ON SOME BOUNDARY VALUE PROBLEMS DEFINED ON SEMI-INFINITE INTERVALS

BY

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To my wife, Regina

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ABSTRACT

The object of this thesis is to discuss some problems which arise in the numerical solution of differential equations defined on semi-infinite intervals. For the problem $y''+f(x)y=0$, known results are made use of to derive properties of the derivatives of the solution. The eigenvalue problem $-y''+f(x)y=\lambda y$, $y(0)=0$ for which there exists a sequence of eigenvalues λ_n, where $\lambda_1<\lambda_2<\lambda_3<\ldots$, is discretized by an infinite system of linear equations using a finite difference scheme. The sequence of eigenvalues μ_i, $i=1,2,\ldots,$ for the discretized system are found. Upper bounds are derived for the difference between the eigenvalues of the continuous and the discretized system. The behaviour of the eigenfunctions as x tends to infinity is also discussed. An example is given to illustrate the theory.

CONTENTS

INTRODUCTION

The behaviour of solutions and their derivatives is of importance in developing an error analysis in the numerical solution of differential systems which are analogous to Sturm-Liouville systems but defined on infinite intervals. Estimating eigenvalues and the discussion of the nature of eigenfunctions in such problems as x tends to infinity is in general a difficult problem. Also, developing an error analysis needs the behaviour of the derivatives. The object of the present work is two-fold. Firstly, for the system $y''+f(x)y=0$, $y(0)=A$, $\lim_{x\to\infty} f(x)=\infty$, we know the behaviour of the solution under some further conditions on $f(x)$. We make use of these results to discuss the behaviour of the derivatives of the solution for all $x \geq 0$. Secondly, for the eigenvalue problem $-y''+f(x)y=\lambda y$, $y(0)=0$, we apply finite difference methods and using known results, we calculate the eigenvalues of the discretized system. The discretized system is a system of infinite linear alegebraic equations. We also develop, for the first time, error bounds for the eigenvalue problems and establish the required result for eigenfunctions, viz., $\lim_{x\to\infty} y(x)=0$. In the process we also develop some useful results for tridiagonal finite and infinite matrices. In fact, we give upper and lower bounds for the inverse elements of a diagonally dominant tridiagonal infinite matrix. A novel procedure adopted is to use different constant step lengths for the finite difference scheme in discussing each eigenvalue problem. Schrödinger's one-dimensional equation with potential x^2 is used to illustrate the theory and some numerical results are given.

CHAPTER 1

PRELIMINARIES

1.1 Boundary Value problems

We are mainly interested in the two systems

$$y''+f(x)y=0, \qquad y(a)=A, \qquad y'(a)=B, \tag{S1}$$

and

$$-y''+f(x)y=\lambda y, \qquad y(a)=A, \tag{S2}$$

under suitable restrictions on $f(x)$. As regards *(S1)*, our interest is in the behaviour of the solution and its higher order derivatives for the entire semi-infinite interval (a,∞). For *(S2)*, we will develop a novel procedure by using simple finite difference methods to discuss eigenvalues and eigenfunctions complete with an error analysis.

For both systems we will assume that $f(x)$ is nonnegative for $x \geq 0$, and that $f(x)$ tends to infinity as x tends to infinity. The analysis of these systems usually leads to application of one of the following topics: continued fractions, infinite series, infinite matrices, or infinite products. The above systems have been studied extensively in the literature particularly when they have been defined on finite intervals. In the use of finite difference methods, the common procedure is to assume either a constant step length $(h>0)$ or a variable step length $(h_k, k=1,2,3,\dots,)$. For *(S2)*, we will use a combination of both procedures of constant and variable step lengths. In problems concerning finite intervals, the error in the evaluation of solutions is usually expressed as $O(h^p)$, for a given integer $p\,(p>0)$ with the implicit understanding that one can reduce the step length to obtain better estimates for error bounds. Clearly, this will not always be possible in the case of infinite intervals, as we need either a constant h or a nest of variable step lengths h_k such that $\sum_{k=1}^{\infty} h_k = \infty$ to enable us to give an error analysis for the entire semi-infinite interval.

To develop an error estimate of a given method for the numerical solution of a differential system, usually additional assumptions are needed about the solution of the system. These assumptions require that the solution possess derivatives of a certain order, belonging to definite function spaces. This puts great demands on the properties of the solution . For example, to get a meaningful error estimate in the numerical solution of a boundary value problem for an equation of second order, a bounded fourth order derivative of the solution is required. This does not present much difficulty in the case of finite intervals, as solutions and their derivatives can reasonably be assumed to be continuous and hence bounded. In the case of infinite intervals, it is usually very difficult to know the behaviour of the solution or its derivatives at infinity.

1.2 An oscillatory system

Let $f(x), (x>0)$ satisfy the conditions

(i) f is positive;

(ii) f', its derivative, is nonnegative and continuous and $\qquad (A1)$

(iii) $\lim_{x\to\infty} f(x) = \infty$.

Then it is well-known (McShane [10]) that each solution of

$$y'' + f(x)y = 0 \quad , \quad x \geq 0 \tag{1}$$

has infinitely many zeros and $|y|$ is bounded and the values of $|y(x)|$ at successive maxima form a decreasing sequence. It has been shown (GMP [5]) that it does not necessarily follow that

$$\lim_{x\to\infty} y(x) = 0 \quad . \tag{2}$$

McShane [10] gives a number of sets of growth conditions on $f(x)$ to insure the behaviour of $y(x)$ as x tends to infinity. One set of conditions states that under (A1), (2) holds for (1) with the additional hypothesis

$$\frac{f'(x)}{f(x)} \text{ is nonincreasing for } x \text{ above some } \bar{x}. \tag{A2}$$

One such example is given by $f(x) = x^2$.

We now consider

$$y'' + p(x)y = 0 \tag{3}$$

where $p(x)$ satisfies $(A1)$ and we will denote $\{t_i\}_{i=1}^{\infty}$ to be the sequence of zeros of $y(x)$, $\{w_i\}_{i=1}^{\infty}$ to be the sequence of zeros of $y'(x)$ and $\{y_i\}_{i=1}^{\infty}$

the sequence formed by $y_i = y(w_i)$. Further, we will denote $w_{i+1} - w_i$ by h_i .

The following results are known to Sansone [15]:

$$\text{(i)} \quad 0 < t_1 < t_2 < \dots \; ; \qquad |y_1| > |y_2| \; \dots \; . \tag{4}$$

$$\text{(ii)} \quad t_i < w_i < t_{i+1}, \quad w_i < t_i < w_{i+1}, \qquad i = 1, 2, 3 \dots .$$

$$\text{(iii)} \quad t_{n+1} - t_n \le t_n - t_{n-1}, \qquad h_{n+1} \le h_n \; .$$

$$\text{(iv)} \quad \sum_{n=1}^{\infty} h_n \text{ and } \sum_{n=1}^{\infty} (t_{n+1} - t_n) \text{ both diverge.}$$

$$\text{(v)} \quad \frac{\pi}{\sqrt{p(w_{n+1})}} \le h_n \le \frac{\pi}{\sqrt{p(w_n)}} \quad , \quad \frac{\pi}{\sqrt{p(t_{n+1})}} \le t_{n+1} - t_n \le \frac{\pi}{\sqrt{p(t_n)}} \quad .$$

For the differential equation (3) we will now consider the properties of higher order derivatives of solutions of (3). To do so, we will consider the expression

$$[\alpha_1(x)y'(x)]'' + \varphi_1(x)[\alpha_1(x)y'(x)]$$

$$= \alpha_1 y''' + 2\alpha_1' y'' + \alpha_1'' y' + \varphi_1 \alpha_1 y'$$

$$= y'[-\alpha_1 p + \alpha_1'' + \alpha_1 \varphi_1] + y[-\alpha_1 p' - 2\alpha_1' p] \qquad \text{(on using (3))}$$

$$= 0 \; ,$$

if we choose

$$-2\frac{\alpha_1'}{\alpha_1} = \frac{p'}{p} \qquad \text{and} \qquad \varphi_1 = \frac{-\alpha_1'' + \alpha_1 p}{\alpha_1} .$$

Integrating we get

$$\alpha_1 = \frac{1}{\sqrt{p}} \qquad \text{and} \quad \text{thus} \quad \varphi_1 = p - \sqrt{p}\left(\frac{1}{\sqrt{p}}\right)'' \tag{5}$$

giving

$$\left(\frac{y'}{\sqrt{p}}\right)'' + \left[p - \sqrt{p}\left(\frac{1}{\sqrt{p}}\right)''\right]\left(\frac{y'}{\sqrt{p}}\right) = 0,$$

which is of the form

$$z'' + \varphi_1(x)z = 0 \quad , \quad z = \alpha_1 y', \tag{6}$$

where α_1 and φ_1 are given by (5).

Similarly, we have

$$[\alpha_2(x)y''(x)]'' + \varphi_2(x)[\alpha_2(x)y'']$$

$$= [-py\alpha_2]'' + \varphi_2[-\alpha_2 p\, y]$$

$$= -y'[2(p\alpha_2)'] + y[p(p\alpha_2) - (p\alpha_2)'' - \alpha_2\varphi_2 p] \qquad \text{(on using (3))}$$

$$= 0\ ,$$

if we choose

$$p\alpha_2 = 1 \qquad \text{and} \qquad \varphi_2 = \frac{p(p\alpha_2) - (p\alpha_2)''}{\alpha_2 p}.$$

Hence

$$\alpha_2 = \frac{1}{p} \qquad \text{and} \qquad \varphi_2 = p\ , \tag{7}$$

giving

$$\left(\frac{y''}{p}\right)'' + p\left(\frac{y''}{p}\right) = 0 \quad ,$$

which is of the form

$$z'' + \varphi_2(x)z = 0 \quad , \quad z = \alpha_2 y'' \quad , \tag{8}$$

where α_2 and φ_2 are given by (7).

For the third order derivative, we have

$$\left[\alpha_3(x)y'''(x)\right]'' + \varphi_3(x)\left[\alpha_3(x)y'''(x)\right]$$

$$= \alpha_3 y^{v} + 2\alpha_3' y^{iv} + \alpha_3'' y''' + \varphi_3\alpha_3 y'''$$

$$= \alpha_3[(-py)'''] + 2\alpha_3'(-py)'' + (\varphi_3\alpha_3 + \alpha_3'')y''' \quad \text{(on using (3))}$$

$$= y'''[-\alpha_3 p + \varphi_3\alpha_3 + \alpha_3'']$$

$$+ y''[-3\alpha_3 p' - 2\alpha_3' p] + y'[-3\alpha_3 p'' - 4\alpha_3' p'] + y[-\alpha_3 p''' - 2\alpha_3' p'']$$

$$= y'''\left\{-\alpha_3 p + \varphi_3\alpha_3 + \alpha_3'' + \frac{1}{p}(3\alpha_3 p'' + 4\alpha_3' p')\right\}$$

$$+ y''\left\{-3\alpha_3 p' - 2\alpha_3' p + (3\alpha_3 p'' + 4\alpha_3' p')\left(\frac{1}{p}\right)' + \left(\frac{1}{p}\right)(\alpha_3 p''' + 2\alpha_3' p'')\right\}$$

on using $y = -y''/p\, , y' = -y'''\left(\frac{1}{p}\right) - y''\left(\frac{1}{p}\right)'$. Equating the coefficient of y'' to zero, we get

$$-2\frac{\alpha_3'}{\alpha_3}=\frac{3p^2p'+3\,p'p''-pp'''}{p^3+2(p')^2-pp''}$$

which on integration yields (with constant of integration assumed to be zero)

$$\ell n\ \ \alpha_3^{-2}=\ell n(p^3+2(p')^2-pp'') \quad ,$$

or

$$\alpha_3=\frac{1}{\sqrt{p^3+2(p')^2-pp''}}\,. \tag{9}$$

Now equating the coefficient of y''' = 0, we get

$$\varphi_3=p-\frac{3p''}{p}-\frac{4\alpha_3'}{\alpha_3}\frac{p'}{p}-\frac{\alpha_3''}{\alpha_3} \quad . \tag{10}$$

Hence we have

$$z''+\varphi_3(x)z=0 \quad , \quad z=\alpha_3 y''', \tag{11}$$

where α_3 and φ_3 are given by (9) and (10) respectively.

