NUMERICAL APPROXIMATION OF
STURM-LIOUVILLE EIGENVALUES

by

J.W. Paine

A thesis submitted to the
Australian National University
for the degree of Doctor of Philosophy
October, 1979.
Some of the work in this thesis was done in collaboration with Frank de Hoog and Bob Anderssen. In particular Chapter 3 is based on results established with Frank de Hoog and Chapter 4 was developed and refined in close collaboration with Frank de Hoog and Bob Anderssen.

Elsewhere in this thesis, unless another source is acknowledged, the work described is my own.

J.W. Paine
29/10/79
ACKNOWLEDGEMENTS

The work for this thesis was undertaken in the Computing Research Group (formerly the Computer Centre) of the Australian National University, and completed in the Department of Pure Mathematics. I am grateful for the support given by both groups and acknowledge the financial assistance provided by the Australian department of Education and the Australian National University.

I wish to express my gratitude to Frank de Hoog and Bob Anderssen for suggesting this problem and for the many discussions which led to the results presented here. I would also like to thank Mike Osborne, Kris Jittorntrum and Graeme Chandler for the help they provided.

My thanks are especially due to Anna Zalucki for typing this thesis, to Mark Lukas for checking the typescript for mathematical and typographical errors, and to Gisela Paine for being herself.
ABSTRACT

This thesis examines some numerical methods for approximating a long sequence of eigenvalues of Sturm-Liouville problems. The aim is to analyse the convergence of these methods and to introduce modifications which improve the numerical performance. The results show that the use of the transformation to Liouville normal form helps considerably in obtaining eigenvalue estimates suitable for this type of eigenvalue problem.

After a brief introduction where notation and basic results on Sturm-Liouville problems are given, Chapter 1 reviews some of the different classes of numerical methods available and examines their limitations.

In Chapter 2 we develop simple eigenvalue error bounds for some initial value methods based on the standard, modified and scaled Prufer substitutions. However, in practice, it is found that these bounds are not always sharp. Improved bounds are then derived for the scaled and modified phase substitutions. These improved bounds show that the eigenvalue error is most uniform for the estimates obtained using the modified or scaled phase associated with an eigenvalue problem which is in Liouville normal form.

When the problem is in Liouville normal form viable numerical schemes for estimating the eigenvalues can be constructed by approximating the coefficient of the differential equation. In Chapter 3 we show that uniformly valid estimates of a long sequence of eigenvalues can be obtained when piecewise constant approximations are used.

Finally, in Chapter 4, we propose a minor modification of a standard finite difference approximation to eigenvalue problems which are in Liouville normal form. The errors in the eigenvalue estimates obtained using this modification are shown to be greatly superior to those of the original problem.
# Table of Contents

PREFACE

ACKNOWLEDGEMENTS

ABSTRACT

CHAPTER 1: INTRODUCTION

1. Outline of Problem and Assumptions 1
   2. Approximation of the Eigenvalues 5
   3. Outline of Approximation Methods 7
   4. Discussion 13

CHAPTER 2: PRUFER PHASE METHODS

1. Introduction 15
   2. Error Bounds for Huen's Method 24
   3. Numerical Examples 27
   4. Improved Bounds for Huen's Method 37
   5. Error Bounds for the Classical Runge-Kutta Method 55

CHAPTER 3: APPROXIMATION OF THE DIFFERENTIAL EQUATION

1. Introduction 72
   2. Approximation of Differential Equations in Normal Form 72
   3. Convergence Results for Problems in Normal Form 77
   4. Approximation of Differential Equations not in Normal Form 83
   5. Numerical Schemes for Piecewise Constant Approximation 87
   6. Numerical Examples 92
CHAPTER 4 : CORRECTION OF FINITE DIFFERENCE ESTIMATES

1. Introduction 100
2. Preliminaries 102
3. Error estimate for $\tilde{\lambda}_k$ 108
4. Numerical Examples 115
5. Extensions 118

APPENDIX 1 126

APPENDIX 2 136

REFERENCES 139
CHAPTER 1

INTRODUCTION

1.1 Outline of Problem and Assumptions

In many applications such as the study of the Earth's free oscillations and the interaction of atomic particles, the underlying problem reduces to finding the eigenvalues of the Sturm-Liouville system

\[- (pu')' + qu = \lambda ru , \quad u' = \frac{du}{dx} , \quad x \in (a,b)\]  \hspace{1cm} (1.1.1)

\[\sigma_1 u(a) + pu'(a) = 0 \hspace{1cm} (1.1.2)\]

\[\sigma_2 u(b) - pu'(b) = 0 \hspace{1cm} (1.1.3)\]

We assume that

\[- \infty < a < b < \infty \]

\[0 < p_m \leq p(x) \leq p_M \]

\[0 < r_m \leq r(x) \leq r_M \]

\[q(x) \geq 0 \]

where \(p_m, p_M, r_m, r_M\) are constants,

\[p, q, r \in PC[a,b] \]

\[\sigma_1 \geq 0 , \quad \sigma_2 \geq 0 .\]

Throughout this thesis \(C^m[a,b]\) will denote the set of functions that are \(m\) times continuously differentiable on \([a,b]\) and \(PC[a,b]\) is the set of functions piecewise continuous on \([a,b]\).
Under the above assumptions the eigenvalue problem (1.1.1) - (1.1.3) has the following properties (compiled from Courant and Hilbert (1953), Tikhonov and Samarskii (1961), Atkinson (1964) and Fix (1967)):

(i) The eigenvalues \( \{ \lambda_k \}_{k=1}^{\infty} \) form a real denumerable set having no finite point of accumulation, and can be ordered

\[
0 < \lambda_1 < \lambda_2 < \ldots < \lambda_k < \infty.
\]

There also exist constants \( C_1 \) and \( C_2 \) such that

\[
C_1 k^2 \leq \lambda_k \leq C_2 k^2. \tag{1.1.4}
\]

(Here and below \( C \) and \( C_i \), \( i = 0, 1, 2, \ldots \) denote constants bounded independently of \( k \)).

(ii) For each eigenvalue \( \lambda_k \) there is a unique (up to sign) eigenfunction \( u_k \) which satisfies

\[
\int_a^b ru_k^2 \, dx = 1
\]

\[
\int_a^b ru_k u_j \, dx = 0 \quad k \neq j.
\]

Furthermore, this eigenfunction has precisely \( (k-1) \) zeroes in \((a,b)\) and

\[
\| u_k \|_\infty \leq C \quad \text{for } k = 1, 2, 3, \ldots \tag{1.1.5}
\]

\[
\| pu_k' \|_\infty \leq C \sqrt{\lambda_k} \tag{1.1.6}
\]

(iii) Define

\[
Lu = -(pu')' + qu, \quad u \in D
\]

where
$$D = \{ u \in L^2([a,b]) \mid u, pu' \text{ are absolutely continuous},$$

$$\sigma_1 u(a) + pu'(a) = 0, \quad \sigma_2 u(b) - pu'(b) = 0, \quad Lu \in L^2([a,b]) \}. $$

Let $H_{\underline{L}}$ be the Hilbert space completion of $D$ with respect to the norm

$$\| u \|_{\underline{L}} := \int_a^b \{ p(u')^2 + qu^2 \} dx, \quad u \in D.$$

Then the eigenvalues have the variational characterisations

$$\lambda_k = \begin{cases} 
\inf \{ R[u] ; u \in H_{\underline{L}}, \int_a^b ru_j dx = 0 \mid j = 1,2,\ldots,k-1\} \\
R[u_k] \\
\inf \{ \sup \{ R[v] \mid v \in T_k \text{ is any } k \text{ dimensional subspace of } H_{\underline{L}} \} \}
\end{cases}$$

where $T_k$ is any $k$ dimensional subspace of $H_{\underline{L}}$, and $R[u]$ is the Rayleigh quotient

$$R[u] := \frac{\int_a^b \{ p(u')^2 + qu^2 \} dx}{\int_a^b ru^2 dx}, \quad u \in H_{\underline{L}}. \quad (1.1.7)$$

(iv) If, in addition to the previous assumptions, we assume $pr \in C^2[a,b]$, then the Liouville transformation

$$t = t(x) = \int_a^x \left( \frac{x}{p} \right)^{1/2} dx; \quad T = \int_a^b \left( \frac{x}{p} \right)^{1/2} dx$$

$$u = wz; \quad w = (pr)^{-1/4} \quad (1.1.8) \quad (1.1.9)$$

transforms (1.1.1) - (1.1.3) to the equivalent Liouville normal form.
I - \ddot{z} + s \dot{z} = \lambda z, \quad \dot{z} = \frac{dz}{dt}, \quad t \in (0,T) \quad (1.1.10)

\sigma_1^* z(0) + \dot{z}(0) = 0 \quad (1.1.11)

\sigma_2^* z(T) - \dot{z}(T) = 0 \quad (1.1.12)

where

s(t) = \left[ t \right] (t) - \left( \frac{\dot{w}}{w} \right)'(t) + \left( \frac{\dot{w}}{w} \right)^2(t) \quad (1.1.13)

\sigma_1^* = \sigma_1 w^2(0) + \left( \frac{\dot{w}}{w} \right)(0) \quad (1.1.14)

\sigma_2^* = \sigma_2 w^2(T) - \left( \frac{\dot{w}}{w} \right)(T) \quad (1.1.15)

The eigenvalues of this problem are identical to those of (1.1.1) - (1.1.3) and the orthonormalised eigenfunctions \{z_k\}_{k=1}^{\infty} have the same properties as the original eigenfunctions.

Define \{\mu_k\}_{k=1}^{\infty}, \{v_k\}_{k=1}^{\infty} to be the ordered eigenvalues and normalised eigenfunctions of (1.1.10) - (1.1.12) for the case \( s(t) \equiv 0 \). Then if we assume that \( s \in C[0,T] \) and that the signs of the \( v_k \) are chosen so that \( (v_k, z_k) \geq 0 \quad k = 1, 2, \ldots \), we have

\[ |\lambda_k - \mu_k| \leq C, \quad (1.1.16) \]

\[ \|z_k - v_k\|_\infty \leq C/\sqrt{\lambda_k}, \quad (1.1.17) \]

\[ \|\dot{z}_k - \dot{v}_k\|_\infty \leq C, \quad (1.1.18) \]

and

\[ |\lambda_k - \mu_k - \frac{1}{T} \int_0^T s dt| \leq C/\lambda_k. \quad (1.1.19) \]
1.2 Approximation of the Eigenvalues

Usually the eigenvalues of (1.1.1) - (1.1.3) cannot be evaluated analytically. Thus a method for approximating them has to be adopted and there are a large number of numerical methods available for this task. Clearly the choice of method will require an assessment of the error characteristics of each scheme in the context of the application.

Often the eigenvalues are related to the energy of the resonant states of the system being studied and only the fundamental and possibly a few (one or two) of its harmonics are required. This is because the first few eigenvalues represent those states which are most easily observed. An example of such a situation arises in the determination of the harmonics of an organ pipe.

Although the calculation of these eigenvalues is not a trivial problem, the first few eigenfunctions are generally smooth slowly varying functions and standard techniques (such as those based on finite differences or Rayleigh quotients) can be used to obtain accurate approximations of the required eigenvalues with reasonable efficiency. Examples of such problems and the techniques for solving them can be found in Collatz (1948) and Kamke (1943).

