)} = \varepsilon$ ($\neq 0, \varepsilon$ shall be taken appropriately so that an overflow doesn't occur). These settings of $y^{(K)}$ and $y^{(K-1)}$ are allowed from the behavior $y^{(k)} \to 0$ $(k \to \infty)$.

Table 6.1 describes how fast the approximated eigenvalues $\lambda^{(k)}$ approach the exact eigenvalue λ with error estimates. In the table, $E^{(k)}_{mn}$ $(k = 1, 2, \ldots)$ represent the RHS of (3.4) without $[1 + o(1)]$ corresponding to the approximated eigenvalue $\lambda^{(k)} = \lambda^{(k)}_{mn}$.

EXPERIMENT 6.2. *Computation of inverse eigenvalues c^2, given m and λ.* The procedure is almost the same as Experiment 6.1. The true value c^2 was computed from a sufficiently large order principal submatrix of (4.4). Then, for each k, we computed all the eigenvalues of $A^{(k)}$ and chose the closest to c^2 to be $c^2_{(k)}$. The values of $x^{(k)}$ $(k = 1, 2, \ldots)$ were obtained by backward-substitution by (1.3), initiating $x^{(K')} = 0$ for sufficiently large K', and $x^{(K'-1)} = \varepsilon$ ($\neq 0, \varepsilon$ shall be taken appropriately so that an overflow doesn't occur). These settings of $x^{(K')}$ and $x^{(K'-1)}$ are allowed from the behavior $x^{(k)} \to 0$ $(k \to \infty)$.

Table 6.2 describes how fast the approximated eigenvalues $c^2_{(k)}$ approach the exact eigenvalue c^2 with error estimates. In the table, $E^{(k)}$ $(k = 1, 2, \ldots)$ represent the RHS of (4.8) without $[1 + o(1)]$ corresponding to the approximated eigenvalue $c^2_{(k)}$.

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TABLE 6.1
Actual errors and estimates of (3.4). Given $m = 0, c^2 = 10$, *compute* $\lambda \equiv \lambda_{00} = 2.305040036\cdots$, $\lambda \equiv \lambda_{01} = 7.285254306\cdots$, $\lambda \equiv \lambda_{02} = 11.79039448\cdots$.

k	$\lambda_{00} - \lambda_{00}^{(k)}$	$E_{00}^{(k)}$	$\lambda_{01} - \lambda_{01}^{(k)}$	$E_{01}^{(k)}$	$\lambda_{02} - \lambda_{02}^{(k)}$	$E_{02}^{(k)}$
2	-2.98E-02	-3.06E-02	-1.57E-02	-1.60E-02	-4.46E-01	-4.29E-01
3	-1.91E-04	-1.93E-04	-6.82E-05	-6.85E-05	-5.85E-03	-5.92E-03
4	-3.64E-07	-3.65E-07	-9.15E-08	-9.17E-08	-1.62E-05	-1.63E-05
5	-2.72E-10	-2.72E-10	-5.02E-11	-5.06E-11	-1.52E-08	-1.52E-08
6					-8.00E-12	-6.21E-12

TABLE 6.2
Actual errors and estimates of (4.8). Given $m = 0, \lambda = 15$, *compute* $c_0^2 = 5.649012143\cdots$, $c_1^2 = 15.46529327\cdots$, $c_2^2 = 32.20360313\cdots$.

k	$c_0^2 - c_{(k)}^2$	$E^{(k)}$	$c_1^2 - c_{(k)}^2$	$E^{(k)}$	$c_2^2 - c_{(k)}^2$	$E^{(k)}$
2	1.90E-01	2.02E-01	1.48E-00	1.65E-00	2.19E-00	2.85E-00
3	5.21E-04	5.23E-04	5.64E-02	5.89E-02	1.04E-01	1.10E-01
4	3.08E-07	3.08E-07	3.95E-04	3.98E-04	1.38E-03	1.40E-03
5	6.62E-11	6.62E-11	9.00E-07	9.02E-07	7.56E-06	7.60E-06
6			8.86E-10	8.87E-10	2.03E-08	2.03E-08
7					2.99E-11	3.00E-11

7. Concluding remarks. By the proposed method, one only has to compute the eigenvalues of the given matrices without further knowledge or skill. The eigensystem routines such as EISPACK [12] with guaranteed error estimates allow one to obtain accurate eigenvalues λ and inverse eigenvalues c^2. The theorems in [8] and [9] are powerful tools for computing eigenvalues of certain classes of infinite matrices, which arise in solving some types of linear differential equations. Further applications of the theorems will be sought by us.

Appendix A.

PROPOSITION. A.1 *The matrix* U *defined in (5.1) is positive definite.*

Proof. One needs to show that $w^TUw \geq 0$ holds for all $w = [w_1, w_2, \ldots]^T \in \ell^2$ and the equality is valid only when $w = 0$. Since $U = S^TS$,

$$w^TUw = w^TS^TSw = ||Sw||^2 \geq 0.$$

The proof for $w^TUw = 0 \Leftrightarrow w = 0$ follows. It is obvious $w = 0$ leads $w^TUw = 0$. Conversely, if one assumes $w^TUw = ||Sw||^2 = 0$, one finds

$$Sw = \begin{bmatrix} 0 & & & 0 \\ e_2 & e_3 & & \\ & e_4 & e_5 & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ e_2w_1 + e_3w_2 \\ e_4w_2 + e_5w_3 \\ e_6w_3 + e_7w_4 \\ \vdots \end{bmatrix} = 0.$$

Therefore,

$$w_2 = -\frac{e_2}{e_3}w_1, w_3 = \frac{e_4}{e_5}\frac{e_2}{e_3}w_1, \ldots, w_n = (-1)^{(n-1)}\left(\Pi_{i=1}^{n-1}\frac{e_{2i}}{e_{2i+1}}\right)w_1.$$

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This shows w_1 has to vanish, since, otherwise,

$$\|w\|^2 = w_1^2 + \left(\frac{e_2}{e_3}\right)^2 w_1^2 + \left(\frac{e_2}{e_3}\right)^2 \left(\frac{e_4}{e_5}\right)^2 w_1^2 + \cdots \to \infty \ \left(, \text{ by } \lim_{i\to\infty} \frac{e_{2i}}{e_{2i+1}} = 1\right)$$

contradicts the premise $w \in \ell^2$. This argument leads to $w_2 = w_3 = \ldots = 0$ or $w = 0$. $\square$

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