Similarly, for the fourth order derivative, we can write

$$(\alpha_4 y^{iv})''+\varphi_4(x)(\alpha_4 y^{iv})$$

$$=\alpha_4 y^{vi}+2\alpha_4' y^{v}+y^{iv}(\alpha_4''+\varphi_4\alpha_4)$$

$$=\alpha_4(-py)^{iv}+2\alpha_4'(-py)'''+y^{iv}(\alpha_4''+\varphi_4\alpha_4) \quad \text{(on using (3))}$$

$$= -\alpha_4[py^{iv} + 4\,p'\,y''' + 6\,p''\,y'' + 4p'''\,y' + p^{iv}\,y]$$

$$-2\alpha_4'(p\,y''' + 3p'\,y'' + 3p''\,y' + p'''\,y)$$

$$+y^{iv}(\alpha_4'' + \varphi_4\alpha_4) \quad .$$

Now using

$$y = -\frac{y''}{p}, \qquad y' = -\frac{y'''}{p} - y''\left(\frac{1}{p}\right)'$$

and

$$y'' = -y^{iv}\left(\frac{1}{p}\right) - 2y'''\left(\frac{1}{p}\right)' - y''\left(\frac{1}{p}\right)'' \quad ,$$

we can solve the last equation to obtain

$$y'' = \frac{\left(\dfrac{2y'''p'}{p^2} - \dfrac{y^{iv}}{p}\right)}{\left(1 + \dfrac{2(p')^2}{p^3} - \dfrac{p''}{p^2}\right)}$$

and thus, we can express y, y', y'' in terms of y''' and y^{iv} to yield

$$(\alpha_4 y^{iv})'' + \varphi_4(\alpha_4 y^{iv})$$

$$= y^{iv}\Big[\,\alpha_4'' + \alpha_4\varphi_4 - 2\,\frac{\alpha_4'}{p}\,\frac{\left(-3p' + \dfrac{p'''}{p} - \dfrac{3p''}{p^2}\,p'\right)}{\left(1 + \dfrac{2(p')^2}{p^3} - \dfrac{p''}{p^2}\right)}$$

$$-\frac{\alpha_4}{p}\,\frac{\left(-6p'' + \dfrac{p^{iv}}{p} - \dfrac{4p'''}{p^2}\,p'\right)}{\left(1 + \dfrac{2}{p^3}\,(p')^2 - \dfrac{p''}{p^2}\right)} - \alpha_4 p\,\Big]$$

$$+y'''\Big[2\alpha_4'\left\{-p + 3\,\frac{p''}{p} + 2\,\frac{p'}{p^2}\,\frac{\left(-3p' + \dfrac{p'''}{p} - 3\,\dfrac{p''}{p^2}\,p'\right)}{\left(1 + \dfrac{2}{p^3}\,(p')^2 - \dfrac{p''}{p^2}\right)}\right\}$$

$$+\alpha_4\left\{4\left(-p' + \frac{p'''}{p}\right) + 2\,\frac{p'}{p^2}\,\frac{\left(-6p'' + \dfrac{p^{iv}}{p} - 4\,\dfrac{p'''}{p^2}\,p'\right)}{\left(1 + \dfrac{2}{p^3}\,(p')^2 - \dfrac{p''}{p^2}\right)}\right\}\Big]\,.$$

Equating the coefficient of y''' = 0, we get

$$-2\,\frac{\alpha_4'}{\alpha_4} = \frac{4p^3p' + 8(p')^3 + 8pp'p'' - 4p^2p''' + 4p''p''' - 2p'p^{iv}}{p^4 + 8p(p')^2 - 4p^2p'' + 3(p'')^2 - 2p'p'''}\,.$$

Since the numerator on the right side is the derivative of the denominator, we can write

$$\alpha_4 = \frac{1}{\sqrt{p^4 + 8p(p')^2 - 4p^2p'' + 3(p'')^2 - 2p'p'''}}\,. \tag{12}$$

Now equating the coefficient of y^{iv} to zero, we get

$$\varphi_4 = -\frac{\alpha_4''}{\alpha_4} + \frac{\alpha_4'}{\alpha_4}\frac{p}{p'}\left(p - 3\frac{p''}{p}\right) + 2\frac{p}{p'}\left(p' - \frac{p'''}{p}\right) + p\,. \tag{13}$$

Hence, we get

$$z'' + \varphi_4(x)\,z = 0 \quad , \qquad z = \alpha_4 y^{iv}\,, \tag{14}$$

where α_4 and φ_4 are given by (12) and (13) respectively.

We can now conclude that, if φ_i satisfies (A1) with $f(x) = \varphi_i$, then $z_i(x) = \alpha_i y^{(i)}$ has all the properties of $y(x)$ in (1) and the respective estimates (4) hold. In particular for $i = 2$, $\frac{y''}{p}$ is oscillatory and its zeros and values of $\left|\frac{y''}{p}\right|$ at successive maxima have the estimates given in (4). If further, φ_i satisfies (A2) with $f(x) = \varphi_i$, then $\lim_{x\to\infty} z_i(x) = 0$ for all i.

1.3 An example

Consider the differential equation

$$y'' + \beta^2\alpha^2 x^{2\beta-2} y = 0\,,$$

which has two linearly independent solutions given by

$$C\sqrt{x}\, J_{\left(\pm\frac{1}{2\beta}\right)}(\alpha x^{\beta})$$

where J_υ represents the Bessel's function of order υ and C is an arbitrary constant. For the particular case

$$y''+x^p\,y=0\quad,\qquad y(0)=1\quad,\quad y'(0)=0\quad,\quad p>0 \tag{14}$$

the unique solution is given by

$$y(x)=C\,\sqrt{x}\,J_{\left(-\frac{1}{p+2}\right)}\left(\frac{2}{p+2}\,x^{\frac{p+2}{2}}\right)$$

for a suitable value of C. From Olver [11], $y(x)$ has the asymptotic expansion given by

$$y(x)\sim C\sqrt{x}\left(\frac{2}{\pi z}\right)^{\frac{1}{2}}\left[\cos\left(z-\frac{\upsilon\pi}{2}-\frac{1}{4}\,\pi\right)\sum_{s=0}^{\infty}(-1)^s\,\frac{A_{2s}(\upsilon)}{z^{2s}}+\sin\left(z-\frac{\upsilon\pi}{2}-\frac{1}{4}\,\pi\right)\sum_{s=0}^{\infty}(-1)^s\,\frac{A_{2s+1}(\upsilon)}{z^{2s+1}}\right]$$

where $z=\dfrac{2}{p+2}x^{\frac{p+2}{2}}$ and $\upsilon=-\dfrac{1}{p+2}$ with explicit formulas for $A_s(\upsilon)$.

Rewriting the expansion, we have

$$y(x)\sim\left(\frac{p+2}{\pi}\right)^{\frac{1}{2}}\frac{1}{x^{\frac{p}{4}}}\Big[\cos\left(\frac{2}{p+2}\,x^{\frac{p+2}{2}}+\frac{\pi}{2p+4}-\frac{1}{4}\,\pi\right)\sum_{s=0}^{\infty}(-1)^s\left(\frac{p+2}{2}\right)^{2s}\frac{A_{2s}}{x^{(p+2)s}}$$

$$+\sin\left(\frac{2}{p+2}\,x^{\frac{p+2}{2}}+\frac{\pi}{2p+4}-\frac{1}{4}\,\pi\right)\sum_{s=0}^{\infty}(-1)^s\left(\frac{p+2}{2}\right)^{2s+1}\frac{A_{2s+1}}{x^{(p+2)(s+\frac{1}{2})}}\Big]$$

as $x\to\infty$. Clearly $y(x)\to 0$ as $x\to\infty$. Assuming the validity of differentiating both sides of the expansion, we can verify that

$$\frac{y'(x)}{x^{\frac{p}{2}}},\quad \frac{y''(x)}{x^{p}},\quad \frac{y'''(x)}{x^{\frac{3p}{2}}},\quad \frac{y^{iv}(x)}{x^{2p}}$$

all tend to zero as $x\to\infty$. For the case $p=2$, it implies that

$$y(x),\quad \frac{y'(x)}{x},\quad \frac{y''(x)}{x^2},\quad \frac{y'''(x)}{x^3},\quad \frac{y^{iv}(x)}{x^4}$$

tend to zero as $x \to \infty$.

Reverting to our results in Section (1.3), we have the following table for

$$(\alpha_i y^{(i)})'' + \varphi_i(\alpha_i y^{(i)}) = 0. \tag{17}$$

	$\varphi_i(x)$	$\alpha_i y^{(i)}$
$i=0$	x^2	$y(x)$
$i=1$	$x^2 - \dfrac{2}{x^2}$	$\dfrac{y'(x)}{x}$
$i=2$	x^2	$\dfrac{y''(x)}{x^2}$
$i=3$	$x^2 + \dfrac{6x^6+108x^2}{(x^4+6)^2}$	$\dfrac{y'''(x)}{(x^6+6x^2)^{\frac{1}{2}}}$
$i=4$	$x^2 + \dfrac{16x^{14}+696x^{10}+1344x^6+3744x^2}{(x^8+24x^4+12)^2}$	$\dfrac{y^{iv}(x)}{(x^8+24x^4+12)^{\frac{1}{2}}}$.

All the functions in the last column tend to zero as x tends to infinity since all the φ's satisfy *(A1)* and *(A2)*. It can easily be seen that the asymptotic expansions in the case $p=2$ give basically the same results as the above table when $x \to \infty$.

CHAPTER 2

SOME RESULTS CONCERNING INFINITE MATRICES

2.1 Diagonally dominant finite matrices

Consider the finite linear system

$$\sum_{j=1}^{n} a_{ij}x_j = b_i \quad , \quad i = 1,2,3,\dots,n \quad . \tag{1}$$

If the matrix $A = (a_{ij})$ is strictly diagonally row dominant, i.e.,

$$\sigma_i |a_{ii}| = \sum_{\substack{j=1 \\ j\neq i}}^{n} |a_{ij}| \quad , \quad 0 \le \sigma_i < 1 \quad , \quad i = 1,2,\dots,n \quad , \tag{2}$$

and if $a_{ii} \neq 0$ for i=1,2,...,n, then it is well-known that (1) has a unique solution and by Cramer's Rule we have

$$x_j = \sum_{k=1}^{n} \frac{A_{kj}}{\det A} b_k \quad , \quad j = 1,2,\dots,n \quad . \tag{3}$$

In the above, A_{ij} represents the cofactor of a_{ij} in A and det A represents the determinant of A. Further, from equations (10) and (13) in Ostrowski [13], we have for the elements $A^{-1} = \left(\frac{A_{ji}}{\det A}\right)$, the inverse of A, the following inequalities:

$$|A_{ij}| \le \sigma_j |A_{ii}| \quad , \quad i \neq j \qquad , \tag{4}$$

and

$$\frac{1}{|a_{ii}|(1+\sigma_i)} \le \left|\frac{A_{ii}}{\det A}\right| \le \frac{1}{|a_{ii}|(1-\sigma_i)} \quad , \quad i = 1,2,\ldots,n. \tag{5}$$

Similar results hold if A is strictly diagonally column dominant. Setting

$$\alpha = \min_{1\le k\le n}[|a_{kk}|(1-\sigma_k)] \quad , \tag{6}$$

Varah [22] establishes that

$$\|A^{-1}\|_\infty = \max_{1\le i\le n} \sum_{k=1}^{n} \left|\frac{A_{ki}}{\det A}\right| < \frac{1}{\alpha} \tag{7}$$

when the matrix A satisfies (2).