Not all applications however are limited to finding a small number of eigenvalues. For example, in quantum mechanics the study of atom-ion interaction often reduces to a radial Schrodinger equation of the (dimensionless) form

\[
-\frac{\hbar^2}{2m} u + Vu = \lambda u
\]

\[
\lim_{x \to 0} u(x) = 0, \quad \lim_{x \to \infty} u(x) = 0
\]
where \( V = V(x) \) is the potential function and the eigenvalues in the (possibly empty) discrete part of the spectrum correspond to the energy levels of the bound states of the system being studied. In contrast with the determination of the harmonics of an organ pipe, it is necessary in this case to compute a large number (twenty or more) of eigenvalues to a given absolute or relative error.

Another example arises in geophysics where the eigenfrequencies of the torsional oscillations of the earth are modelled by

$$
- \frac{d}{dr} \left( r^4 \frac{du}{dr} \right) + (\ell+1)(\ell-2)\mu r^2 u = r^4 \rho \lambda u
$$

$$
\mu \frac{du}{dr}(a) = 0 = \mu \frac{du}{dr}(b).
$$

Here, \( u = u(r) \) is the radial displacement, \( \rho = \rho(r) \) denotes the density, \( \mu = \mu(r) \) the rigidity, \( \ell \) is the angular order number and \( a \) and \( b \) denote the radius of the Earth and the core-mantle boundary respectively. The eigenvalues \( \{\lambda_k\}_{k=1}^{\infty} \) denote the squares of the eigenfrequencies of the torsional oscillations.

The aim of such models is to compare the eigenvalues computed for various models of the density \( \rho \) and rigidity \( \mu \) with the corresponding observed values. The spread of observations over values of \( k \) and \( \ell \) is such that it is necessary to compare long sequences of harmonics for many values of \( \ell \). Since the observed values have a uniformly bounded relative error (see e.g. Gilbert and Dziewonski (1975)), we therefore need eigenvalue estimates that have a similar error.

The problem of choosing an efficient method which will give the required eigenvalue estimates in the last two examples is much more difficult than in the case when only a few eigenvalues are required. The reason for drawing
the distinction between calculating a few or many harmonics is the fact
that the eigenfunctions of the higher harmonics are very oscillatory. It
is intuitively clear that, with respect to a given grid, the higher
eigenfunctions cannot be approximated very well by piecewise polynomials.
As a consequence, numerical schemes based on piecewise polynomial
approximation of the eigenfunctions (such as finite differences and finite
elements) will yield poor estimates of the higher eigenvalues.

More specifically the error in the eigenvalues calculated by discretizing
(1.1.1) - (1.1.3) in the obvious manner has the form $C(k)h^p$ where $h$ is
the stepsize and $C(k)$ increases very rapidly with $k$. Typically the
eigenvalue error has the form

$$|\lambda_k - \tilde{\lambda}_k| \leq Ch^{p+k^2}$$

which is to be compared with the requirement of a bounded absolute or
relative error.

1.3 Outline of Approximation Methods

We now give brief descriptions of some of the available methods and
also the corresponding eigenvalue error bounds when these are available. We
use $\Delta_N$ to denote a partition of $[a,b]$ which has the general form

$$\Delta_N = \{x_i, i = 0,1,\ldots,N \mid x_0 = a, x_N = b, x_{i+1} > x_i\}.$$

For each partition $\Delta_N$ we define

$$h = \max_{0 \leq i \leq N-1} |x_{i+1} - x_i|$$

and say the partition is uniform if
\[ x_{i+1} - x_i = h \quad i = 0,1, \ldots, N-1. \]

Also \( C \) and \( C_i \) \( i = 0,1, \ldots \) will denote constants which are bounded independently of \( k \) and \( h \), unless a specific dependence such as \( C(k) \) is shown.

(a) Finite difference methods

At each point \( x_i \in \Delta_N \) the differential equation (1.1.1) is replaced by a finite difference approximation. The resulting linear equations, in conjunction with finite difference approximations of the boundary conditions (1.1.2) - (1.1.3), yields an algebraic eigenvalue problem of the form

\[ Au = \lambda Bu \]

where \( A \) and \( B \) are \((N-1) \times (N-1)\) matrices and \( u \) is an \((N-1)\) dimensional vector.

Keller (1968; Theorem 5.3.3) has shown that, when \( \Delta_N \) is uniform, \( A \) symmetric and \( B \) symmetric positive definite, then the error in the eigenvalue estimates \( \{ \lambda_k \}_{k=1}^{N-1} \) is directly proportional to the truncation error associated with the particular finite difference approximation used. For example, if \( \sigma_1 = \sigma_2 = \infty \), and if the standard centred differences are used, then

\[ |\lambda_k - \lambda_k^-| \leq Ch^2k^4 \quad k < \alpha N \]

for some positive constant \( \alpha < 1 \).

(b) Shooting methods

The aim of these methods is to replace (1.1.1) - (1.1.3) by an equivalent first order (possibly non-linear) boundary value problem of the form
\[ \theta' = f(x, \theta, \lambda) \] (1.3.1)
\[ \theta(a, \lambda) = \alpha(\lambda) \] (1.3.2)
\[ \theta(b, \lambda) = \beta(\lambda) . \] (1.3.3)

The eigenvalues then correspond to the values of \( \lambda \) for which the solution of the initial value problem (1.3.1) - (1.3.2) also satisfies (1.3.3). In general it is necessary to integrate (1.3.1) - (1.3.2) numerically.

If we assume that (1.3.3) is satisfied exactly with respect to the numerical solution of (1.3.1) - (1.3.2) and rounding error effects are ignored, then Keller (1968; Theorem 5.2.3) has shown that the error in the eigenvalue estimates \( \{ \tilde{\lambda}_k \}_{k=1}^M \) (where \( M \) depends on \( N \) and the method used) will have the same order of convergence as that of the method used in the integration. Thus, if a fourth order Runge-Kutta method is used on the uniform partition \( \Delta_N \), then

\[ |\lambda_k - \tilde{\lambda}_k| \leq C(k)h^4 \quad k < k_0(h) . \]

It has been observed by a number of authors (see e.g. Keller (1968), Bailey et al (1978), Pryce (1979)) that \( C(k) \) is determined by two factors. The first is the error in the approximation of \( \theta(b, \lambda) \) and the second is the behaviour of \( \theta(b, \lambda) - \beta(\lambda) \) near its zeroes.

(c) Rayleigh-Ritz methods

As we noted before, eigenvalues have a variational characterisation and this can be used to obtain numerical approximations. If we let \( T_{\leq N} \) denote an \( N \)-dimensional subspace of \( H_L \) with basis \( \{ \phi_i(x) \}_{i=1}^N \), then the Rayleigh-Ritz method consists of finding the stationary points of
\[ R[u] = \frac{\int_a^b \{p(u')^2 + qu^2\} \, dx}{\int_a^b ru^2 \, dx} \]

on \( T_N \). The restriction of \( R[u] \) to \( T_N \) yields the algebraic eigenvalue problem

\[ A\tilde{\alpha} = \tilde{\lambda} B\tilde{\alpha} \]

where \( A \) and \( B \) denote \( N \times N \) matrices with entries

\[ A_{ij} = \int_a^b \{p\phi_i^j + q\phi_i^j\} \, dx \]

\[ B_{ij} = \int_a^b r\phi_i^j \, dx \]

and \( \tilde{a}^T = (a_1, a_2, \ldots, a_N) \). Since \( A \) and \( B \) are symmetric and positive definite, the matrix eigenvalue problem yields the approximations

\[ 0 \leq \tilde{\lambda}_1 \leq \tilde{\lambda}_2 \leq \ldots \leq \tilde{\lambda}_N. \]

The behaviour of these approximations depends heavily on the choice of the basis \( \{\phi_i\}_{i=1}^N \). On the one hand, if the \( \{\phi_i\}_{i=1}^N \) correspond to arbitrarily chosen globally defined coordinate functions, then the rate of growth of \( \tilde{\lambda}_N \) can often greatly exceed that of \( \lambda_N \). On the other hand, if the \( \{\phi_i\}_{i=1}^N \) correspond to the eigenfunctions of an operator similar to (1.1.1) - (1.1.3) then the rate of growth of \( \tilde{\lambda}_N \) matches that of \( \lambda_N \) (A fuller discussion of this point can be found in Mikhlin (1976; Chapter VII)).

Often the \( \{\phi_i\}_{i=1}^N \) are chosen to be piecewise polynomials on the uniform partition \( \Delta_N \) of \([a,b]\) (cf. Mikhlin (1976; Chapter VII) and Schultz (1973; Chapter 8)). When the polynomials are linear, the eigenvalue error
is essentially the same as that for the second order finite difference method. (cf. Andrew (1970)). If a cubic Hermite basis is used, Birkhoff et al (1966) have shown that

$$|\lambda_k - \tilde{\lambda}_k| \leq C_1 h^{6} k^9 \quad k < C_2 N^{8/9}.$$ 

An alternative approach is to take as the \{\phi_i\}_{i=1}^N a subset of the (exact) eigenfunctions of a simpler operator which is either similar or semi-similar in the sense of Mikhlin (1976) to the original one (viz positive definite operators are semi-similar (similar) if their energy spaces (domains) coincide).

The usefulness of this approach has been demonstrated in a geophysical context by Geller and Stein (1978), who showed that approximations generated by their variational method (which corresponds to the implementation of a similar operator approach) are superior to those generated by first and second order perturbation methods. This method has also been used by Shore (1973) to study a quantum mechanics problem.

Although studies of this type clearly show the effectiveness of this approach, convergence bounds of the form $C(k)h^P$ are, in general, not available. However some measure of it's usefulness can be obtained from the result of Mikhlin (1976) that

$$\lambda_k \leq \tilde{\lambda}_k \leq C\lambda_k \quad k = 1, 2, \ldots, N$$

which indicates that the approximate eigenvalues at least have the correct growth as a function of $k$.

(d) Approximation of the differential equation

An alternative approach based on approximating the differential equation itself has been suggested by a number of authors (see e.g. Haskell (1953),
and Pruess (1973)). Specifically we replace \( p, q \) and \( r \) in (1.1.1) - (1.1.3) by the approximations \( \tilde{p}, \tilde{q} \) and \( \tilde{r} \) respectively, and then calculate approximations \( \{ \tilde{\lambda}_k \}_{k=1}^{\infty} \) of the eigenvalues by solving

\[
- (\tilde{p}u')' + \tilde{q}u = \lambda \tilde{r}u, \quad x \in (a,b)
\]  
\[ \sigma_1 u(a) + \tilde{p}u'(a) = 0 \]  
\[ \sigma_2 u(b) - \tilde{p}u'(b) = 0 . \]

If we assume that this eigenvalue problem can be solved exactly, then Pruess (1973) has shown that if \( \tilde{p}(a) = p(a) \) and \( \tilde{p}(b) = p(b) \),

\[ |\lambda_k - \tilde{\lambda}_k| \leq C_k \lambda^M h^{k+1} , \]

for piecewise \( M \)-th order polynomial interpolation of the coefficients on a partition \( \Delta_N \) of \([a,b] \). He also extends this basic result to show that, for piecewise polynomial interpolation at the gaussian points,

\[ |\lambda_k - \tilde{\lambda}_k| \leq C_k \alpha^M h^{2M+2} , \]

where \( \alpha = \max \{1 + \frac{1}{2}M, 5\} \).

For the special case when the eigenvalue problem is in the Liouville normal form (1.1.10) - (1.1.12) and \( s \) is approximated by midpoint interpolation on a uniform partition \( \Delta_N \) of \([a,b] \), Ixaru (1972) has shown that

\[ |\lambda_k - \tilde{\lambda}_k| \leq C_k h^2 . \]
1.4 Discussion

In each of the examples mentioned in §1.2, the requirement is to obtain eigenvalue approximations which satisfy either

\[ |\lambda_k - \tilde{\lambda}_k| \leq \varepsilon \quad k = 1,2,\ldots,n \]

or

\[ |\lambda_k - \tilde{\lambda}_k| \leq C k^2 \quad k = 1,2,\ldots,n . \]

This contrasts with the eigenvalue errors given in §1.3 which are of the form

\[ |\lambda_k - \tilde{\lambda}_k| \leq C(k) h^p \]

where, in general, \( C(k) \) grows rapidly with \( k \).

As we noted before, when \( n \) (the number of eigenvalues required) is small, the growth of \( C(k) \) will have very little influence on the choice of method and hence any of the standard methods will suffice. However when \( n \) is not small (say \( n > 20 \)), then the growth of \( C(k) \) needs to be taken into consideration.

The naive remedy to overcome the growth of \( C(k) \) is to consider the approximation of each eigenvalue as a separate problem and reduce \( h \) appropriately until the required accuracy is obtained. This will of course lead to very inefficient numerical algorithms. A more efficient approach to the problem is to consider how the growth of \( C(k) \) may be reduced.

One very efficient means for achieving this reduction is to use an asymptotic expansion for the eigenvalues (see e.g. Fix (1967)). The use of such expansions gives eigenvalue estimates whose error actually decreases with \( k \). However in most practical problems the asymptotic expansion will
only give the required accuracy for the very large eigenvalues, and these are of little practical interest. Therefore a numerical method will still be needed to approximate the remaining eigenvalues and the asymptotic expansion will only be useful in overcoming the difficulties caused by the growth of $C(k)$ when $k$ is sufficiently large.

In this thesis we pursue three methods for reducing the growth of $C(k)$. They are:

(i) Transforming the eigenfunctions so that the resulting function is no longer highly oscillatory.

(ii) Transforming the differential equation so that the particular method, when applied to the transformed problem, will yield better approximations than if applied to the original problem.

(iii) Using specific properties of the approximate and exact eigenvalues and eigenfunctions to correct the eigenvalue estimates in order to reduce their growth as a function of $k$.

The approaches (i) and (ii) have been widely used in practice, especially in shooting methods. In chapter 2 we study shooting methods based on ordinary, modified and scaled Prufer phases.

In chapter 3 we examine the special case when the coefficients are approximated by piecewise constants.

Finally, in chapter 4, we apply the third approach to the finite difference approximation of an eigenvalue problem in Liouville normal form.

In all cases examined it is found that the eigenvalue problem should be transformed to Liouville normal form before the methods are applied.
CHAPTER 2

PRUFER PHASE METHODS

2.1 Introduction

There are many possible forms of the eigenvalue problem (1.1.1) - (1.1.3) which can be used to construct shooting techniques for approximating the eigenvalues (see, for example Wax (1961), Bailey (1966, 1978), Godart (1966), Scott, Shampine and Wing (1969), Sirohi and Srivastava (1972), Hargrave (1976), Pryce (1979)). A particularly important class of formulations which has received much attention recently are those obtained by Prufer type phase transformations

\[ \tan \theta = \rho \frac{u'}{pu}, \quad \theta = \theta(x, \lambda), \]  

(2.1.1)

where \( \rho = \rho(x, \lambda) \) is some appropriately chosen scaling function. Such transformations lead to non-linear boundary value problems

\[ \theta' = f(x, \theta, \lambda) \]  

(2.1.2)

\[ \theta(a) = \alpha(\lambda) \]  

(2.1.3)

\[ \theta(b) = \beta(\lambda) \]  

(2.1.4)

where

(a) for the standard Prufer phase,

\[ \rho(x, \lambda) = 1 \]

\[ f(x, \theta, \lambda) = \frac{1}{\rho} \cos^2 \theta + (\lambda r-q) \sin^2 \theta \]

\[ \tan \alpha(\lambda) = -1/\sigma_1 \]

\[ \tan \beta(\lambda) = 1/\sigma_2 \]
(b) for the scaled Prüfer phase proposed by Bailey (1978),

\[
\rho(x,\lambda) = \lambda^{\frac{1}{2}} \\
f(x,\theta,\lambda) = \frac{\lambda^{\frac{1}{2}}}{\rho} \cos^2 \theta + \lambda^{\frac{1}{2}}(r - \frac{q}{\lambda}) \sin^2 \theta \\
\tan \alpha(\lambda) = -\frac{\lambda^{\frac{1}{2}}}{\sigma_1} \\
\tan \beta(\lambda) = \frac{\lambda^{\frac{1}{2}}}{\sigma_2}
\]

(c) for the modified phase,

\[
\rho(x,\lambda) = (\lambda^{pr-pq})^{\frac{1}{2}} \\
f(x,\theta,\lambda) = \left(\frac{\lambda r-q}{\rho}\right)^{\frac{1}{2}} + \left(\frac{\lambda^{pr} - (pq)'}{\lambda^{pr-pq}}\right) \frac{\sin 2\theta}{4} \\
\tan \alpha(\lambda) = -\frac{\rho(a,\lambda)}{\sigma_1} \\
\tan \beta(\lambda) = \frac{\rho(b,\lambda)}{\sigma_2}.
\]

Clearly, in each of the above formulations, the eigenvalues \(\{\lambda_k\}_{k=1}^\infty\) will be precisely those values of \(\lambda\) for which \(\tan \theta(b,\lambda) - \tan \beta(\lambda) = 0\), where \(\theta(x,\lambda)\) is the solution of the initial value problem (2.1.2) - (2.1.3) with \(\alpha(\lambda) = \arctan(-\rho(a,\lambda)/\sigma_1)\). A more useful characterization of the eigenvalues is obtained if we put \(\beta(\lambda) = \arctan(\rho(b,\lambda)/\sigma_2)\). Then the eigenvalues are precisely the zeroes of

\[
\omega(\lambda) = \sin(\theta(b,\lambda) - \beta(\lambda))
\]

and for the \(k'\)th eigenvalue

\[
\theta(b,\lambda) - \beta(\lambda) = k\pi.
\]
If, for a given value of $\lambda$, we replace $\theta(b,\lambda)$ by the approximation $\tilde{\theta}(b,\lambda)$ then the approximate eigenvalues are found as the zeroes of

$$\tilde{\omega}(\lambda) = \sin(\tilde{\theta}(b,\lambda) - \beta(\lambda)) .$$

Such approximations can be constructed by numerical integration of the initial value problem (2.1.2) - (2.1.3).

In the sequel we ignore rounding error effects and assume that the roots $\{\lambda_k\}_{k=1}^\infty$ are evaluated exactly. Under these assumptions the accuracy of the eigenvalue estimates is determined by the accuracy of $\tilde{\theta}(b,\lambda)$ and by the behaviour of $\omega(\lambda)$ near its zeroes.

For the Prüfer phases defined above we have

**Lemma 2.1**  
Let $u(x)$ denote the solution of the initial value problem (1.1.1) - (1.1.2) normalised so that $\int_a^b ru^2 \, dx = 1$. Then, for any $\lambda > 0$,

$$\frac{\partial \omega}{\partial \lambda} = \left[ \frac{\rho + upu(b)\frac{\partial \rho}{\partial \lambda}}{\rho^2 u^2(b) + (pu)^2(b)} + \frac{2}{\rho^2 + \sigma^2} \right] \cos(\theta(b,\lambda) - \beta(\lambda)) .$$  

(2.1.5)

**Proof**  
Let $\lambda$ be given and assume $pu(b) \neq 0$. Then, from Atkinson (1964; Theorem 8.4.2) $u(b), pu(b)$ are continuously differentiable functions of $\lambda$ and

$$\frac{\partial}{\partial \lambda} \left[ \frac{u}{pu} \right](b) = (pu)^{-2}(b) .$$

Therefore on differentiating (2.1.1) with respect to $\lambda$ we obtain

$$\frac{\partial \theta}{\partial \lambda} = \frac{\rho + upu(b)\frac{\partial \rho}{\partial \lambda}}{\rho^2 u^2(b) + (pu)^2(b)} .$$
Similarly

\[ \frac{\partial \rho}{\partial \lambda} = \frac{\sigma_2 \frac{\partial \rho}{\partial \lambda}}{\rho^2 + \sigma_2^2}, \]

and the result follows from the definition of \( \omega \).

On the other hand if \( \lambda \) is such that \( pu(b) = 0 \),

\[ \frac{\partial}{\partial \lambda} \left( \frac{pu}{u} \right)(b) = -u^{-2}(b), \]

and the result follows as before on differentiating the relation \( \cot \theta = \frac{pu}{u} \).

When \( \lambda \) is an eigenvalue, we have from the boundary condition (1.1.3),

\[ \frac{upu(b)}{\rho^2 u^2(b) + (pu)^2(b)} = \frac{\sigma_2}{\rho^2 + \sigma_2^2}. \]

Hence

\[ \frac{\partial \omega}{\partial \lambda}(\lambda) = \frac{(-1)^k \rho}{\rho^2 u^2(b) + (pu)^2(b)}, \quad (2.1.6) \]

which implies that the eigenvalues are simple zeroes of \( \omega \). We also note that \( \frac{\partial \omega}{\partial \lambda} \) is a continuously differentiable function of \( \lambda \).

**Lemma 2.2** Let \( \mu \) be an eigenvalue of (2.1.2) - (2.1.4), define

\[ \gamma = \min \{ |\lambda - \mu| : \frac{\partial \omega}{\partial \lambda}(\lambda) = 0 \}, \]

\[ \hat{\gamma} = \frac{|\frac{\partial \omega}{\partial \lambda}(\mu)|}{\max_{|\lambda - \mu| < \gamma} \left| \frac{\partial^2 \omega}{\partial \lambda^2}(\lambda) \right|} . \]
\[ \hat{\eta} = \min \left\{ \frac{\partial \omega}{\partial \lambda}(\lambda) \mid |\lambda - \mu| < \frac{\hat{\nu}}{2} \right\} \]

and assume that

\[ \max \left| \theta(b, \lambda) - \bar{\theta}(b, \lambda) \right| \leq \frac{\hat{\eta}}{2} \quad \text{for some } \lambda \text{ between } \lambda \text{ and } \mu. \]

Then

\[ |\mu - \bar{\mu}| \leq \frac{1}{\hat{\eta}} \left| \theta(b, \mu) - \bar{\theta}(b, \mu) \right| \]

for some zero \( \bar{\mu} \) of \( \tilde{\omega} \). Furthermore

(a) for the Pruefer phase,

\[ \hat{\eta} \geq C \mu^{-1}, \quad \hat{\nu} \geq C \mu^{-\frac{1}{2}} \]

(b) for the scaled phase,

\[ \hat{\eta} \geq C \mu^{-\frac{1}{2}}; \quad \hat{\nu} \geq C \]

(c) for the modified phase,

\[ \hat{\eta} \geq C \mu^{-\frac{1}{2}}, \quad \hat{\nu} \geq C. \]

**Proof** From the Taylor series for \( \frac{\partial \omega}{\partial \lambda} \) expanded about \( \lambda = \mu \),

\[ \frac{\partial \omega}{\partial \lambda}(\lambda) = \frac{\partial \omega}{\partial \lambda}(\mu) + (\lambda - \mu) \frac{\partial^2 \omega}{\partial \lambda^2}(\lambda^*) \] (2.1.7)

for some \( \lambda^* \) between \( \lambda \) and \( \mu \).