We will now prove an important theorem using mathematical induction concerning M-matrices.

<u>Definition:</u> An M-matrix is an n × n real matrix, $A = (a_{ij})$, such that

(i) $a_{ij} \le 0$, $i \ne j$,

(ii) A is nonsingular, and

(iii) $A^{-1} \ge 0$.

If A is a strictly diagonally dominant matrix, then Price [14] proves that $\det A > 0$ if $a_{ii} > 0$ for all i.

<u>Theorem 1.</u>

Let $A^{(p)} = (a_{ij}^{(p)})$ be a real strictly row diagonally dominant $p \times p$ matrix in the sense that

$$a_{ii}^{(p)} - \sum_{\substack{j=1 \\ j\ne i}}^{n} |a_{ij}| > 0 \quad ,$$

where $a_{ij}^{(p)} \le 0, i \ne j$. Then $(A^{(p)})^{-1} > 0$ and hence $A^{(p)}$ is an M-matrix.

<u>Proof:</u> We will show that $(A^{(p)})^{-1} > 0$ by induction. Since for $p = 1$, the statement is true, we will verify the statement for $p = 2$. Since $\det A^{(2)} > 0$, then

$$(A^{(2)})^{-1} = \frac{1}{\det A^{(2)}} \begin{pmatrix} a_{22}^{(2)} & -a_{12}^{(2)} \\ -a_{21}^{(2)} & a_{11}^{(2)} \end{pmatrix} \ge 0,$$

in view of $a_{ij}^{(2)} \le 0, i \ne j$ and $a_{ii}^{(2)} > 0$. Assume the theorem to be true for $p = n$, i.e., $A_{ij}^{(n)} > 0, a_{ij}^{(n)} \le 0, i \ne j$. Since $A^{(n)}$ is strictly diagonally dominant, $\det A^{(n)} > 0$. To prove the result for $p = n+1$, we will consider the linear system

$$\sum_{j=1}^{n+1} a_{ij}^{(n+1)} x_j = b_i \quad , \quad i = 1, 2, \dots, n+1 \quad . \tag{8}$$

Since $a_{ii}^{(n+1)} > 0$ and $A^{(n+1)}$ is strictly diagonally dominant, we can solve the system to give

$$x_j = \sum_{k=1}^{n+1} \frac{A_{kj}^{(n+1)}}{\det A^{(n+1)}} b_k \quad , \quad j = 1, 2, \dots, n+1 \quad . \tag{9}$$

Putting $j = n+1$, we get

$$x_{n+1} = \sum_{k=1}^{n+1} \frac{A_{k,n+1}^{(n+1)}}{\det A^{(n+1)}} b_k \quad . \tag{10}$$

From (8), we get for $i = n+1$,

$$x_{n+1} = \frac{b_{n+1}}{a^{(n+1)}_{n+1,n+1}} - \sum_{j=1}^{n} \frac{a^{(n+1)}_{n+1,j}}{a^{(n+1)}_{n+1,n+1}} x_j \ , \qquad (11)$$

which we will use to eliminate x_{n+1} in (8) for $i = 1,2,\dots,n$ to get

$$\sum_{j=1}^{n} c^{(n)}_{i,j} x_j = b_i - \frac{a^{(n+1)}_{i,n+1}}{a^{(n+1)}_{n+1,n+1}} b_{n+1} \quad , \quad i = 1,2,\dots,n \, , \qquad (12)$$

where the matrix $C^{(n)} = (c^{(n)}_{ij})$, $i,j = 1,2,\dots,n$ is given by

$$c^{(n)}_{ij} = a^{(n+1)}_{ij} - \frac{a^{(n+1)}_{n+1,j}\, a^{(n+1)}_{i,n+1}}{a^{(n+1)}_{n+1,n+1}} \quad .$$

For $i = j$,

$$c^{(n)}_{ii} = a^{(n+1)}_{ii} - \frac{a^{(n+1)}_{n+1,i} a^{(n+1)}_{i,n+1}}{a^{(n+1)}_{n+1,n+1}}$$

$$\geq a^{(n+1)}_{ii} - |a^{(n+1)}_{n+1,i}| \frac{|a^{n+1}_{i,n+1}|}{a^{(n+1)}_{n+1,n+1}}$$

$$\geq a^{(n+1)}_{ii} - |a^{(n+1)}_{n+1,i}|$$

$$> 0 \, .$$

For $i \neq j$, clearly

$$c^{(n)}_{ij} \leq a^{(n)}_{ij} \leq 0 \qquad \text{(by def. of } c^{(n)}_{ij}\text{)} \, .$$

Further, $C^{(n)}$ is strictly diagonally dominant since for $i = 1,2, \dots , n$,

$$c_{ii}^{(n)} - \sum_{\substack{j=1\\j\neq i}}^{n} |c_{ij}^{(n)}| \geq a_{ii}^{(n+1)} - \frac{|a_{i,n+1}^{(n+1)}||a_{n+1,j}^{(n+1)}|}{a_{n+1,n+1}^{(n+1)}} - \sum_{\substack{j=1\\j\neq i}}^{n} |a_{ij}^{(n+1)}| + \frac{\left|a_{i,n+1}^{(n+1)}\right|\left|a_{n+1,j}^{(n+1)}\right|}{a_{n+1,n+1}^{(n+1)}} \sum_{j=1}^{n} \left|a_{n+1,j}\right|$$

$$\geq a_{ii}^{(n+1)} - \sum_{\substack{j=1\\j\neq i}}^{n} |a_{ij}^{(n+1)}| - |a_{i,n+1}^{(n+1)}|$$

$$\geq a_{ii}^{(n+1)} - \sum_{j=1}^{n+1} |a_{ij}^{(n+1)}|$$

$$> 0 \quad .$$

Now solving (12) by Cramer's Rule, in the usual notation

$$x_j = \sum_{k=1}^{n} \frac{C_{kj}^{(n)}}{\det C^{(n)}} \left[b_k - \frac{a_{k,n+1}^{(n+1)}}{a_{n+1,n+1}^{(n+1)}} b_{n+1} \right] \quad , \quad j = 1,2,\dots,n \quad . \tag{13}$$

It is clear that the coefficients of $b_i (i = 1,2,\dots,n)$ in (13) are nonnegative and by comparing the coefficients of $b_i (i = 1,2,\dots,n)$ from (9) and (13) we conclude that

$$\frac{A_{kj}^{(n+1)}}{\det A^{(n+1)}} \geq 0 \quad , \quad j = 1,2,\dots,n \ , \ k = 1,2,\dots,n+1 \, ,$$

since the b_i's are arbitrary.

It only remains to show that

$$A_{k,n+1}^{(n+1)} \geq 0 \ , \ k = 1,2,\dots,n+1 \quad . \tag{14}$$

From (11) and (13), we get

$$x_{n+1} = \frac{b_{n+1}}{a_{n+1,n+1}^{(n+1)}} - \sum_{j=1}^{n} \frac{a_{n+1,j}^{(n+1)}}{a_{n+1,n+1}^{(n+1)}} \left\{ \sum_{k=1}^{n} \frac{C_{kj}^{(n)}}{\det C^{(n)}} \left[b_k - \frac{a_{k,n+1}^{(n+1)}}{a_{n+1,n+1}^{(n+1)}} b_{n+1} \right] \right\} \quad .$$

Observing as before that the coefficients of the b_i's are nonnegative and comparing with (10), we conclude (14). Hence the theorem.

Now we will prove a theorem on tridiagonal matrices which will express all the cofactors in terms of principal subdeterminants. We are concerned with the tridiagonal $p \times p$ matrix $A = (a_{ij})$ where every off diagonal element is -1. We will use the notation $A^{(r,s)}$ to represent a principal tridiagonal submatrix of size $(s-r+1) \times (s-r+1)$ whose diagonal entry in the first row is a_{rr} and the diagonal entry in the last row is a_{ss}.

Theorem 2. Let $A = A^{(1,n)}$ be an $n \times n$ tridiagonal symmetric matrix with each nonzero off diagonal element being equal to -1. If $A^{-1} = \left(\frac{A_{ji}}{\det A}\right)$, then we can express the cofactors A_{ji} in terms of principal subdeterminants as follows:

$$A_{ij} = \det A^{(1,i-1)} \det A^{(j+1,n)} \quad , \; 1 \le i \le j \le n \quad ,$$

where $\det A^{(1,0)}$ and $\det A^{(n+1,n)}$ are each defined to be unity. A similar result holds for $1 \le j \le i \le n$.

Proof. Due to symmetry, we need only consider $1 \le i \le j \le n$. The cases when $i = 1, j = 1$ and $i = n, j = n$ hold trivially, while when $i = 1$, $j = n$, we have

$$A_{1n} = (-1)^{n+1} \det \begin{bmatrix} -1 & a_{22} & & -1 & & \\ & -1 & & a_{33} & -1 & \\ & & \ddots & & & \\ & & & & -1 & a_{n-1,n-1} \\ & & & & & -1 \end{bmatrix}$$

$$= (-1)^{n+1}(-1)^{n+1}$$

$$= 1$$

For the case i = 1, 1 < j < n ,

$$A_{1j} = (-1)^{1+j} \det \left[\begin{array}{cccccc|cc} -1 & a_{22} & & -1 & & & & \\ & -1 & & a_{33} & & -1 & & \\ & & \ddots & & & & & \\ & & & -1 & & a_{j-1,j-1} & & \\ & & & & & -1 & -1 & \\ \hline & & & & & 0 & & A^{(j+1,n)} \end{array} \right]$$

$$= (-1)^{1+j}(-1)^{j-1} \det A^{(j+1,n)}$$

$$= \det A^{(j+1,n)} .$$

Similarly, we can establish for $1 < i < n$, $j = n$, that $A_{i,n} = 1$. For the case 1 < i = j ≤ n,

$$A_{ii} = \left[\begin{array}{c|c} A^{(1,i-1)} & 0 \\ \hline 0 & A^{(i+1n)} \end{array} \right]$$

$$= \det A^{(1,i-1)} \det A^{(i+1,n)} \quad .$$

Finally, for the case 1 < i < j < n ,

$$A_{ij} = (-1)^{i+j}\det\left[\begin{array}{c|ccccc|c}
A^{(1,i-1)} & & & & & & 0 \\
 & -1 & & & & & \\ \hline
 & -1 & a_{i+1,i+1} & -1 & & & \\
0 & & -1 & a_{i+2,i+2} & -1 & & \\
 & & & \ddots & & & \\
 & & & & -1 & a_{j+1,j+1} & \\
 & & & & & -1 & -1 \\ \hline
0 & & & & & 0 & A^{(j+1,n)}
\end{array}\right]$$