Hence
\[
\gamma = \frac{\frac{\partial \omega}{\partial \lambda}(\mu)}{\frac{\partial^2 \omega(\lambda^*)}{\partial \lambda^2}}
\]

Therefore we certainly have \( \hat{\eta} > 0 \).

Let \( \varepsilon(\lambda) = \omega(\lambda) - \tilde{\omega}(\lambda) \), then

\[
|\varepsilon(\lambda)| \leq |\theta(b, \lambda) - \tilde{\theta}(b, \lambda)|.
\]

Now, for \( \lambda \in [\mu - \frac{\hat{\gamma}}{2}, \mu + \frac{\hat{\gamma}}{2}] \)

\[
|\omega(\lambda)| \geq |\lambda - \mu| \hat{\eta}.
\]

Hence for some \( \lambda_1^* \in [\mu - \frac{\hat{\gamma}}{2}, \mu] \) and some \( \lambda_2^* \in [\mu, \mu + \frac{\hat{\gamma}}{2}] \),

\[
|\omega(\lambda_i^*)| \geq \max_{|\lambda - \mu| < \frac{\hat{\gamma}}{2}} |\theta(b, \lambda) - \tilde{\theta}(b, \lambda)|
\]

\[
\geq |\varepsilon(\lambda_i^*)|, \quad i = 1, 2.
\]

Since the zeroes of \( \omega \) are simple and \( \tilde{\omega} \) is a continuous function of \( \lambda \),
this implies that \( \tilde{\omega}(\tilde{\mu}) = 0 \) for some \( \tilde{\mu} \in [\mu - \frac{\hat{\gamma}}{2}, \mu + \frac{\hat{\gamma}}{2}] \).

But
\[ 0 = \omega(\mu) - \tilde{\omega}(\tilde{\mu}) \]
\[ = \omega(\mu) - \omega(\tilde{\mu}) + \omega(\tilde{\mu}) - \tilde{\omega}(\tilde{\mu}) \]
\[ = (\mu - \tilde{\mu}) \frac{\partial \omega}{\partial \lambda}(\lambda^*) + \varepsilon(\tilde{\mu}) \]

for some \( \lambda^* \) between \( \mu \) and \( \tilde{\mu} \). Thus
\[ |\mu - \tilde{\mu}| \hat{\eta} \leq |\varepsilon(\tilde{\mu})|, \]

and the first result follows.

From (2.1.7)
\[ \hat{\eta} \geq \left| \frac{\partial \omega}{\partial \lambda}(\mu) \right| - \frac{\varphi^2}{2} \left| \frac{\partial^2 \omega}{\partial \lambda^2}(\lambda^*) \right| \]
\[ \geq \left| \frac{\partial \omega}{\partial \lambda}(\mu) \right| - \frac{1}{2} \left| \frac{\partial \omega}{\partial \lambda}(\mu) \right| \]
\[ = \frac{1}{2} \left| \frac{\partial \omega}{\partial \lambda}(\mu) \right| . \]

Thus to prove the remaining results, we only need to bound \( \frac{\partial \omega}{\partial \lambda}(\mu) \) and \( \frac{\partial^2 \omega}{\partial \lambda^2} \).

(a) The Prüfer phase.

From (2.1.6)
\[ \left| \frac{\partial \omega}{\partial \lambda}(\mu) \right| \geq \frac{\rho^2}{\rho^2 \| u \|^2_\infty + \| pu' \|^2_\infty} \]

which, on using (1.1.5) - (1.1.6), implies
\[ \left| \frac{\partial \omega}{\partial \lambda}(\mu) \right| \geq \frac{C_1}{\mu}, \]

and hence
In addition, we obtain on differentiating (2.1.5) and noting that
\[ |\frac{\partial}{\partial \lambda}(pu')| \leq C, \]
\[ |\frac{\partial^2 \omega}{\partial \lambda^2}| \leq C_2\lambda^{-\frac{3}{2}}. \]

Therefore
\[ \gamma \geq \frac{C_1\lambda^{\frac{3}{2}}}{C_2\mu} \]
\[ \geq C\mu^{\frac{3}{2}}, \]
and hence
\[ \gamma \geq C\mu^{-\frac{1}{2}}. \]

(b) The scaled phase.

By the same argument, we have
\[ |\frac{\partial \omega}{\partial \lambda}(\mu)| \geq C_1\mu^{-\frac{3}{2}}, \]
and
\[ |\frac{\partial^2 \omega}{\partial \lambda^2}| \leq C_2\lambda^{-1}. \]

Hence
\[ \gamma \geq \frac{C_1\lambda}{C_2\mu^{\frac{3}{2}}} \geq C\mu^{\frac{3}{2}}, \]
\[ \gamma \geq \frac{C_1}{2} \mu^{\frac{3}{2}}, \]
and
\[ \gamma \geq C. \]
(c) The modified phase.

Again we have

\[ \left| \frac{\partial \omega}{\partial \lambda}(u) \right| \geq C_1 u^{-\frac{1}{2}}, \]

and

\[ \left| \frac{\partial^2 \omega}{\partial \lambda^2} \right| \leq C_2 \lambda^{-\frac{1}{2}}. \]

Therefore

\[ \gamma \geq C_1 \lambda \geq C_1 \mu^\frac{1}{2}, \]

\[ \hat{\eta} \geq C_1 2 \mu^\frac{1}{2}, \]

and

\[ \hat{\eta} \gamma \geq C. \]

We now consider the numerical integration of (2.1.2) - (2.1.3) and restrict attention to explicit one step methods of the form

\[ \tilde{\theta}_0 = \theta(a, \lambda) = \alpha(\lambda) \]

\[ \tilde{\theta}_{i+1} = \tilde{\theta}_i + h\Phi(x_i, \tilde{\theta}_i; h) \quad i = 0, 1, \ldots, N-1 \]

where \( x_i = a + ih \), \( h = (b-a)/N \) and \( \Phi(x, \theta; h) \) is called the increment function (the dependence on \( \lambda \) being understood).

Let \( e_i = \theta_i - \tilde{\theta}_i \), \( i = 0, 1, \ldots, N \) (where \( \theta_i = \theta(x_i, \lambda) \) is the exact solution of the initial value problem). Then under appropriate conditions on the increment function, it follows from Henrici (1962; Chapter 2, Theorem 2.2) that

\[ |e_i| \leq \delta E_L(b-a) \]
where $E_L(x) = (\exp(Lx)-1)/L$, \(L = L(\lambda)\) is the Lipschitz constant of \(\phi(x,\theta;h)\) with respect to \(\theta\), and

$$\delta = \max_{0 \leq i \leq N-1} |\delta_i|; \quad \delta_i = \phi(x_i, \theta_i;h) - (\theta_{i+1} - \theta_i)/h.$$  

Once the Lipschitz constant \(L(\lambda)\) and the local truncation errors \(\delta_i\) are determined, this global error bound can be used in conjunction with Lemma 2.1 to obtain a bound on the eigenvalue error of a given method.

### 2.2 Error Bounds for Huen’s Method

To determine \(L(\lambda)\) and \(\delta\) it is necessary to examine the increment function and the local truncation error for each scheme separately. To illustrate, we consider Huen’s method for which

$$\phi(x, \theta;h) = \frac{1}{2}(f(x, \theta, \lambda) + f(x+h, \theta + h f(x, \theta, \lambda), \lambda).$$

In Henrici (1962; p.126) it is shown that

$$L(\lambda) \leq (1 + \frac{h}{2} L_0(\lambda)) L_0(\lambda),$$

where \(L_0(\lambda)\) is the Lipschitz constant of \(f(x, \theta, \lambda)\) with respect to \(\theta\). If we assume that \(p, q, r \in C^3[a,b]\) then using the appropriate Taylor series to expand \(\phi(x_i, \theta_i;h)\) and \((\theta_{i+1} - \theta_i)/h\) in terms of function values at \(x = x_i\), the local truncation error is given by

$$\delta_i = h^2 \left[ \frac{1}{2} f^2(x_i, \theta_i, \lambda) \frac{\partial f}{\partial x}(x+h, \theta^*, \lambda) + \frac{1}{2} f(x_i, \theta_i, \lambda) \frac{\partial^2 f}{\partial \theta \partial x}(x_i, \theta_i, \lambda) \right]$$

$$+ \frac{1}{4} \frac{\partial^2 f}{\partial x^2}(x_i, \theta_i, \lambda) - \frac{1}{6} \frac{d^2 f}{dx^2}(x^*, \theta(x^*, \lambda), \lambda) \right].$$
where \( x^* \), \( x_1^* \) and \( x_2^* \) are some points in \((x_i, x_{i+1})\) and \( \theta^* \) is some point between \( \theta_i \) and \( \theta_i + hf(x_i, \theta_i, \lambda) \).

With these results we are now in a position to obtain explicit bounds for each of the methods.

(a) Prufer substitution

Since \( f(x, \theta, \lambda) = \frac{1}{p} \sin^2 \theta + (\lambda r-q) \cos^2 \theta \), we have

\[
L_0(\lambda) = \| \lambda r-q - \frac{1}{p} \|_{\infty}
\]

and

\[
\delta \leq C h^2 \lambda^3.
\]

Therefore from (2.1.8) and Lemma 2.2

\[
|\lambda_k - \tilde{\lambda}_k| \leq C h^2 \lambda^3 E L (b-a)
\]

provided \( |e_N| \leq \frac{\sqrt{\eta}}{2} \).

(b) Scaled phase

Since

\[
L_0(\lambda) = \sqrt{\lambda} \| \frac{1}{P} - r + \frac{q}{\lambda} \|_{\infty}
\]

it is necessary to consider two cases.

(i) If \( pr \neq 1 \),

\[
\delta \leq C h^2 \lambda^{3/2}
\]

and hence from (2.1.8) and Lemma 2.2

\[
|\lambda_k - \tilde{\lambda}_k| \leq C h^2 \lambda^{3/2} E L (b-a)
\]
provided \(|e_N| < \frac{\hat{\gamma}}{2}\).

(ii) If \(pr \equiv 1\), \(E_L(b-a)\) is bounded independently of \(\lambda\) and

\[\delta \leq Ch^2\lambda^\frac{1}{2}\]

Therefore

\[|\lambda_k - \tilde{\lambda}_k| \leq Ch^2\lambda_k^{\frac{1}{2}}\lambda_k^{-\frac{1}{2}}\]

\[\leq Ch^2k^2,\quad (2.2.3)\]

if \(|e_N| < \frac{\hat{\gamma}}{2}\) or, equivalently if \(\sqrt{\lambda}h < C^*\) for some fixed constant \(C^*\).

(c) Modified phase

For this phase transformation

\[f(x,\theta,\lambda) = \left(\frac{\lambda r-q}{p}\right)^{\frac{1}{2}} + \left(\frac{(pr)'-(pq)'}{\lambda pr - pq}\right)\frac{\sin 2\theta}{4},\]

and

\[L_0(\lambda) = \|\left(\frac{pr}{p}\right)\|_{\infty} + C\lambda^{-1}.\]

Hence \(E_L(b-a)\) is bounded independently of \(\lambda\) and we only need to consider the local truncation error. This error depends on the behaviour of \((pr)'\) and also \(\left(\sqrt{\frac{r}{p}}\right)''\).

(i) If \((pr)' \neq 0\),

\[\delta \leq Ch^2\lambda\]

and hence
\[ |\lambda_k - \tilde{\lambda}_k| \leq C \lambda_k^{\frac{1}{2}} \]
\[ \leq Cy^2 \]  
(2.2.4)

if \( \sqrt{\lambda_k} h \leq C^* \) for some fixed constant \( C^* \).

(ii) When \((pr)\)' = 0 and \[ (\sqrt{\frac{r}{p}})^n \neq 0 , \]
\[ \delta \leq C \lambda^{\frac{1}{2}} \]
and hence
\[ |\lambda_k - \tilde{\lambda}_k| \leq C \lambda_k^{\frac{1}{2}} \]
\[ \leq Cy^2 \]  
(2.2.5)

if \( \sqrt{\lambda_k} h^2 \leq C^* \).

(iii) When \((pr)\)' = 0 and \[ (\sqrt{\frac{r}{p}})^n \equiv 0 \]
\[ \delta \leq Cy^2 \]
and hence
\[ |\lambda_k - \tilde{\lambda}_k| \leq Cy^2 \]  
(2.2.6)

for all \( k \).

2.3 Numerical Examples

In order to examine the validity of the above bounds we now consider numerical results for the eigenvalue problem

\[ -\ddot{u} + e^t u = \lambda u \]  
(2.3.1)

\[ u(0) = 0 = u(1) \]  
(2.3.2)
or some of its equivalent formulations.

In each of the examples the eigenvalue estimates are found using Huen's method with \( N = 40 \). We estimate the error by comparing them with estimates found using the classical fourth-order Runge-Kutta method to integrate the modified phase of (2.3.1) - (2.3.2) with \( N = 1024 \). Numerical experimentation indicates that these latter estimates have an absolute accuracy of better than \( 10^{-6} \) for the first forty eigenvalues.

(a) Prufer phase

The errors in the eigenvalue estimates obtained by integrating the Prufer phase of (2.3.1) - (2.3.2) are given in figure 2.1. Although the exponential growth predicted in (2.2.1) is not observed, it is clear that the eigenvalue estimates obtained are of little value.

(b) Scaled phase

If we introduce the transformations

\[
    x = e^t, \quad v = e^t u
\]

in (2.3.1) - (2.3.2) we obtain the eigenvalue problem

\[
    - \frac{d}{dx} \left( \frac{1}{x} \frac{dv}{dx} \right) + \left( \frac{1}{x^2} - \frac{1}{x^3} \right) v = \frac{\lambda}{x^3} v \quad (2.3.3)
\]

\[
    v(1) = 0 = v(e) \quad (2.3.4)
\]

for which \( \text{pr} \neq 1 \).

Integrating the scaled phase of (2.3.3) - (2.3.4) gives eigenvalue estimates whose errors behave in the same manner as those in figure 2.1.
Figure 2.1  Eigenvalue error in using Huen's method to integrate the Prufer phase for (2.3.1) - (2.3.2).
Although the exponential growth predicted by (2.2.2) is again not observed, the estimates obtained are of little practical use.

If however we make the change of variable $x = e^t$ in (2.3.1) - (2.3.2) we obtain

$$\frac{d}{dx}\left(\frac{du}{dx}\right) + u = \frac{\lambda}{x}u$$

(2.3.5)

$$u(1) = 0 = u(e)$$

(2.3.6)

for which $\text{pr} \equiv 1$.

The errors in the eigenvalue estimates obtained by integrating the scaled phase of (2.3.5) - (2.3.6) are given in figure 2.2 and show good agreement with the bound (2.2.3).

On the other hand the errors for the eigenvalue estimates obtained from the scaled phase for (2.3.1) - (2.3.2), given in figure 2.3, are in fact superior to that predicted by (2.2.3).

(c) Modified phase

(i) For (2.3.3) - (2.3.4), $(\text{pr})' \neq 0$ and the errors obtained for the modified phase are given in figure 2.4. If we divide the errors by $k^2$ then the ratios, given in Table 2.1, indicate that the errors are better than that predicted by (2.2.4) and appear to satisfy

$$|\lambda_k - \lambda_k^*| \leq Ch^2k^2, \quad k \leq N/2.$$  

(ii) For (2.3.5) - (2.3.6), $(\text{pr})' \equiv 0$ but $\left[\sqrt{\frac{r}{p}}\right]'' \neq 0$. The errors obtained by integrating the modified phase, given in figure 2.5, show excellent agreement with the bound (2.2.5).
Figure 2.2 Eigenvalue error in using Huen's method to integrate the scaled phase for (2.3.5) - (2.3.6).
Figure 2.3  Eigenvalue error in using Huen's method to integrate the scaled phase for (2.3.1) - (3.2.2).
Figure 2.4  Eigenv alue error in using Huen's method to integrate the modified phase for (2.3.3) - (2.3.4).
Table 2.1  Eigenvalue errors in using Huen's method to integrate the modified phase for (2.3.3) - (2.3.4).

<table>
<thead>
<tr>
<th>$k$</th>
<th>$\lambda_k$</th>
<th>$(\tilde{\lambda}_k - \lambda_k)/k^2$</th>
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Figure 2.5  Eigenvalue error in using Huen's method to integrate the modified phase for
(2.3.5) - (2.3.6)
Figure 2.6  Eigenvalue error in using Huen's method to integrate the modified phase for (2.3.1) - (2.3.2)
(iii) For (2.3.1) - (2.3.2), we have both \((pr) \cdot 0\) and \(\left(\frac{\sqrt{r}}{p}\right) ^\prime \equiv 0\) so, from (2.2.6) we predict that the errors should behave like \(Ch^2 k\). However the actual errors given in figure 2.6 appear to satisfy

\[ |\lambda_k - \tilde{\lambda}_k| \leq Ch^2, \quad k = 1, 2, \ldots, 20, \]

and only agree with (2.2.6) when \(k \sim 40\).

2.4 Improved Bounds for Huen's Method

From these numerical results we see that the bounds obtained in §2.2 are not always sharp. The question of whether the bounds can be improved therefore arises.

Clearly, improving the bounds for the Prufer phase and for the scaled phase when \(pr \neq 1\) is not useful because of the poor eigenvalue estimates obtained. However for the remaining cases in which the bound does not appear to be sharp (i.e. for the scaled phase when \(pr \equiv 1\), for the modified phase for the general problem, and also for the modified phase when both \((pr) \cdot 0\) and \(\left(\frac{\sqrt{r}}{p}\right) ^\prime \equiv 0\) there is a clear need for improvement.

To investigate this question we define

\[ T_i(y) = \frac{1}{2}(y_i + y_{i+1}) \]

\[ = \frac{1}{2}(y(x_i) + y(x_{i+1})) , \]

\[ ET_i(y) = \int_{x_i}^{x_{i+1}} y(x)dx - hT_i(y) , \]

and note that, for Huen's method,
\[ e_{i+1} - e_i = E_T(f(x, \theta, \lambda)) \]
\[ + h(T_i(f(x, \theta, \lambda) - \Phi(x_i, \tilde{\theta}_i; h)). \tag{2.4.1} \]

We also note that
\[ e_N = \sum_{i=0}^{N-1} (e_{i+1} - e_i), \]

and from Conte and de Boor (1972; equation (5.26), p.287)
\[ E_T(y) = -\frac{h^3}{12} \frac{d^2 y}{dx^2}(\xi), \quad \xi \in (x_i, x_{i+1}) \tag{2.4.2} \]

if \( y \in C^2[a,b] \).

(i) We consider the modified phase for a problem in Liouville normal form.

From (2.1.8)
\[ |e_i| \leq Ch^2, \]

and hence
\[ h|T_i(f(x, \theta, \lambda) - \Phi(x_i, \tilde{\theta}_i; h))| \leq Ch^3/\lambda. \]

In addition, from (2.4.2) it follows that
\[ |E_T(\sqrt{\lambda - q})| = \frac{h^3}{12} \left| \frac{d^2 (\sqrt{\lambda - q})(\xi)}{dx^2} \right| \leq Ch^3/\sqrt{\lambda}. \]

Therefore, from (2.4.1),
\[ |e_{i+1} - e_i - ET_i(g \sin 2\theta)| \leq Ch^3/\sqrt{\lambda}, \]
which implies

\[ |e_N| \leq \sum_{i=0}^{N-1} E T_i (g \sin 2\theta) + Ch^2/\sqrt{\lambda} , \]

where \( g(x) = -q'/4(\lambda-q) \). We can therefore obtain an improved eigenvalue error bound once we obtain a more explicit bound for the error in the trapezoidal integration of \( g \sin 2\theta \). In fact we have

**Lemma 2.3** For an eigenvalue problem in Liouville normal form with \( q \in C^3[a,b] \),

\[
|e_N| \leq \begin{cases} 
\frac{C_1 h^2}{\sqrt{\lambda}} & \text{if } \sin \sqrt{\lambda}h \neq 0 \\
\frac{1}{\sqrt{\lambda}h} \left| \frac{\cot \sqrt{\lambda}h}{\sqrt{\lambda}h} - \frac{1}{\lambda h^2} \right| \max_{1 \leq p \leq N} |p\sqrt{\lambda}h| + \frac{C_2 h^2}{\sqrt{\lambda}} & \text{if } \sin \sqrt{\lambda}h = 0 
\end{cases}
\]

when Huen's method is used to integrate the differential equation for the modified phase.

**Proof** If we replace \( g \) by its linear interpolate

\[ g_h(x) = \frac{1}{h} \{ g_i(x_{i+1} - x) + g_{i+1}(x-x_i) \} , \quad i = 0,1, \ldots, N-1 , \]

and note, from Conte and de Boor (1972; Theorem 4.3, p. 211), that

\[
|(g-g_h)(x)| \leq \frac{\|g\|_{\infty} h^2}{8} \quad x \in [x_i, x_{i+1}] \\
\leq Ch^2/\lambda
\]

then
\[ |E_T(g \sin 2\Theta) - E_T(g_h \sin 2\Theta)| = |E_T(g-g_h)\sin 2\Theta)| \]

\[ = \left| \int_{x_i}^{x_{i+1}} (g-g_h)\sin 2\Theta \, dx \right| \]

\[ \leq Ch^{3/\lambda} \cdotp \tag{2.4.3} \]

For the modified phase, it is shown in Birkhoff and Rota (1969; Theorem 7, p. 300) that

\[ |\theta(x,\lambda) - \phi(x,\lambda)| \leq C/\sqrt{\lambda} \]

where \( \phi = \phi(x,\lambda) = \alpha(\lambda) + \sqrt{\lambda}(x-a) \).