By expanding the determinant according to the column i, (0,0, .. , 0,-1, -1,0, ... , 0), we get

$$A_{ij} = (-1)^{i+j}\{(-1)(-1)^{i+i-1}\det\left[\begin{array}{c|ccccc|c}
A^{(1,i-2)} & & & & & & \\
 & -1 & & & & & \\ \hline
 & 0 & a_{i+1,i+1} & -1 & & & \\
 & & -1 & a_{i+2,i+2} & -1 & & \\
 & & & \ddots & & & \\
 & & & & -1 & a_{j-j-1} & \\
 & & & & & -1 & -1 \\ \hline
 & & & & & & A^{(j+1,n)}
\end{array}\right]$$

$$+(-1)(-1)^{i+i}\det\left[\begin{array}{c|ccccc|c}
A^{(1,i-1)} & & & & & & \\ \hline
 & -1 & a_{i+2,i+2} & -1 & & & \\
 & & -1 & a_{i+3,i+3} & -1 & & \\
 & & & \ddots & & & \\
 & & & -1 & a_{j-1,j-1} & & \\
 & & & & -1 & & -1 \\ \hline
 & & & & & & A^{(j+1,n)}
\end{array}\right]\}$$

$$= D_1 + D_2$$

Expanding the first determinant again according to the column i, (0,0 ... 0,–1,0, ... , 0) we get,

$$D_1 = (-1)^{i+j}(-1)^{i-1+i-2}\det\left[\begin{array}{c|cccc|c} A^{(1,i-3)} & -1 & & & & \\ \hline & 0 & a_{i+1,i+1} & -1 & & \\ & & -1 & a_{i+2,i+2} & -1 & \\ & & & \ddots & & \\ & & & -1 & a_{j-1,j-1} & \\ & & & & -1 & -1 \\ \hline & & & & & A^{(j+1,n)} \end{array}\right]$$

Proceeding in the same manner by expanding the above determinant according to column i, (0,0, ... , 0,-1,0,0 ... 0) we get

$$D_1 = (-1)^{i+j}\det\left[\begin{array}{ccccc|c} a_{11} & -1 & 0 & & & \\ & 0 & a_{i+1,i+1} & -1 & & \\ & & -1 & a_{i+2,i+2} & -1 & \\ & & & \ddots & & \\ & & & -1 & a_{j-1,j-1} & \\ & & & & -1 & -1 \\ \hline & & 0 & & & A^{(i+n,n)} \end{array}\right]$$

$= 0$ (on expanding according to the first column)

The second term of the expansion of A_{ij} is

$$D_2 = (-1)^{i+j} \det \left[\begin{array}{c|cccccc|c} A^{(1,i-1)} & & & & & & & \\ \hline & -1 & a_{i+3,i+3} & -1 & & & & \\ & & -1 & a_{i+4,i+4} & -1 & & & \\ & & & & \ddots & & & \\ & & & & & -1 & a_{j-1,j-1} & \\ & & & & & & -1 & -1 \\ \hline & & & & & & & A^{(i+1,n)} \end{array} \right]$$

Proceeding in the same manner, we finally get, after some simplifications,

$$A_{ij} = \det \left[\begin{array}{c|c} A^{(1,i-1} & 0 \\ \hline 0 & A^{(j+1,n)} \end{array} \right]$$

$$= \det A^{(1,i-1)} \cdot \det A^{(j+1,n)} \quad .$$

2.2 Diagonally dominant infinite matrices

Consider the infinite linear system

$$\sum_{j=1}^{\infty} a_{ij} x_j = b_i \ , \ i = 1,2,\ldots, \tag{16}$$

where the infinite matrix $A = (a_{ij})$ is strictly diagonally row dominant in the sense

$$\sigma_i |a_{ii}| = \sum_{\substack{j=1 \\ j \neq i}}^{\infty} |a_{ij}| \ , \ 0 \le \sigma_i < 1 \, , i = 1,2,\ldots, \ . \tag{17}$$

Shivakumar and Wong [19] have established the following theorem.

<u>Theorem 3:</u> Let, for the system (16) and (17) the following hypotheses hold:

(*i*) $\sum_{i=1}^{\infty} \frac{1}{|a_{ii}|} < \infty$,

(*ii*) $\sum_{\substack{j=1 \\ j \neq i}}^{\infty} |a_{ij}| \leq M$ for some M and all i

(*iii*) $\sum_{i=1}^{\infty} |a_{ij}| < \infty$ for each fixed j

(*iv*) the sequence $\{b_i\}_{i=1}^{\infty}$ is bounded.

Then the system has only one bounded solution. The theorem implies the existence of A^{-1}, the inverse of A and (i) and (ii) imply

$$\sum_{i=1}^{\infty} \sigma_i < \infty \quad . \tag{19}$$

Note that if $a_{ii} > 0$, one can establish that det A and all the principal minors A_{ii} are positive. If in addition, $a_{ij} \leq 0$, $i \neq j$, then $A^{-1} \geq 0$ and we will term the matrix A as an infinite M-matrix. By assuming

$$|a_{ii}|(1 - \sigma_i) \geq \delta > 0 ,$$

and by the method of truncations, it can be shown using Shivakumar [17] that

$$|A_{ij}| \leq \sigma_i |A_{ii}| \ , \ j \neq i ,$$

$$\frac{1}{|a_{ii}|(1+\sigma_i)} \le \left|\frac{A_{ii}}{\det A}\right| \le \frac{1}{|a_{ii}|(1-\sigma_i)} \ , \quad i = 1,2,\dots, \ . \tag{20}$$

Also if $\{|a_{ii}|(1-\sigma_i)\}$ is a strictly increasing sequence, we can extend (7) to

$$\|A^{-1}\|_\infty = \max_{1\le i\le\infty} \sum_{k=1}^{\infty} \left|\frac{A_{ki}}{\det A}\right| < \frac{1}{\alpha} \ ,$$

where

$$\alpha = |a_{11}|(1-\sigma_1) \ .$$

2.3 Comparison of two matrices

For the two matrices (finite or infinite)

$$B(\lambda) = D - \lambda h^2 I \, , \quad B(\mu) = D - \mu h^2 I \, ,$$

we have, formally,

$$B(\lambda) = B(\mu) - (\lambda - \mu) h^2 I \ ,$$

yielding after some calculations

$$B^{-1}(\lambda) = B^{-1}(\mu) + (\lambda - \mu) h^2 B^{-1}(\lambda) B^{-1}(\mu)$$

and

$$B^{-1}(\lambda) = B^{-1}(\mu)[I - (\lambda - \mu) h^2 B^{-1}(\mu)]^{-1} \ .$$

Hence

$$\|B^{-1}(\lambda)\|_\infty \leq \frac{\|B^{-1}(\mu)\|_\infty}{1-\beta} \quad , \tag{22}$$

where

$$\beta = |(\lambda-\mu)|h^2\|B^{-1}(\mu)\|_\infty < 1 \quad . \tag{23}$$

As a consequence of the above, we obtain

$$\frac{B_{jj}(\lambda)}{\det B(\lambda)} - \frac{B_{jj}(\mu)}{\det B(\mu)} = (\lambda-\mu)h^2\sum_{k=1}^{\infty}\frac{B_{kj}(\lambda)}{\det B(\lambda)}\frac{B_{jk}(\mu)}{\det B(\mu)} . \tag{24}$$

Similarly, if $A(\lambda)=\lambda h^2 I - D$, $A(\mu)=\mu h^2 I - D$, we will have

$$\frac{A_{jj}(\lambda)}{\det A(\lambda)} - \frac{A_{jj}(\mu)}{\det A(\mu)} = (\mu-\lambda)h^2\sum_{k=1}^{\infty}\frac{A_{kj}(\lambda)}{\det A(\lambda)}\frac{A_{jk}(\mu)}{\det B(\mu)} \quad . \tag{25}$$

2.4 A Computational procedure

For computation, we reproduce the procedure given in [18] with some modifications, to expand an infinite matrix $A^{(1,\infty)} = D - \mu h^2 I$, where D is tridiagonal with diagonal elements d_{ii} and each off-diagonal element being -1. The method is based on the row expansion of a determinant. We note that under our conditions, $\det A^{(1,k)}$ diverges as $k \to \infty$. Therefore, we will consider $\det A^{(1,k)}$ for a fixed large k . Starting the expansion for $A^{(1,k)}$ by its first row, we can write

$$\det A^{(1,k)} = (d_{11} - \mu h^2)\det A^{(2,k)} - \det A^{(3,k)}$$

$$= (d_{11} - \mu h^2)[(d_{22} - \mu h^2)\det A^{(3,k)} - \det A^{(4,k)}] - \det A^{(3,k)}$$

$$= [(d_{11} - \mu h^2)(d_{22} - \mu h^2) - 1]\det A^{(3,k)} - (d_{11} - \mu h^2)\det A^{(4,k)} .$$

Proceeding similarly, we get

$$\det A^{(1,k)} = p_s \det A^{(s,k)} - p_{s-1} \det A^{(s+1,k)} \quad ,$$

where

$$p_s = p_{s-1}(d_{s-1,s-1} - \mu h^2) - p_{s-2} , \quad s = 2,3,\dots,$$

and

$$p_0 = 0 , \quad p_1 = 1 .$$

We can now formally write

$$\frac{\det A^{(1,k)}}{\det A^{(s,k)}} = p_{s-1}\left\{\frac{p_s}{p_{s-1}} - \frac{\det A^{(s+1,k)}}{\det A^{(s,k)}}\right\}.$$

If $A^{(1,\infty)}$ is strictly diagonally dominant and if

$$\left\{ d_{ii} - \mu h^2 - \sum_{\substack{j-1 \\ j \neq i}}^{\infty} |d_{ij}| \right\}_{i=1}^{\infty}$$

is a strictly increasing sequence, we can write

$$\frac{1}{d_{s,s} - \mu h^2 + 1} \leq \frac{\det A^{(s+1,k)}}{\det A^{(s,k)}} \leq \frac{1}{d_{s,s} - \mu h^2 - 1} .$$

We wish to find an eigenvalue μ for A, i.e., "$\det A^{(1,\infty)} = 0$" . However, this determinant diverges, as noted earlier. Also, since $\det A^{(s,k)} > 0$ for $k > s > n$ by Price [13], the sign of $\det A^{(1,k)}$ is the same as that of $\dfrac{\det A^{(1,k)}}{\det A^{(s,k)}}$ and this ratio tends to a limit as $k \to \infty$ as seen in [17, Corollaries 1 and 2]. We will denote this limit as $\dfrac{\det A^{(1,\infty)}}{\det A^{(s,\infty)}}$, which has the same sign as $\dfrac{\det A^{(1,k)}}{\det A^{(s,k)}}$ for all $k > s > n$. We will now consider the following cases to determine the sign of $\det A^{(1,k)}$:

(i) If p_{s-1} and p_s are of opposite signs then $\det A^{(1,k)}$ has the same sign as $(-p_{s-1})$.

(ii) If p_{s-1} and p_s are of the same sign, and if

(*a*) $\dfrac{p_s}{p_{s-1}} > \dfrac{1}{d_{s,s} - \mu h^2 - 1}$, then $\det A^{(1,k)}$ is of same sign as p_{s-1}.

(*b*) $\dfrac{p_s}{p_{s-1}} < \dfrac{1}{d_{s,s} - \mu h^2 + 1}$, then $\det A^{(1,k)}$ is of the same sign as $(-p_{s-1})$.

(iii) If neither (i) or (ii) holds, p_{s-1} and p_s are calculated for higher values of s till (i) or (ii) holds. There is a remote possibility that neither of the conditions (i) and/or (ii) are satisfied for a reasonable value of s. The main idea in finding the sign of $\dfrac{\det A^{(1,\infty)}}{\det A^{(s,\infty)}}$ is to use the method of bisection to locate a value of μ such that $\frac{\det A^{(1,\infty)}}{\det A^{(s,\infty)}} = 0$. This of course needs two values of μ such that $\det A^{(1,k)}$ has opposite signs for the two values of μ . By this process, one can achieve upper and lower bounds for the eigenvalues μ to any required degree of accuracy.