If we define

\[ \varepsilon(x) = \sin 2\Theta(x,\lambda) - \sin 2\phi(x,\lambda) \]

and note that

\[ \left\| \frac{d^j \varepsilon}{dx^j} \right\|_{\infty} \leq C\lambda^{(j-1)/2} \quad j = 0,1,2 \cdotp \]

then by (2.4.2)

\[ |E_T(g_h \sin 2\Theta) - E_T(g_h \sin 2\phi)| = |E_T(g_h \varepsilon)| \]

\[ \leq \frac{h^3}{12} \left\| \frac{d^2}{dx^2}(g_h \varepsilon) \right\|_{\infty} \]

\[ \leq Ch^{3/\sqrt{\lambda}} \cdotp \]

Combined with (2.4.3), this shows that

\[ \left| \sum_{i=0}^{N-1} E_T(g \sin 2\Theta) \right| \leq \left| \sum_{i=0}^{N-1} E_T(g_h \sin 2\phi) \right| + Ch^{2/\sqrt{\lambda}} \cdotp \tag{2.4.4} \]
where by direct computation

\[
ET_j(g_h \sin 2\phi) = \frac{h}{2} \cos 2\phi (g_i^1 + g_i^1 - g_i^1) \left[ \frac{\sin \sqrt{\lambda h}}{\lambda h^2} - \frac{\cos \sqrt{\lambda h}}{\sqrt{\lambda h}} - \sin \sqrt{\lambda h} \right]
\]

\[
+ \frac{h}{2} \sin 2\phi (g_i^1 + g_i^1) \left[ \frac{\sin \sqrt{\lambda h}}{\sqrt{\lambda h}} - \cos \sqrt{\lambda h} \right].
\]

Now

\[
| (g_i^1 - g_i^1) \left[ \frac{\sin \sqrt{\lambda h}}{\lambda h^2} - \frac{\cos \sqrt{\lambda h}}{\sqrt{\lambda h}} - \sin \sqrt{\lambda h} \right] | \leq Ch^2 / \sqrt{\lambda}.
\]

Also, by Lemma A1.1,

\[
\frac{1}{2} \sum_{i=0}^{N-1} (g_i^1 + g_i^1) \sin 2\phi \left[ \frac{\sin \sqrt{\lambda h}}{\sqrt{\lambda h}} - \cos \sqrt{\lambda h} \right] \leq \frac{N-1}{2} \sum_{i=0}^{N-1} g_i^1 \sin 2\phi \left[ \frac{\sin \sqrt{\lambda h}}{\sqrt{\lambda h}} - \cos \sqrt{\lambda h} \right] + Ch / \lambda
\]

\[
\leq (\|g\|_\infty + (b-a) \|g\|_\infty) \max_{1 \leq p \leq N} \left| \sin \frac{p \sqrt{\lambda}}{\lambda} \right| + \frac{Ch}{\lambda}
\]

\[
\leq \frac{C_1}{\lambda} \max_{1 \leq p \leq N} \left| \sin \frac{p \sqrt{\lambda}}{\lambda} \right| + \frac{Ch}{\lambda}
\]

if \( \sin \sqrt{\lambda} \neq 0 \). On the other hand if \( \sin \sqrt{\lambda} = 0 \)

\[
\frac{1}{2} \sum_{i=0}^{N-1} g_i^1 \sin 2\phi \left[ \frac{\sin \sqrt{\lambda h}}{\sqrt{\lambda h}} - \cos \sqrt{\lambda h} \right] \leq N(\|g\|_\infty + (b-a) \|g\|_\infty)
\]

and the result follows from (2.4.4).

\[\#\]

**THEOREM 2.1** For an eigenvalue problem in Liouville normal form with \( q \in C^3[a,b] \), the eigenvalue estimates satisfy

\[
|\lambda_k - \tilde{\lambda}_k| \leq Ch^2 \quad \sqrt{\lambda_k} h \leq \frac{\pi}{2}
\]

when Huen's method is used to integrate the differential equation for the modified phase.
Proof. We can obtain an eigenvalue error bound once we verify that the conditions of Lemma 2.2 are satisfied. Since $|e_N| \leq Ch^2$, it is clear that there is an $h_1$ (which is independent of $k$) such that Lemma 2.2 will hold if $h \leq h_1$.

Now we have already shown that $|\lambda_k - \tilde{\lambda}_k| \leq Ch^2/\lambda_k$ when $h \leq h_1$. Therefore there is an $h_0 \leq h_1$ such that $\sqrt{\lambda}_k h \leq \frac{3\pi}{4}$ and $\tilde{\lambda}_k \geq \frac{1}{4}\lambda_k$ whenever $h \leq h_0$ and $\sqrt{\lambda}_k h \leq \frac{\pi}{2}$. But when $h \leq h_0$, we have from Lemmas 2.3 and 2.2 that

$$|\lambda_k - \tilde{\lambda}_k| \leq h^2 \left( \frac{\lambda_k}{\tilde{\lambda}_k} \right)^{\frac{1}{2}} \left[ C_1 \left| \cot \frac{\sqrt{\lambda}_k h}{\sqrt{\tilde{\lambda}_k} h^2} \right| - \frac{1}{\tilde{\lambda}_k h^2} \right] + C_2.$$

The result then follows from this bound since

$$\left| \frac{\cot \frac{\sqrt{\lambda}_k h}{\sqrt{\tilde{\lambda}_k} h^2}}{\sqrt{\lambda}_k h} - \frac{1}{\tilde{\lambda}_k h^2} \right| \leq 1$$

and

$$\left( \frac{\lambda_k}{\tilde{\lambda}_k} \right)^{\frac{1}{2}} \leq 2$$

when $\sqrt{\lambda}_k h \leq \frac{\pi}{2}$.

From Courant and Hilbert (1953; equation (19a), p.415) we have

$$|\sqrt{\lambda}_k h - k\pi| \leq Ch.$$

Therefore the condition $\sqrt{\lambda}_k h \leq \frac{\pi}{2}$ is essentially equivalent to the condition $k \leq \frac{N}{2}$. Thus the bound given in the above theorem is in good agreement with the numerical results.
(ii) Scaled phase

From (2.1.8) $|e_i| \leq C h^2/\lambda$, and hence

$$h|T_i(f(x,\theta,\lambda)) - \Phi(x_i,\tilde{\theta}_i;h)| \leq Ch^3, \quad i = 0,1,\ldots,N-1.$$  

If we then apply the argument used in Lemma 2.3 we obtain the improved bound

$$|e_i| \leq Ch^2 \quad h/\lambda \leq \frac{\pi}{2}, \quad i = 0,1,\ldots,N. \quad (2.4.5)$$

However this improved global error bound is still not sufficiently sharp and needs to be improved further.

To achieve this we note, from (2.4.5), that

$$h|T_i(f(x,\theta,\lambda)) - \Phi(x_i,\tilde{\theta}_i;h)| \leq Ch^3/\lambda, \quad \sqrt{\lambda}h \leq \frac{\pi}{2}, \quad i = 0,1,\ldots,N-1$$

and we only need to improve the bound on the quadrature error. Such a bound is obtained in the following Lemma.

**Lemma 2.4** Let $h > 0$, $q \in C^3[a,b]$ and $\mu$ be any eigenvalue for which $h/\mu \leq \frac{\pi}{2}$. Further let $C^*$ be the constant for which $\gamma$ and $\hat{\gamma}$ as defined in Lemma 2.2 satisfy $\gamma \hat{\gamma} \geq C^*$. Then

$$\left| \sum_{i=0}^{N-1} ET_i(f(x,\theta,\lambda)) \right| \leq Ch^2/\sqrt{\lambda} \quad \sqrt{\lambda}h \leq \frac{\pi}{2}, \quad |\lambda-\mu| \leq \frac{1}{2}C^*,$$

when Huen's method is used to integrate the differential equation for the scaled phase.

**Proof** Since $\theta$ satisfies

$$\dot{\theta} = \sqrt{\lambda} - \frac{q}{2\sqrt{\lambda}} + \frac{q \cos 2\theta}{2\sqrt{\lambda}} \quad (2.4.6)$$
we observe that

$$|\theta(x, \lambda) - \hat{\phi}(x, \lambda)| \leq \frac{1}{2\sqrt{\lambda}} \left| \int_a^x q \cos 2\theta dx \right|, \quad x \in [a, b] \quad (2.4.7)$$

where

$$\hat{\phi}(x, \lambda) = \phi(x, \lambda) - \frac{1}{2\sqrt{\lambda}} \int_a^x q dx$$

and $\phi$ is as defined previously. Hence from (2.4.7) we have

$$|\theta(x, \lambda) - \hat{\phi}(x, \lambda)| \leq C/\sqrt{\lambda}.$$

If we define $\eta = \theta - \hat{\phi}$, then $\|\eta\|_{\infty} \leq C/\sqrt{\lambda}$ and (from (2.4.6)) $\|\eta\|_{\infty} \leq C$. Therefore

$$\left| \int_a^x (q \sin 2\eta) \sin 2\hat{\phi} dx \right| \leq \left| \int_a^x \frac{\cos 2\hat{\phi}}{(\sqrt{\lambda} - q/2\sqrt{\lambda})} dx \right|$$

$$+ \int_a^x \frac{\cos 2\hat{\phi}}{(\sqrt{\lambda} - q/2\sqrt{\lambda})} (q \sin 2\eta)' dx$$

$$\leq C/\sqrt{\lambda}$$

and, similarly,

$$\left| \int_a^x (q \cos 2\eta) \cos 2\hat{\phi} dx \right| \leq C/\sqrt{\lambda}.$$

Hence

$$\left| \int_a^x q \cos 2\theta dx \right| \leq \left| \int_a^x (q \cos 2\eta) \cos 2\hat{\phi} dx \right|$$

$$+ \left| \int_a^x (q \sin 2\eta) \sin 2\hat{\phi} dx \right|$$

$$\leq C/\sqrt{\lambda},$$

and, from (2.4.7)
\[
\|\theta - \hat{\theta}\|_\infty \leq C/\lambda .
\]

Now
\[
\begin{align*}
\text{ET}_i(f(x, \theta, \lambda)) &= \text{ET}_i \left( \sqrt{\lambda} - \frac{1}{2\sqrt{\lambda}} \right) \\
&\quad + \text{ET}_i \left( \frac{1}{2\sqrt{\lambda}} q(\cos 2\theta - \cos 2\hat{\theta}) \right) \\
&\quad - 2\text{ET}_i \left( \frac{q}{2\sqrt{\lambda}} \sin^2 \left( \frac{1}{2\sqrt{\lambda}} \int_a^x qdx \cos 2\phi \right) \right) \\
&\quad + \text{ET}_i \left( \frac{q}{2\sqrt{\lambda}} \sin \left( \frac{1}{\sqrt{\lambda}} \int_a^x qdx \sin 2\phi \right) \right) \\
&\quad + \text{ET}_i \left( \frac{q}{2\sqrt{\lambda}} \cos 2\phi \right).
\end{align*}
\]

But
\[
\left\| \frac{d^j}{dx^j} (\cos 2\theta - \cos 2\hat{\theta}) \right\|_\infty \leq C\lambda^{(j-2)/2} \quad j = 0,1,2
\]
and
\[
\left\| \frac{d^j}{dx^j} \left( \frac{1}{\sqrt{\lambda}} \int_a^x qdx \right) \right\|_\infty \leq C/\sqrt{\lambda} \quad j = 0,1,2 .
\]

Therefore, using (2.4.2),
\[
\begin{align*}
|\text{ET}_i(f(x, \theta, \lambda)) - \text{ET}_i \left( \frac{q}{2\sqrt{\lambda}} \cos 2\phi \right) - \text{ET}_i \left( \frac{q}{2\sqrt{\lambda}} \sin \left( \frac{1}{\sqrt{\lambda}} \int_a^x qdx \sin 2\phi \right) \right)| \\
&\leq C\lambda^3/\sqrt{\lambda} .
\end{align*}
\]

In addition if we put \( g = \frac{q}{2\sqrt{\lambda}} \sin \left( \frac{1}{\sqrt{\lambda}} \int_a^x qdx \right) \) in (2.4.4) and apply the subsequent argument in Lemma 2.3 we obtain
\[
\left| \sum_{i=0}^{N-1} \text{ET}_i(g \sin 2\phi) \right| \leq C\lambda^2/\sqrt{\lambda} , \quad \sqrt{\lambda} h \leq \frac{\pi}{2} .
\]

Hence
where $q_h$ is the linear interpolate of $q$ defined in Lemma 2.3 and

$$
ET_i \left[ \frac{q_h \cos 2\phi}{2\sqrt{\lambda}} \right] = \frac{h}{4\sqrt{\lambda}} \sin 2\phi_{i+\frac{1}{2}}(q_{i+1} - q_i) \left[ \frac{\sin \sqrt{\lambda}h}{\sqrt{\lambda}h^2} - \frac{\cos \sqrt{\lambda}h}{\sqrt{\lambda}h} - \frac{\sin \sqrt{\lambda}h}{\sqrt{\lambda}h} \right] - \frac{h}{4\sqrt{\lambda}} \cos 2\phi_{i+\frac{1}{2}}(q_{i+1} + q_i) \left[ \frac{\sin \sqrt{\lambda}h}{\sqrt{\lambda}h} - \frac{\cos \sqrt{\lambda}h}{\sqrt{\lambda}h} \right].
$$

From Lemma A1.1,

$$
\sum_{i=0}^{N-1} (q_{i+1} - q_i) \sin 2\phi_{i+\frac{1}{2}} \leq \sum_{i=0}^{N-1} hq'_{i+\frac{1}{2}} \sin 2\phi_{i+\frac{1}{2}} \leq \frac{(b-a)}{24} h^2 \|q''\|_\infty
$$

$$
\leq h\left(\|q\|_\infty + (b-a)\|q''\|_\infty\right) \max_{1 \leq p \leq N} \left| \frac{\sin p\sqrt{\lambda}h}{\sin \sqrt{\lambda}h} \right| + \frac{(b-a)}{24} h^2 \|q''\|_\infty
$$

$$
\leq \frac{C_1h}{\sin \sqrt{\lambda}h} + C_2h^2.
$$

In addition from Lemma A1.2,

$$
\sum_{i=0}^{N-1} (q_{i+1} + q_i) \cos 2\phi_{i+\frac{1}{2}} \leq 2 \sum_{i=0}^{N-1} q'_{i+\frac{1}{2}} \cos 2\phi_{i+\frac{1}{2}} + \frac{(b-a)}{4} h\|q''\|_\infty
$$

$$
\leq \frac{C_1}{\sqrt{\lambda} \sin \sqrt{\lambda}h} (\|q\|_\infty + \|q'\|_\infty) + \frac{C_2}{\sin \sqrt{\lambda}h} h^2 \|q''\|_\infty
$$

$$
+ \frac{h}{2 \sin^2 \sqrt{\lambda}h} (\|q''\|_\infty + (b-a)\|q''\|_\infty) + \frac{(b-a)}{4} h\|q''\|_\infty
$$

$$
\leq \frac{C_3}{\sqrt{\lambda} \sin \sqrt{\lambda}h} + \frac{C_4}{\sin^2 \sqrt{\lambda}h} + C_5 h.
$$
Now applying Lemma A2.1 we obtain

\[
\sum_{i=0}^{N-1} E_i \left( \frac{q_i \cos 2\phi}{2\sqrt{\lambda}} \right) \leq \frac{h}{4\sqrt{\lambda}} \left( \frac{C_1}{\sin \sqrt{\lambda h}} + C_2 h^2 \right) \left| \frac{\sin \sqrt{\lambda h} - \cos \sqrt{\lambda h} - \sin \sqrt{\lambda h}}{\sqrt{\lambda h}} \right|
\]

\[
+ \frac{h}{4\sqrt{\lambda}} \left( \frac{C_3}{\sqrt{\lambda} \sin \sqrt{\lambda h}} + \frac{C_4}{\sin^2 \sqrt{\lambda h}} + C_5 h \right) \left| \frac{\sin \sqrt{\lambda h} - \cos \sqrt{\lambda h}}{\sqrt{\lambda h}} \right|
\]

\[
\leq \frac{h}{4\sqrt{\lambda}} \left( \frac{C_1}{\sin \sqrt{\lambda h}} + C_2 h^2 \right) \sin \sqrt{\lambda h}
\]

\[
+ \frac{h}{4\sqrt{\lambda}} \left( \frac{C_3}{\sqrt{\lambda} \sin \sqrt{\lambda h}} + \frac{C_4}{\sin^2 \sqrt{\lambda h}} + C_5 h \right) \sqrt{\lambda h} \sin \sqrt{\lambda h}
\]

\[
\leq \frac{C_1 h^2}{4\sqrt{\lambda}} + \frac{C_2 h^3}{4\sqrt{\lambda}} + \frac{C_3 h^2}{4\sqrt{\lambda}} + \frac{C_4 h^3}{4\sqrt{\lambda}} + \frac{C_5 h^2}{4\sqrt{\lambda}} \frac{\pi}{2}
\]

\[
\leq Ch^2 / \sqrt{\lambda}
\]

and the result follows from (2.4.8) and (2.4.9). #

With this improved quadrature error bound we now have

**THEOREM 2.2** Let the eigenvalue problem (1.1.1) - (1.1.3) be in Liouville normal form and \( q \in C^3[a,b] \). Then there is an \( h_0 > 0 \) such that whenever \( h < h_0 \), the eigenvalue estimates satisfy

\[
|\lambda_k - \tilde{\lambda}_k| \leq Ch^2 \quad h \sqrt{\tilde{\lambda}_k} \leq \frac{\pi}{2}
\]

when Huen's method is used to integrate the differential equation for the scaled phase.

**Proof** Since \( |e_N| \leq Ch^2 \) when \( \sqrt{\lambda h} \leq \frac{\pi}{2} \), there is an \( h_1 \) such that the conditions of Lemma 2.2 are satisfied when \( h < h_1 \) and \( \sqrt{\lambda h} \leq \frac{\pi}{2} \).
Hence the eigenvalue estimates satisfy

\[ |\lambda_k - \tilde{\lambda}_k| \leq C_1 h^2 \sqrt{\lambda_k} \]

whenever \( h < h_1 \). Therefore there is an \( h_0 \leq h_1 \) such that the conditions of Lemma 2.4 will be satisfied and

\[
|e_N| \leq \left| \sum_{i=0}^{N-1} E_T \left( f(x, \theta, \tilde{\lambda}_k) \right) \right| + h \sum_{i=0}^{N-1} \left| T_i \left( f(x, \theta, \tilde{\lambda}_k) - \Phi(x_i, \tilde{\theta}_i, h) \right) \right|
\]

\[
\leq C_1 h^2 / \sqrt{\tilde{\lambda}_k} + C_2 h^2 / \sqrt{\lambda_k}
\]

\[
\leq Ch^2 / \sqrt{\tilde{\lambda}_k}
\]

whenever \( h < h_0 \) and \( \sqrt{\tilde{\lambda}_k} h \leq \frac{\pi}{2} \). Applying Lemma 2.2 then yields

\[
|\lambda_k - \tilde{\lambda}_k| \leq C_1 \left( \frac{\lambda_k}{\tilde{\lambda}_k} \right)^{1/2} h^2
\]

\[
\leq Ch^2 .
\]

(iii) Modified phase for general self-adjoint form.

The analysis of this case is rather more involved than for the Liouville normal form since the \( k^3 \) term in the eigenvalue error arises not only from the trapezoidal error but also from the Euler predictor step.

To obtain a sharper bound on the eigenvalue error we firstly bound the quadrature error.

**Lemma 2.5** For an eigenvalue problem in general self-adjoint form with \( p, q, r \in C^3(a, b) \)

\[
\left| \frac{1}{i} \sum_{i=0}^{j} E_T \left( f(x, \theta, \lambda) \right) \right| \leq Ch^2 \sqrt{\lambda} , \quad \sqrt{\lambda} h \leq \frac{\pi}{2\| (x) \|_\infty} , \quad j = 1, 2, \ldots, N-1 ,
\]
when Huen's method is used to integrate the differential equation for the modified phase.

**Proof** If we make the change of variable

\[ t = t(x) = \int_a^x \left( \frac{x}{p} \right)^\frac{1}{2} \, dx ; \quad T = \int_a^b \left( \frac{x}{p} \right)^\frac{1}{2} \, dx \]

in (2.1.2), we obtain

\[ \frac{d\theta}{dt} = \sqrt{\lambda - \frac{q}{r}} + g(t) \sin \theta \]

(2.4.10)

where \( g = \frac{1}{4} \left( \frac{\lambda(pr)' - (pq)'}{\lambda pr - pq} \right) \).

Since \( |\sqrt{\lambda - \frac{q}{r}} - \sqrt{\lambda}| \leq C / \sqrt{\lambda} \), we observe that

\[ |\theta(t,\lambda) - (\theta_0 + \sqrt{\lambda} t + \int_0^t g(t) \sin 2\theta \, dt)| \leq C / \sqrt{\lambda} \]

(2.4.11)

Hence we have

\[ |\theta(t,\lambda) - \phi(t,\lambda)| \leq C \]

where

\[ \phi(t,\lambda) = \theta_0 + \sqrt{\lambda} t \]

If we define \( \eta = \theta - \phi \), note that \( |\eta| \leq C \) and (from (2.4.10)) \( |\eta| \leq C \), then

\[ \int_0^t g(t) \sin 2\theta \, dt = \int_0^t g(t) \sin(2\phi + 2\eta) \, dt \]

\[ = \int_0^t g(t) \cos 2\eta \sin 2\phi \, dt + \int_0^t g(t) \sin 2\eta \cos 2\phi \, dt \]