CHAPTER 3

Eigenvalue Problems

3.1 Introduction.

In this chapter we study the solution of the system

$$-y'' + f(x)y = \lambda y , \qquad (1)$$

$$y(0) = 0 , \qquad (2a)$$

$$y(\infty) = 0 , \qquad (2b)$$

where $f(x)$ monotonically increases to infinity as x increases to infinity. This system is an analog of the classical Sturm-Liouville eigenvalue problem which is defined on a closed interval [a,b]. The theoretical study of boundary value problems on semi-infinite intervals has not substantially contributed to the numerical solutions of such problems, as in most cases the restrictions concern the solution $y(x)$ and its derivatives and are not easily verifiable. Numerical methods of solution (see Aziz [2])frequently involve replacing the given problem by one on a finite interval or involve experimentation with a succession of finite intervals. These procedures have been used to considerable advantage by Lentini and Keller [8]. Gerek and d'Oliveira [6] use a continued fraction calculation using the replacement of the boundary conditions method. The methods preclude the matching of solutions to the expected exponentially decaying nature of the solution. Other numerical experiments are described by Fox [4] and an account of the WKB method can be found in Bender and Orszag [3]. Truhlar [21] uses the finite difference technique to discuss the one dimensional Schrödinger equation on $(0,\infty)$ and the method again involves finite matrices. Recently Lund and Riley [9] have given a collocation method using sinc collocation basis elements and Whittaker Cardinal functions. For finite element techniques, see Schoombie and Botha [16].

It is well-known that (1), (2a) together with $y(a) = 0$ in a Sturm-Liouville equation has an infinite number of eigenvalues $\lambda_1, \lambda_2, \ldots,$ ($\lambda_n \to \infty$ as $n \to \infty$) which are all real and positive if $f(x)$ is chosen to be a positive function tending to infinity as x tends to infinity. For details concerning the nature of solutions, including exponential decay, see [7].

We use finite difference techniques to get an eigenvalue problem for infinite linear algebraic systems. In this study, we do not truncate the infinite system nor do we replace the given problem on a finite interval. Existence, uniqueness and boundedness concerning the inverse of the infinite matrix along with suitable estimates are used to aid the analysis. We assume for the error analysis the boundedness of the fourth derivative of the solution $y(x)$ (see section 3.3) which, we will later observe, implies the exclusion of the unbounded solution of (1) and (2). In Section (2) we give details of the system and its discretization by using a finite difference scheme.

3.2 The eigenvalue problem (continuous case)

We will now consider the system given by (1), (2a) and discretize it using the points $x_k = kh$, $k = 0,1,\dots$ for an arbitrary but fixed step size $h > 0$. Using Taylor's expansion for $y(x)$ with the differential form of the remainder, we can write

$$y''(x) - \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} = \frac{y^{iv}(\xi_k)}{12}, \qquad \text{where} \quad \xi_k \in (x_{k-1}, x_{k+1})$$

and thus, (1) and (2a,b) will be equivalent to

$$-y_{k-1} + 2y_k - y_{k+1} + h^2 f_k y_k = \lambda h^2 y_k + h^2 t_k(h) \ , \quad k = 1,2,3,\dots \tag{3}$$

with $y_0 = 0$ and in the above notation $f(x_k) = f_k$ and $y(x_k) = y_k$. The error term is given by

$$t_k(h) = \frac{h^2}{12} y^{iv}(\xi_k) \ , \quad \xi_k \in (x_{k-1}, x_{k+1}) . \tag{4}$$

Writing (3) in matrix form we have

$$D\underset{\sim}{y} = \lambda h^2 \underset{\sim}{y} + h^2 \underset{\sim}{T}(h) \tag{5}$$

where

$$\underset{\sim}{y} = (y_1, y_2 \dots)^T \qquad \textit{and} \qquad \underset{\sim}{T}(h) = (t_1(h), t_2(h), \dots)^T \tag{6}$$

and the matrix $D = (d_{ij})$, $i, j = 1,2,3,\dots$ is given by

$$d_{ij} = \begin{cases} -1, & i = j-1, j+1, \\ 2 + h^2 f_i, & i = j, \\ 0, & \textit{otherwise.} \end{cases} \tag{7}$$

The system (5) can be written as

$$(D-\lambda h^2 I)\underset{\sim}{y}=h^2\underset{\sim}{T}(h) \tag{8}$$

or alternately, for a fixed integer $n \geq 1$, we have our equations decomposed into three portions

$$y_{k-1}+[\lambda h^2-(2+h^2 f_k)]y_k+y_{k+1}=-h^2 t_k(h)\,, \tag{9}$$

$$k=1,2,\ldots,n-1\,,$$

$$y_{n-1}+[\lambda h^2-(2+h^2 f_n)]y_n+y_{n+1}=-h^2 t_n(h)\,, \tag{10}$$

$$-y_{k-1}+[2+h^2 f_k-\lambda h^2]y_k-y_{k+1}=h^2 t_k(h)\,, \tag{11}$$

$$k=n+1,n+2,\ldots\ .$$

Where $y_0 = 0$. Note that, if n = 0, (9) and (10) do not exist and (11) is really (8). If n = 1, (9) does not exist. For n > 1, (9)–(11) all exist. For n > 1, we will denote the finite $(n-1)\times(n-1)$ matrix in (9) by $A=(a_{ij})$ and treat (9) as a set of equations in $y_1, y_2 \cdots y_{n-1}$ which can be expressed in terms of y_n and the $t_k(h)$'s. We will denote the inverse of A by

$$A^{-1}=\left(\frac{A_{ji}}{\det A}\right),$$

where A_{ij} and $\det A$ have the usual meanings. Similarly, we will denote the infinite matrix in (11) by B and treat the equations in (10) as a set of equations in $y_{n+1}, y_{n+2}, \ldots$ which can be expressed in terms of y_n. Also we can write

$$B^{-1}=\left(\frac{B_{ji}}{\det B}\right).$$

We now proceed formally to solve (8) or (9)–(11) with $y_0 = 0$. We will justify the inverting of the matrices in the next section (Section 3.3). To do this, we will consider three cases, case (A) being the consideration of (8), case (B) being the consideration of (10) and (11) when n = 1 and case (C) being the consideration of (9)–(11) when n >1.

Case A (n=0). For the system (8)

$$(D - \lambda h^2 I)\underset{\sim}{y} = h^2 \underset{\sim}{T}(h)$$

we put $(D - \lambda h^2 I) = B(\lambda)$ which is consistent with our earlier notation. Using Cramer's Rule to solve

$$B(\lambda)\underset{\sim}{y} = h^2 \underset{\sim}{T}(h), \tag{12}$$

we get

$$y_j = h^2 \sum_{k=1}^{\infty} \frac{B_{kj}(\lambda)}{\det B(\lambda)} t_k(h) \quad , \quad j = 1, 2, \dots, \infty. \tag{13}$$

where

$$B^{-1}(\lambda) = \left(\frac{B_{kj}(\lambda)}{\det B(\lambda)} \right). \tag{14}$$

This gives a formal expression for the eigenvector corresponding to the eigenvalue λ .

Case B (n=1). We get from (10) and (11),

$$[\lambda h^2 - (2 + h^2 f_1)]y_1 + y_2 = -h^2 t_1(h) \tag{15}$$

and

$$-y_{k-1} + [(2 + h^2 f_k) - \lambda h^2]y_k - y_{k+1} = h^2 t_k(h)\,, \tag{16}$$

$$k = 2, 3, \dots, \ .$$

Treating (16) as a system of linear equations in $y_2, y_3, \dots$ and denoting the infinite matrix by $B(= B(\lambda))$, we get

$$B\begin{pmatrix} y_2 \\ y_3 \\ \vdots \end{pmatrix} = h^2 \begin{pmatrix} t_2(h) \\ t_3(h) \\ \vdots \end{pmatrix} + \begin{pmatrix} y_1 \\ 0 \\ \vdots \end{pmatrix}.$$

Again using Cramer's Rule, we get

$$y_j = h^2 \sum_{k=2}^{\infty} \frac{B_{kj}}{\det B} t_k(h) + \frac{B_{2j}}{\det B} y_1\,, \qquad j = 2, 3, \dots \ . \tag{17}$$

In particular,

$$y_2 = h^2 \sum_{k=2}^{\infty} \frac{B_{k2}}{\det B} t_k(h) + \frac{B_{22}}{\det B} y_1$$

which with (15) gives on eliminating y_2,

$$\left[\lambda h^2 - (2 + h^2 f_1) + \frac{B_{22}(\lambda)}{\det B(\lambda)}\right] y_1 = -h^2 t_1(h) - h^2 \sum_{k=2}^{\infty} \frac{B_{k2}(\lambda)}{\det B(\lambda)} t_k(h) \tag{18}$$

where we have taken note of the fact that the elements of B and B^{-1}

are functions of λ. Now substituting for y_1 in (17), we get y_j, $j = 2,3,\ldots$ where y_1 is given by (18). For convenience, we will rewrite (18) as

$$F_1(\lambda)y_1 = -h^2 G_1(\lambda) \tag{19}$$

where

$$F_1(\lambda) = \lambda h^2 - (2 + h^2 f_1) + \frac{B_{22}(\lambda)}{\det B(\lambda)} \tag{20}$$

and

$$G_1(\lambda) = t_1(h) + \sum_{k=2}^{\infty} \frac{B_{k2}(\lambda)}{\det B(\lambda)} t_k(h). \tag{21}$$

Using (19) in (17) we get

$$y_j = h^2 \sum_{k=2}^{\infty} \frac{B_{kj}(\lambda)}{\det B(\lambda)} t_k(h) - h^2 \frac{B_{2j}(\lambda)}{\det B(\lambda)} \frac{G_1(\lambda)}{F_1(\lambda)}, \qquad j = 2,3,\ldots, \tag{22}$$

thereby giving the eigenfunctions corresponding to the eigenvalue λ.

<u>Case (C) ($n \geq 2$).</u> The equation (9) can be written as

$$A \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-1} \end{pmatrix} = -h^2 \begin{pmatrix} t_1(h) \\ t_2(h) \\ \vdots \\ t_{n-1}(h) \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \vdots \\ -y_n \end{pmatrix}.$$

Solving the above system in terms of y_n, we get

$$y_j = -h^2 \sum_{k=1}^{n-1} \frac{A_{kj}(\lambda)}{\det A(\lambda)} t_k(h) - \frac{A_{n-1,j}}{\det A} y_n , \qquad j = 1,2,\dots,n-1 . \tag{23}$$

In particular

$$y_{n-1} = -h^2 \sum_{k=1}^{n-1} \frac{A_{k,n-1}(\lambda)}{\det A(\lambda)} t_k(h) - \frac{A_{n-1,n-1}}{\det A} y_n . \tag{24}$$

Similarly the equations (11) can be written as

$$B \begin{pmatrix} y_{n+1} \\ y_{n+2} \\ \vdots \end{pmatrix} = h^2 \begin{pmatrix} t_{n+1}(h) \\ t_{n+2}(h) \\ \vdots \end{pmatrix} + \begin{pmatrix} y_n \\ 0 \\ \vdots \end{pmatrix} .$$

Solving the above system in terms of y_n, we get

$$y_j = h^2 \sum_{k=n+1}^{\infty} \frac{B_{kj}(\lambda)}{\det B(\lambda)} t_k(h) + \frac{A_{n+1,j}(\lambda)}{\det A(\lambda)} y_n ,$$

$$j = n+1, n+2, \dots \infty . \tag{25}$$

In particular,

$$y_{n+1} = h^2 \sum_{k=n+1}^{\infty} \frac{B_{k,n+1}(\lambda)}{\det B(\lambda)} t_k(h) + \frac{B_{n+1,n+1}(\lambda)}{\det B(\lambda)} y_n . \tag{26}$$

Substituting for y_{n-1} and y_{n+1} in (10) from (25) and (26), and rearranging we get

$$F_n(\lambda) y_n = -h^2 G_n(\lambda) \tag{27}$$

where

$$F_n(\lambda) = \lambda h^2 - (2 + h^2 f_n) - \frac{A_{n-1,n-1}}{\det A} + \frac{B_{n+1,n+1}}{\det B} \tag{28}$$

and

$$G_n(\lambda) = t_n(h) - \sum_{k=1}^{n-1} \frac{A_{k,n-1}}{\det A} t_k(h) + \sum_{k=n+1}^{\infty} \frac{B_{k,n+1}}{\det B} t_k(h) \quad . \tag{29}$$

Note that (27) gives y_n which on using in (24) and (25) gives $y_1, y_2, \ldots$ y_{n-1} and $y_{n+1}, y_{n+2} \;\cdots$.

We will now make suitable assumptions to justify the previous formal results in each of the three cases A, B and C. We will make the following assumption on *f(x)* for fixed $h > 0$:

$$\sum_{k=1}^{\infty} \frac{1}{f_k} < \infty \quad . \tag{A3}$$

The nature of the matrices A and B will now be discussed in the following intervals for λ:

<u>Case A (continued):</u> For the decomposition given in case A, we will choose the interval for λ as

$$-\infty < \lambda h^2 < 1 + h^2 f_1 \quad . \tag{30}$$

Then $B(\lambda) = D - \lambda h^2 I$ is diagonally row dominant and satisfies all the conditions of Theorem (3) in view of (A3) and (30) implying the existence of the inverse $B^{-1}(\lambda)$ thereby justifying (13). In fact, $B^{-1}(\lambda)$ will be an infinite M-matrix.

<u>Case B (continued).</u> For the decomposition of the infinite system given in Case B, we will chose h so that

$$1 + h^2 f_1 < \lambda h^2 < 4 + h^2 f_1 \quad , \quad h^2 f_2 > 4 + h^2 f_1 \quad . \tag{31}$$

Again, we can easily verify that the matrix $B^{(2,\infty)}(\lambda)=B(\lambda)$ satisfies all the conditions of Theorem 1 and hence B^{-1} exists and is an infinite M-matrix thereby justifying (17). In addition, results given in (20) and (21) of Chapter 2 hold.

Case C (continued). For the decomposition of the infinite system given in case C, we will choose the interval for λ as

$$4+h^2 f_{k-1}<\lambda h^2<4+h^2 f_k \tag{32}$$

where

$$h^2 f_{k+1}>4+h^2 f_k \quad , \quad k=1,2,3,\dots .$$

The finite matrix A in this case is strictly diagonally dominant with a positive diagonal although the off diagonal elements might not be negative. Hence A^{-1} exists justifying (23) and the results given in equations (20) and (21) of Chapter 2 still hold. As before, we can establish that the matrix B satisfies all the conditions of Theorem (1) on matrix A and hence $B^{-1}(\lambda)$ exists and is in fact an infinite M-matrix. Hence (25) holds and results of (20) and (21) of Chapter 2 are applicable.

In summary, we have derived the solution to (1) and (2) for the decompositions given in cases A, B and C to values of λ as follows:

$$(a) \qquad Case\ A: \qquad -\infty < \lambda h^2 \le 1 + h^2 f_1 \quad , \quad h^2 f_2 > 4 + h^2 f_1 ,$$

$$(b) \qquad Case\ B: \qquad 1 + h^2 f_1 \le \lambda h^2 \le 4 + h^2 f_1 \quad , \quad h^2 f_2 > 4 + h^2 f_1 , \tag{33}$$

$$(c) \qquad Case\ C: \qquad 4 + h^2 f_k \le \lambda h^2 \le 4 + h^2 f_{k+1} \quad , \quad h^2 f_{k+1} > 4 + h^2 f_k ,$$

$$k = 1,2,3, \ldots \quad .$$

3.3 The eigenvalue problem (discretized case).

The approximate eigenvalue problem is given by putting $t_k(h) = 0$, $k = 1,2,3,\ldots$, in (8) with λ replaced by μ and the equations can now be written as

$$D \underset{\sim}{\bar{y}} = \mu h^2 \underset{\sim}{\bar{y}} \quad , \quad \underset{\sim}{\bar{y}} = (\bar{y}_1, \bar{y}_2, \ldots)^T \quad . \tag{34}$$

All the results of section (3.2) hold under (A1). We will now discuss the existence or otherwise of eigenvalues μh^2 in all the three cases described in (33).

<u>Case A'.</u> In the interval

$$-\infty < \mu h^2 < 1 + h^2 f_1 \quad , \tag{35}$$

we have from (13) and the results in Case A (continued), the infinite system of linear equations (34) has only the null solution. We thereby conclude that there are no eigenvalues μh^2 of D in the interval (35).

<u>Case B'.</u> In the interval

$$1 + h^2 f_1 < \mu h^2 < 4 + h^2 f_1 \quad , \tag{36}$$

we have from (18)

$$F_1(\mu)\bar{y}_1 = \left[\mu h^2 - (2+h^2 f_1) + \frac{B_{22}(\mu)}{\det B(\mu)}\right]\bar{y}_1 = 0\,. \tag{37}$$

For μh^2 to be an eigenvalue of D in the interval given by (36), we need $F_1(\mu)$ to vanish in that interval. We note that $B_{22}(\mu)/\det B(\mu)$ is positive in view of B being a diagonally dominant infinite matrix. We will now show that

(i) $F_1(\mu)$ attains values of opposite signs in (36) and

(ii) $F_1(\mu_1) \geq F_1(\mu_2)$ whenever $\mu_1 > \mu_2$ for all μ in (36).

This will enable us to conclude that there exists one and only one eigenvalue in the interval given by (36).

To prove (i), we note from (20) in Section 2.2,

$$\frac{1}{3+h^2 f_2 - \mu h^2} \leq \frac{B_{22}(\mu)}{\det B(\mu)} \leq \frac{1}{1+h^2 f_2 - \mu h^2}\ . \tag{38}$$

At the left end point of the interval, $\mu h^2 = 1 + h^2 f_1$, we have from (37) and (38)

$$F_1(\mu) \le 1 + h^2 f_1 - (2 + h^2 f_1) + \frac{1}{h^2 f_2 - h^2 f_1}$$

$$= -1 + \frac{1}{h^2(f_2 - f_1)}$$

$$\le -1 + \frac{1}{4} \qquad \text{by virtue of (31)}$$

$$< 0 .$$

Similarly, at the right end of the interval, $\mu h^2 = 1 + 4h^2 f_1$, and we have from (37) and (38)

$$F_1(\mu) \ge 4 + h^2 f_1 - (2 + h^2 f_1) + \frac{B_{22}(\mu)}{\det B(\mu)}$$

$$= 2 + \frac{B_{22}(\mu)}{\det B(\mu)}$$

$$> 0 ,$$

thereby proving (i). To demonstrate (ii), we have

$$F_1(\mu_1) - F_1(\mu_2) = h^2(\mu_1 - \mu_2) + \left[\frac{B_{22}(\mu_1)}{\det B(\mu_1)} - \frac{B_{22}(\mu_2)}{\det B(\mu_2)} \right].$$

using the results of section (2.3) and (24) in particular,

$$F_1(\mu_1) - F_1(\mu_2) = (\mu_1 - \mu_2)h^2 \left\{ 1 + \sum_{k=2}^{\infty} \frac{B_{kj}(\mu_1)}{\det B(\mu_1)} \frac{B_{kj}(\mu_2)}{\det B(\mu_2)} \right\}$$

which establishes the fact $F_1(\mu_1) \geq F_1(\mu_2)$ whenever $\mu_1 \geq \mu_2$ since $B^{-1}(\mu)$ is an infinite M-matrix. Hence we have established the existence of one and only one eigenvalue μh^2 of D in the interval (36).

Case C'. Let for fixed $n \geq 2$,

$$4 + h^2 f_n \leq \mu h^2 \leq 4 + h^2 f_{n+1} \quad , \quad h^2 f_{n+1} > 4 + h^2 f_n \quad , \tag{39}$$
$$n = 1, 2, 3, \ldots ,$$

hold.

We have from (27)

$$[F_n(\mu)]\bar{y}_n = \left[\mu h^2 - (2 + h^2 f_n) - \frac{A_{n-1,n-1}(\mu)}{\det A(\mu)} + \frac{B_{n+1,n+1}(\mu)}{\det B(\mu)}\right]\bar{y}_n = 0. \tag{40}$$

We can establish the diagonal dominance of the finite matrix $A(\mu)$ with positive diagonal elements, which yields on using (39) and (A3),

$$\frac{1}{\mu h^2 - h^2 f_{n-1} - 1} \leq \frac{A_{n-1,n-1}(\mu)}{\det A(\mu)} \leq \frac{1}{\mu h^2 - h^2 f_{n-1} - 3} \ . \tag{41}$$

Similarly we can establish the diagonal dominance of $B(\mu)$ and that $B(\mu)$ is an infinite M-matrix, which yields on using (39) and (A3),

$$\frac{1}{3 + h^2 f_{n+1} - \mu h^2} \leq \frac{B_{n+1,n+1}(\mu)}{\det B(\mu)} \leq \frac{1}{1 + h^2 f_{n+1} - \mu h^2}. \tag{42}$$

As in case B', we will now show that $F_n(\mu)$ as given in (40) changes sign once and only once in the interval (39). Using (41) and (42), we get

$$F_n(\mu) \geq \mu h^2 - (2 + h^2 f_n) - \frac{1}{\mu h^2 - h^2 f_{n-1} - 3} + \frac{1}{3 + h^2 f_{n+1} - \mu h^2}.$$

At the right hand end point of (39),

$$F_n(\mu) \ge 4 + h^2 f_n - (2 + h^2 f_n) - \frac{1}{4 + h^2 f_n - h^2 f_{n-1} - 3} + \frac{1}{3 + h^2 f_{n-1} - 4 - h^2 f_n}$$

$$= 2 - \frac{1}{1 + h^2 (f_n - f_{n-1})} + \frac{1}{h^2 (f_{n+1} - f_n) - 1}$$

$$\ge 2 - \frac{1}{5} + \frac{1}{h^2 (f_{n+1} - f_n) - 1}$$

$$> 0 \qquad \text{on using (39)} \ .$$

Similarly, from (40)–(42) we have

$$F_n(\mu) \le \mu h^2 - (2 + h^2 f_n) - \frac{1}{\mu h^2 - h^2 f_{n-1} - 1} + \frac{1}{1 + h^2 f_{n+1} - \mu h^2} .$$

At the left hand end point of the interval,

$$F_n(\mu) \le 4 + h^2 f_{n-1} - (2 + h^2 f_n) - \frac{1}{3} + \frac{1}{h^2 (f_{n+1} - f_{n-1}) - 3}$$

$$= -\frac{5}{3} - h^2 (f_n - f_{n-1}) + \frac{1}{h^2 (f_{n+1} - f_{n-1}) - 3}$$

$$< 0$$

after repeated applications of (39). It now remains to show that

$F_n(\mu_1) > F_n(\mu_2)$ whenever $\mu_1 > \mu_2$. From (40), we have

$$F_n(\mu_1) - F_n(\mu_2) = (\mu_1 - \mu_1) h^2 + \left[\frac{A_{n-1,n-1}(\mu_2)}{\det A(\mu_2)} - \frac{A_{n-1,n-1}(\mu_1)}{\det A(\mu_1)}\right]$$

$$+ \left[\frac{B_{n+1,n+1}(\mu_1)}{\det B(\mu_1)} - \frac{B_{n+1,n+1}(\mu_2)}{\det B(\mu_2)}\right]$$

Making suitable application of (25) of Section (2.3) for the first square bracket and of (24) of Section (2.3) for the second square bracket above, we get

$$F_n(\mu_1)-F_n(\mu_2)=h^2(\mu_1-\mu_2)\left\{1+\sum_{k=1}^{n-1}\frac{A_{k,n-1}(\mu_1)}{\det A(\mu_1)}\frac{A_{n-1,k}(\mu_2)}{\det A(\mu_2)}+\sum_{k=n+1}^{\infty}\frac{B_{k,n+1}(\mu_1)}{\det B(\mu_1)}\frac{B_{n+1,k}(\mu_2)}{\det B(\mu_2)}\right\}.$$

The third term in the bracket involving elements of B^{-1} is nonnegative and if we show that the second term is also nonnegative and the result $F_n(\mu_1) > F_n(\mu_2)$ whenever $\mu_1 > \mu_2$ follows. To do this we need only observe that since A is a symmetrix tridiagonal matrix, $A_{k,n-1}(\mu)$ and $A_{n-1,k}(\mu)$ for any μ satisfying (39) will have the same sign. Hence we conclude that there is one and only one eigenvalue μh^2 of D in each of the intervals (39).

In fact, we can improve the bounds for eigenvalues μh^2 of D in each of the intervals by considering the decomposition of (34) for $n \geq 2$ to be as follows:

$$\bar{y}_{k-1}+\left[\mu h^2-(2+h^2 f_k)\right]\bar{y}_k+\bar{y}_{k+1}=0 \quad , \quad k=1,2,\ldots,n-1. \tag{43}$$

$$-\bar{y}_{k-1}+\left[(2+h^2 f_k)-\mu h^2\right]\bar{y}_k-\bar{y}_{k+1}=0 \quad , \quad k=n,n+1,\ldots\ . \tag{44}$$

In each of the fixed intervals for μh^2 given by (36) and (37) we has already established that there exists one and only one eigenvalue μh^2 of D. If we now consider the subinterval

$$4+h^2 f_{n-1} \leq \mu h^2 \leq 1+h^2 f_n \quad , \tag{45}$$

the matrices in (43) and (44) are suitably diagonally dominant and we can write

$$\bar{y}_{n-1} = -\frac{A_{n-1,n-1}(\mu)}{\det A(\mu)}\,\bar{y}_n$$

and similarly from (44)

$$\bar{y}_n = \frac{B_{n,n}(\mu)}{\det B(\mu)}\,\bar{y}_{n-1}$$

which together gives

$$\left\{1+\frac{A_{n-1,n-1}(\mu)}{\det A(\mu)}\frac{B_{n,n}(\mu)}{\det B(\mu)}\right\}\bar{y}_n = 0\,.$$

In view of the fact that the expression in the bracket is positive, we have $\bar{y}=0$ implying that there are no eigenvalues μh^2 of D in the interval (45).

Proceeding in the same manner, we now decompose (34) for fixed $n \geq 1$, as follows:

$$\bar{y}_{k-1} + [\mu h^2 - (2+h^2 f_k)]\bar{y}_k + \bar{y}_{k+1} = 0 \quad , \quad k = 1,2,\dots,n$$

$$-\bar{y}_{k-1} + [2+h^2 f_k - \mu h^2]\bar{y}_k - \bar{y}_{k+1} = 0 \quad , \quad k = n+1, n+2, \dots, \infty\,,$$

in the subinterval

$$3 + h^2 f_n \leq \mu h^2 \leq 4 + h^2 f_n \tag{46}$$

we can show that the matrices involved are suitably diagonally dominant and that there are no eigenvalues μh^2 of D in the interval (46).

In summary, we have established the existence of one and only one eigenvalue μh^2 of D in each of the intervals

$$1+h^2 f_n < \mu h^2 < 3+h^2 f_n \quad , \quad n=1,2,3,\ldots \quad . \tag{47}$$

3.4 Error Analysis.

In this section, we will derive error bounds for $|\lambda_n - \mu_n|$, $n=1,2,3,\ldots$, where λ_n represents the eigenvalues of the continuous system described in Section (3.2) and μ_n represents the eigenvalues of the discretized case described in Section (3.3). We note that the results derived in these sections hold for all values of h and we will assume that for a given h, we can calculate by the numerical procedure of section (2.4) the values of μ for any required degree of accuracy. In each of these cases, we will select that value h which will give an upper bound for $|\lambda - \mu|$. The process of selection of h in each of the cases A, B, C of Section 3.2 will be dealt with later. In this process we will also give information regarding the eigenvector $\underset{\sim}{y} = (y_1, y_2, \ldots)^T$ in Section (3.2) and in particular the behaviour of y_j as j tends to infinity.

If λ is an eigenvalue of (1) and (2), λh^2 will be in one of the intervals for any given h,

$$I_1 = (0, 4+h^2 f_1)$$

and

$$I_n = (4+h^2 f_{n-1}, 4+h^2 f_n) \quad , \quad n=1,2,\ldots \quad .$$

Also we know that there exists one and only one eigenvalue μh^2 of D in each of the following intervals:

$$J_n = (1+h^2 f_n \,, 3+h^2 f_n) \quad , \quad h^2 f_{n+1} > h^2 f_n \quad , \quad n = 1,2,3, \dots \, .$$

Case (i). If λh^2 lies in I_1 and μh^2 in J_1 for a given h, we have from (18) and (37),

$$F_1(\lambda_1) - F_1(\mu_1) = -\frac{h^2}{y_1} G_1(\lambda_1) \quad , \quad y_1 \neq 0$$

or

$$(\lambda_1 - \mu_1)h^2 + \frac{B_{22}(\lambda_1)}{\det B(\lambda_1)} - \frac{B_{22}(\mu_1)}{\det B(\mu_1)} = \frac{-h^2}{y_1}\left[t_1(h) + \sum_{k=2}^{\infty} \frac{B_{k2}(\lambda_1)}{\det B(\lambda_1)} t_k(h) \right]$$

On using (24) of Chapter 2, the left side of the above equation becomes

$$(\lambda_1 - \mu_1)h^2 \left[1 + \sum_{k=2}^{\infty} \frac{B_{k2}(\lambda_1)}{\det B(\lambda_1)} \frac{B_{2k}(\mu_1)}{\det B(\mu_1)} \right].$$

Now using the results of Theorem 2 of Section 2.1, we get

$$\lambda_1 - \mu_1 = -\frac{1}{y_1} \frac{\left[t_1(h) + \sum_{k=2}^{\infty} \frac{B_{k2}(\lambda_1)}{\det B(\lambda_1)} t_k(h) \right]}{\left[1 + \sum_{k=2}^{\infty} \frac{B_{k2}(\lambda_1)}{\det B(\lambda_1)} \frac{B_{2k}(\mu_1)}{\det B(\mu_1)} \right]} . \tag{48}$$

If we assume from (5), for some positive constant M,

$$\max | t_k(h) | \leq M \frac{h^2}{12} \tag{A4}$$

then (48) yields on using (21) and (22) of Chapter 2,

$$|\lambda_1-\mu_1| \le \frac{Mh^2}{12|y_1|}\left[1+\frac{\|B^{-1}(\mu_1)\|}{1-\beta_1}\right] \tag{49}$$

provided that $\beta_1 = |\lambda_1-\mu_1|\, h^2 \|B^{-1}(\mu_1)\| < 1$ holds.

For numerical work, we can use the initial estimate

$$|\lambda_1-\mu_1| \le \frac{3}{h^2}+f_1 \tag{50}$$

where we are assuming that λ_1 lies I_1 and μ_1 lies in J_1. We can use also the initial estimate

$$|\lambda_1-\mu_1| \le \frac{2}{h^2} \tag{51}$$

where we are assuming that both λ_1 and μ_1 lie in the interval $(1+h^2 f_1\,, 3+h^2 f_1)$. Numerical work now consists of finding a value of h leading to a value of μ such that Q_1 the right side of (49) viz:

$$Q_1 = h^2\left[1+\frac{\|B^{-1}(\mu_1)\|}{1-\beta_1}\right]$$

is a minimum. We note that (48) can be expressed in terms of principal subdeterminants for which we can write upper and lower bounds, by using the results of Theorem 2 as follows:

$$|\lambda_1-\mu_1| = \frac{-1}{y_1}\frac{\left[t_1(h)+\dfrac{B_{22}(\lambda_1)}{\det B(\lambda_1)}t_2(h)+\displaystyle\sum_{k=3}^{\infty}\frac{\det B^{(k-1,\infty)}(\lambda_1)}{\det B(\lambda_1)}t_k(h)\right]}{\left[1+\dfrac{B_{22}(\lambda_1)}{\det B(\lambda_1)}\dfrac{B_{22}(\mu_1)}{\det B(\mu_1)}+\displaystyle\sum_{k=3}^{\infty}\frac{\det B^{(k-1,\infty)}(\lambda_1)}{\det B(\lambda_1)}\frac{\det B^{(k-1,\infty)}(\mu_1)}{\det B(\mu_1)}\right]} \tag{52}$$

with an initial estimate for λ as $0 < \lambda < \frac{4}{h^2} + f_1$ or $\frac{1}{h^2} + f_1 < \lambda < \frac{3}{h^2} + f_1$. Numerical work can be carried out to find a h and the corresponding μ_1 such that the right side of (52) is a minimum.

Case (ii). If $\lambda_n h^2$ lies in I_n and $\mu_n h^2$ lies in J_n, we have from (27) and (40),

$$F_n(\lambda_n) - F_n(\mu_n) = -\frac{h^2}{y_n} G_n(\lambda_n) \quad , \quad y_n \neq 0$$

where $F_n(\mu) = 0$. Rewriting the above equation, we have

$$(\lambda_n - \mu_n)h^2 + \left[\frac{A_{n-1,n-1}(\mu_n)}{\det A(\mu_n)} - \frac{A_{n-1,n-1}(\lambda_n)}{\det A(\lambda_n)}\right]$$

$$-\left[\frac{B_{n+1,n+1}(\mu_n)}{\det B(\mu_n)} - \frac{B_{n+1,n+1}(\lambda_n)}{\det B(\lambda_n)}\right]$$

$$= \frac{-h^2}{y_n}\left[t_n(h) - \sum_{k=1}^{n-1} \frac{A_{k,n-1}(\lambda_n)}{\det A(\lambda_n)} t_k(h) + \sum_{k=n+1}^{\infty} \frac{B_{k,n+1}(\lambda_n)}{\det B(\lambda_n)} t_k(h)\right].$$

Using the results of Section 2.3, the left hand side of the above equation becomes

$$(\lambda_n - \mu_n)h^2\left[1 + \sum_{k=1}^{n-1} \frac{A_{k,n-1}(\lambda_n)}{\det A(\lambda_n)} \frac{A_{n-1,k}(\mu_n)}{\det A(\mu_n)} + \sum_{k=n+1}^{\infty} \frac{B_{k,n+1}(\lambda_n)}{\det B(\lambda_n)} \frac{B_{n+1,k}(\mu_n)}{\det B(\mu_n)}\right]. \tag{53}$$

Noting that each of the terms in the above bracket is nonnegative we can now estimate for $|\lambda_n - \mu_n|$ using (A4), as

$$|\lambda_n - \mu_n| \le \frac{Mh^2}{12|y_n|}\{1+\|A^{-1}(\lambda_n)\|+\|B^{-1}(\lambda_n)\|\}$$

$$\le \frac{M}{12|y_n|}\left\{h^2\left[1+\frac{\|A^{-1}(\mu_n)\|}{1-\alpha_n}+\frac{\|B^{-1}(\mu_n)\|}{1-\beta_n}\right]\right\} \tag{54}$$

where

$$\alpha_n = |\lambda_n - \mu_n| h^2 \|A^{-1}(\mu_n)\| < 1 \qquad \text{and}$$

$$\beta_n = |\lambda_n - \mu_n| h^2 \|B^{-1}(\mu_n)\| < 1 \qquad \text{hold.}$$

Again, as in Case B, we will select an h with its corresponding value for μ_n which will make Q_n, the right side of (54), minimum where

$$Q_n = h^2\left[1+\frac{\|A^{-1}(\mu_n)\|}{1-\alpha_n}+\frac{\|B^{-1}(\mu_n)\|}{1-\beta_n}\right] \tag{55}$$

n = 2,3, ... Once $\mu'_n s$ are known, the norms involved in Q_n, $n = 1,2,3, \ldots$, are given by (21) of Section 2. An initial estimate for $|\lambda_n - \mu_n|$ in Q_n is either

$$|\lambda_n - \mu_n| \le \max\left\{\frac{3}{h^2}, (f_n - f_{n-1}) - \frac{1}{h^2}\right\} \tag{56}$$

if we assume λ_n lies in I_n and μ_n in J_n, or

$$|\lambda_n - \mu_n| \le \frac{2}{h^2} \tag{57}$$

if we assume that λ_n and μ_n both are in the interval $\left(\frac{1}{h^2}+f_n, \frac{3}{h^2}+f_n\right)$.

Note also that we can express all the cofactors in (53) and its previous equation in terms of principal submatrices from Theorem 2, for which upper and lower bounds are easily given.

3.5 The solution of the continuous system.

We will now revert to the system given by (1) and (2) which is equivalent to (5). For values of λh^2 which are not eigenvalues of D we need to show that y_j tends to zero as j tends to infinity in (5) implying that (2b) is satisfied. We will assume that λh^2 is not an eigenvalue of D hence, implying that the expression $F_n(\lambda)$ is not zero for $n = 1,2,3,$ ... . We will assume the usual a-priori estimate (A4) to discuss the behaviour of the solution as x tends to infinity.

<u>Case A:</u> Let $-\infty < \lambda h^2 < 1 + h^2 f_1$ From (13) and (A4), we have

$$|y_j| \leq \frac{M}{12} h^4 \sum_{k=1}^{\infty} \frac{B_{kj}^{(1,\infty)}}{\det B^{(1,\infty)}} \quad .$$

Since B is an infinite diagonally dominant M-matrix, and from (5) of Chapter 2,

$$|y_j| \le \frac{M}{12} h^4 \left\{ \frac{B_{jj}}{\det B} + \sigma_j \left[\sum_{\substack{k=2 \\ k \ne j}}^{\infty} \frac{B_{kk}}{\det B} + \frac{B_{11}}{\det B} \right] \right\} \quad , \quad j > 1$$

$$\le \frac{Mh^4}{12} \left\{ \frac{1}{h^2 f_j - \lambda h^2} + \sigma_j \left[\sum_{k=2}^{\infty} \frac{1}{h^2 f_k - \lambda h^2} + \frac{B_{11}}{\det B} \right] \right\}.$$

By an elementary argument based on expanding det B by the first row, the boundedness of $\frac{B_{11}}{\det B}$ can be established. In view of (A3), we conclude that y_j tends to zero as j tends to infinity since σ_j tends to zero as j tends to infinity.

Case B. Now let $1 + h^2 f_1 < \lambda h^2 < 4 + h^2 f_1$. From (19) and using the fact that B is an infinite M-matrix and that $F_1(\lambda) \ne 0$ when λh^2 is not an eigenvalue of D, we have for $j = 2,3, \ldots$, from (17),

$$|y_j| \le \frac{M}{12} h^4 \sum_{k=2}^{\infty} \frac{B_{kj}}{\det B} + \sigma_j \frac{B_{22}}{\det B} |y_1|$$

$$\le \frac{M}{12} h^4 \sigma_j \sum_{k=2}^{\infty} \frac{B_{kk}}{\det B} + \sigma_j \frac{B_{22}}{\det B} |y_1| \quad .$$

Using arguments analogous to Case A, we can establish that y_j tends to zero as j tends to infinity.

Case C. Let $4 + h^2 f_{n-1} < \lambda h^2 < 4 + h^2 f_n$, $n = 2,3,\ldots$ From (25),

$$|y_j| \le \frac{M}{12} h^4 \sum_{k=n+1}^{\infty} \frac{B_{kj}}{\det B} + \frac{B_{n+1,j}}{\det B} |y_n|$$

$$\le \frac{Mh^4}{12}\left[\frac{B_{jj}}{\det B} + \sigma_j \sum_{k=n+1}^{\infty} \frac{B_{kk}}{\det B}\right] + \sigma_j \frac{B_{n+1,n+1}}{\det B} |y_n| \quad .$$

In view of the fact that $\frac{B_{jj}}{det\,B}$ and σ_j tend to zero as j tends to infinity and since the infinite sum is bounded, we conclude that y_j tends to zero as j tends to infinity.

We now collect the main resuls of this chapter in the following two theorems.

<u>Theorem 4.</u> For the system (1)–(2a,b), and for $x_k = kh$, $k= 0,1,2,3, \ldots$, $h > 0$ and fixed, let the following hypotheses hold:

(i) $\sum_{k=1}^{\infty} \frac{1}{f(x_k)} < \infty$ $\qquad (A3)$

(ii) $h^2 f(x_{k+1}) > h^2 f(x_k) + 4 \quad , \quad k = 1,2,3,\ldots$ $\qquad (A4)$

(iii) $|y^{iv}(x)| \le M \quad , \quad x \ge 0 \quad .$ $\qquad (A5)$

Then, for all values of λh^2 which are not eigenvalues of the matrix D in (8), the system (1)–(3) has a solution. Also if λh^2 is an eigenvalue of matrix D in (8), then also the system has a solution.

Note that in the above theorem, assumption of a common value of h is made for all cases A, B and C to ensure the inclusion for discussion of all values of λh^2 (other than the eigenvalues of D) in $-\infty < \lambda h^2 < \infty$. It should be noted, however, that the value of h in each of the cases can be different and we have the following theorem.

Theorem 5. For the system (1)–(3), let $(h_n)_{n=1}^{\infty}$ be an infinite sequence of positive numbers satisfying

$$h_n^2 f[(n+1)h_n] > h_n^2 f(nh_n) + 4 \tag{58}$$

then there exists one and only one eigenvalue $\mu_n h_n^2$ of D in each of the intervals

$$1 + h_n^2 f(nh_n) < \mu_n h_n^2 < 3 + h_n^2 f(nh_n) \quad , \tag{59}$$

$$n = 1,2,3,\ldots \quad .$$

3.6 An example: Schrödinger equation

Consider the one-dimensional Schrödinger equation [19] satisfying

$$\frac{d^2x}{dx^2} + (\lambda - x^2)y = 0 \quad , \quad y(0) = 0 \quad , \quad y(\infty) = 0 \quad ,$$

where x is the distance displaced, λ's represent the permitted energy levels of a particle in the potentials $f(x) = x^2$. It is known that the eigenvalues λ_n are given by $4n\text{-}1$, $n = 1,2,3, \ldots$, and in fact a solution ψ_n corresponding to λ_n is given by

$$\psi_n(x) = e^{-x^2/2} H_{2n+1}(x)$$

where $H_n(x)$ is the Hermite polynomial of degree n. Clearly, the results of the earlier sections are applicable. For $\lambda = 3$, $y(x) = 2xe^{-x^2/2}$ with the corresponding $|\psi^{iv}(x)| \leq M \approx 11.5661$ occuring at x = 0.6167. For $\lambda = 7$, $\psi(x) = (8x^3 - 12x)e^{-x^2/2}$ with the corresponding $|\psi^{iv}(x)| \leq M \approx 216.3994$ occuring at $x \approx 0.5124$.

We select a value of h and then calculate μ from the computational procedure of Section 2.4 to derive lower and upper bounds to μ . Care is taken to ensure the selected h satisfies requirements of Theorem 4 which in this case reduces h from (58) to

$$h_n^2[(n+1)^2 h_n^2 - n^2 h_n^2] > 4$$

or

$$h_n^4 > \frac{4}{2n+1} \quad , \quad n = 1,2,3,\dots, \tag{60}$$

and similarly the bisection method is carried on in the interval (59) which in this case becomes

$$\frac{1}{h^2} + n^2 h_n^2 < \mu_n < \frac{3}{h^2} + n^2 h_n^2 \quad , \quad n = 1,2,3,\dots, \quad . \tag{61}$$

Table 1 gives the values of μ_1 for various values of h, with μ_1 and h_1 satisfying (60) and (61). The table also gives the evaluated values of the upper bound Q_1^* of Q_1 by applying (22) and (23) of Chapter 2 and we choose that value of h_1 and hence μ_1 that Q_1^* a minimum. In the table Q_1^* was evaluated with the estimate (50).

Table 1

h_1	$\mu_1 \approx \lambda_1$ (*lower bound* *upper bound*)	Q_1^*
1.31	2.81623518	2.5732687
	2.81623523	
1.32	2.82782022	2.5414171
	2.82782027	
1.33	2.83985554	2.5172919
	2.83985560	
1.34	2.85233751	2.4995137
	2.85233761	
1.35	2.86526235	2.4870207
	2.86526244	
1.36	2.87867656	2.4789827
	2.87867666	
1.37	2.89242618	2.4747405
	2.89242627	
1.38	2.90665758	2.4737649
	2.90665767	
1.39	2.92131674	2.4756255
	2.92131685	
1.40	2.93640002	2.4799689
	2.93640011	
1.45	3.01804438	2.5301781
	3.01804447	
1.50	3.10972542	2.6134532
	3.10972550	

From the above table, we find that the minimum value of Q_1 occurs when h is between 1.37 and 1.39. On further refinement we conclude that $\mu_1 = 2.90410157$ gives an approximate value for λ_1 .

Table 2 gives the summary of calculations for the first 5 eigenvalues.

Table 2

n	h_n	$\mu_n \approx \lambda_n$	*Exact value of* λ_n
1	1.3782	2.9041	3
2	1.0747	6.4304	7
3	0.9464	10.3626	11
4	0.8635	14.8156	15
5	0.8165	19.7366	19

In this example, we have shown that even with the crude approximation that $y^{iv}(x)$ is bounded for all x , we can derive meaningful eigenvalues for the continuous problem. If the value of M is specifically known one could set up an iteration for $|\lambda-\mu|$ using (49) and (54). It is useful to note that the expected exponential decay in $y^{iv}(x)$ can lead to an assumption of the form $|y^{iv}(x)| \le M_1 e^{-\alpha x}$ for suitable values of M_1 and α . Also we note from (60)

$$\sum_{k=1}^{\infty} h_k > \sum_{k=1}^{\infty} \frac{\sqrt{2}}{(2k+1)^{1/4}}$$

showing that $\sum_{k=1}^{\infty} h_k$ is divergent as expected.

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