For a general function \( y \in C^1[0,T] \),
\[
\int_0^t y \sin 2\phi \, dt = \left[ -\frac{y \cos 2\phi}{2\sqrt{\lambda}} \right]_0^t + \int_0^t \frac{\dot{y} \cos 2\phi}{2\sqrt{\lambda}} \, dt,
\]
and hence
\[
\left| \int_0^t y \sin 2\phi \, dt \right| \leq (2\|y\|_{\infty} + T\|\dot{y}\|_{\infty})/2\sqrt{\lambda}.
\]
Similarly
\[
\left| \int_0^t y \cos 2\phi \, dt \right| \leq (2\|y\|_{\infty} + T\|\dot{y}\|_{\infty})/2\sqrt{\lambda}.
\]
Therefore
\[
\left| \int_0^t g \sin 2\theta \, dt \right| \leq C/\sqrt{\lambda}
\]
and hence, from (2.4.11) we have
\[
|\theta(t,\lambda) - \phi(t,\lambda)| \leq C/\sqrt{\lambda}.
\]
Applying the change of variable \( t = \int_a^x \left( \frac{r}{p} \right)^{1/2} dx \) to the trapezoidal rule we obtain
\[
ET_1(f(x,\theta,\lambda)) = ET_1(F(t,\theta,\lambda))
\]
\[
-\frac{1}{2} \left\{ \left[ h\left( \frac{r}{p} \right)^{1/2} \delta_i \right] F(t_{i+1},\theta_{i+1},\lambda) + \left[ h\left( \frac{r}{p} \right)^{1/2} \delta_i \right] F(t_i,\theta_{i},\lambda) \right\}(2.4.12)
\]
where
\[
F(t,\theta,\lambda) = \left( \frac{p}{r} \right)^{1/2} (x(t)) f(x(t),\theta(x(t),\lambda),\lambda),
\]
\[
t_i = \int_a^{t_i} \left( \frac{r}{p} \right)^{1/2} dx \quad i = 0,1,2,\ldots,N
\]
and
\[\delta_i = t_{i+1} - t_i = \int_{x_i}^{x_{i+1}} \left( \frac{p}{r} \right)^{\frac{1}{2}} dx, \quad i = 0, 1, \ldots, N-1.\]

We note, for later use, that

\[mh \leq \delta_i \leq Mh, \quad i = 0, 1, \ldots, N-1\]

where

\[m = \min_{x \in [a, b]} \left( \frac{p}{r} \right)^{\frac{1}{2}},\]

and

\[M = \max_{x \in [a, b]} \left( \frac{r}{p} \right)^{\frac{1}{2}}.\]

Expanding \(\left( \frac{r}{p} \right)^{\frac{1}{2}}\) in its Taylor series about \(x = x_i\), we obtain

\[|\delta_i - h \left( \frac{r}{p} \right)^{\frac{1}{2}} - \frac{h^2}{2} \frac{d}{dx} \left( \frac{r}{p} \right)^{\frac{1}{2}}| \leq Ch^3,\]

and similarly, expanding about \(x = x_{i+1}\),

\[|\delta_i - h \left( \frac{r}{p} \right)^{\frac{1}{2}}_{i+1} + \frac{h^2}{2} \frac{d}{dx} \left( \frac{r}{p} \right)^{\frac{1}{2}}_{i+1}| \leq Ch^3.\]

Therefore

\[\left| \left( h \left( \frac{r}{p} \right)^{\frac{1}{2}}_{i+1} - \delta_i \right) F(t_{i+1}, \theta_{i+1}, \lambda) + \left( h \left( \frac{r}{p} \right)^{\frac{1}{2}}_{i} - \delta_i \right) F(t_i, \theta_i, \lambda) \right| \]

\[\leq \frac{h^2}{2} |F(t_{i+1}, \theta_{i+1}, \lambda) \frac{d}{dx} \left( \frac{r}{p} \right)^{\frac{1}{2}}_{i+1} - F(t_i, \theta_i, \lambda) \frac{d}{dx} \left( \frac{r}{p} \right)^{\frac{1}{2}}_{i}| + Ch^3/\lambda\]

\[= \frac{h^3}{2} \left| \frac{d}{dx} \left( \frac{p}{r} \right)^{\frac{1}{2}} f(x, \theta, \lambda) \right| (\xi) \bigg| + Ch^3/\lambda\]

\[\leq Ch^3/\lambda. \quad (2.4.13)\]
Defining \( e(t) \) and \( g_h(t) \) as before, we find

\[
|E_T\left(\sqrt{\lambda - \frac{q}{r}}\right)| \leq C h^3/\lambda
\]

and

\[
|E_T(\sin 2\theta) - E_T(g_h \sin 2\phi)| \leq |E_T((\sin 2\theta) - |E_T(g_h \sin 2\phi)| |E_T(g_h e)|
\]

\[
\leq C h^3/\lambda .
\]

Hence from \((2.4.12)\) and \((2.4.13)\)

\[
\sum_{i=0}^{j} |E_T(f(x, \theta, \lambda))| \leq \sum_{i=0}^{j} |E_T(g_h \sin 2\phi)| + Ch^2/\lambda \quad j = 1, 2, \ldots, N-1
\]

(2.4.14)

where

\[
E_T(g_h \sin 2\phi) = \frac{\delta_i}{2} \cos 2\phi_1 (g_{i+1} - g_i) \left[ \frac{\sin \sqrt{\lambda \delta_i}}{\lambda \delta_i^2} - \frac{\cos \sqrt{\lambda \delta_i}}{\sqrt{\lambda \delta_i}} - \sin \sqrt{\lambda \delta_i} \right]
\]

\[
+ \frac{\delta_i}{2} \sin 2\phi_1 (g_i + g_{i+1}) \left[ \frac{\sin \sqrt{\lambda \delta_i}}{\sqrt{\lambda \delta_i}} - \cos \sqrt{\lambda \delta_i} \right].
\]

Since

\[
|g_{i+1} - g_i| \left| \frac{\sin \sqrt{\lambda \delta_i}}{\lambda \delta_i^2} - \frac{\cos \sqrt{\lambda \delta_i}}{\sqrt{\lambda \delta_i}} - \sin \sqrt{\lambda \delta_i} \right| \leq Ch^2 \sqrt{\lambda} \|g\|
\]

\[
\leq Ch^2 \sqrt{\lambda}
\]

and

\[
|g_i + g_{i+1} - 2g_{i+n}| \leq Ch^2
\]

we have
\[
| \sum_{i=0}^{j} ET_1(g_i \sin 2\phi) | \leq \frac{1}{2\sqrt{\lambda}} \left| \sum_{i=0}^{j} (\sin \sqrt{\lambda \delta_i} - \sqrt{\lambda \delta_i} \cos \sqrt{\lambda \delta_i}) g_{i+\frac{1}{2}} \sin 2\phi_{i+\frac{1}{2}} \right|
+ \frac{\lambda}{2} \delta, \quad j = 1, \ldots, N-1 . \tag{2.4.15}
\]

In Lemma Al.3 it is shown that
\[
| \sum_{i=0}^{j} (\sin \sqrt{\lambda \delta_i} - \sqrt{\lambda \delta_i} \cos \sqrt{\lambda \delta_i}) g_{i+\frac{1}{2}} \sin 2\phi_{i+\frac{1}{2}} | \leq C(||g||_\infty + \|\tilde{g}\|_\infty) h^2 \lambda , \quad j = 1, 2, \ldots, N-1 \tag{2.4.16}
\]
provided \( M \lambda h \leq \frac{\pi}{2} \). The stated bound then follows from (2.4.15) and (2.4.14).

With this result we can now prove

**Lemma 2.6** For a general eigenvalue problem with \( p, q, r \in C^3[a,b] \),
\[
|e_N| \leq \lambda \sqrt{\lambda} , \quad \sqrt{\lambda} h \leq \frac{\pi}{2 \|\frac{\lambda}{\lambda} \|_\infty} \]
when Huen's method is used to integrate the differential equation for the modified phase.

**Proof** By the definitions already given
\[
e_{i+1} - e_i = ET_1(f(x,\theta,\lambda)) + h(T_1(f(x,\theta,\lambda) - \tilde{\phi}(x_i,\tilde{\theta}_i;h)) .
\]
Hence
\[
e_{j+1} = \sum_{i=0}^{j} ET_1(f(x,\theta,\lambda)) + S_j \tag{2.4.17}
\]
where
\[
S_j = h \sum_{i=0}^{j} (T_1(f(x,\theta,\lambda) - \tilde{\phi}(x_i,\tilde{\theta}_i;h)) .
\]
Since \( \tilde{\theta}_0 = \theta_0 \), we have that

\[
|S_0| \leq C_1 h^2 \theta
\]

\[
\leq Ch^2 \theta
\]

From (2.4.17) and Lemma 2.5

\[
|e_{j+1}| \leq Ch^2 \theta + |S_j|
\]

(2.4.18)

In addition

\[
|\sin 2\theta_j - \sin 2\tilde{\theta}_j| \leq 2|e_j|
\]

and

\[
|\theta_{j+1} - \theta_j - h\theta_j| \leq Ch^2 \theta
\]

Therefore

\[
|S_j| \leq |S_{j-1}| + h|T_j(f(x, \theta, \lambda) - \Phi(x_j, \tilde{\theta}_j; h)|
\]

\[
\leq |S_{j-1}| + \frac{h}{2}|g_j(\sin 2\theta_j - \sin 2\tilde{\theta}_j)|
\]

\[
+ \frac{h}{2}|g_{j+1}(\sin 2\theta_{j+1} - \sin 2(\tilde{\theta}_j + hf(x, \tilde{\theta}_j, \lambda)))|
\]

\[
\leq |S_{j-1}| + \frac{h}{2}\|g\|_\infty |e_j|
\]

\[
+ \frac{h}{2}\|g\|_\infty \{2h\|g\|_\infty |e_j| + 2|e_j| + Ch^2 \theta\}
\]

\[
\leq |S_{j-1}|(1 + hA) + h^3 \sqrt{\lambda} B
\]

where, using (2.4.18),
From Henrici (1962; equation (1.13), p.18) we have

\[ A = 2\|g\|_\infty + h\|g\|_\infty^2 \]

\[ B = C(2\|g\|_\infty + \|g\|_\infty^2 + \frac{1}{2}) . \]

Since \( A \) and \( B \) are bounded independently of \( \lambda \), this result when substituted in (2.4.18) with \( j = N-1 \) gives the desired estimate. #

Using this improved error bound in conjunction with Lemma 2.2 then gives

**THEOREM 2.3**

Let the eigenvalue problem (1.1.1) - (1.1.3) be such that \( p, q, r \in C^3[a,b] \). Then there is an \( h_0 > 0 \) such that whenever \( h < h_0 \) the eigenvalue estimates satisfy

\[ |\lambda_j - \hat{\lambda}_j| \leq Ch^2k^2 \quad , \quad |\sqrt{\lambda_j}h| \leq \frac{\pi}{2\|\frac{\partial}{\partial p}\|^2\|\infty} \]

when Huen's method is used to integrate the differential equation for the modified phase.

2.5 **Error bounds for the classical Runge-Kutta method**

Usually more sophisticated methods than Huen’s are used to integrate initial value problems. It is therefore natural to examine whether the foregoing analysis can be generalised.

Clearly, bounds of the form given in §2.2 can easily be obtained for any one step method once the Lipschitz constant and local truncation error are known. The generalisation of the analysis which gave the improved
bounds in §2.4 is however not so obvious.

If we take the proof of Theorem 2.2 as the basis of the analysis, then we can identify two main steps in the derivation of improved bounds. The first is to obtain an error bound for the quadrature of \( f(x,\theta,\lambda) \) using exact values of \( \theta \). The second is to bound the error resulting from the use of approximate values of \( \theta \) in the quadrature rule.

Because the analysis in each of these steps requires an explicit examination of the increment function, we cannot give a complete answer to the question of obtaining improved bounds. We do however conjecture that improved bounds can be obtained for those methods which are based on symmetric quadrature rules.

This is of course true for Huen's method since it corresponds to the trapezoidal rule. It is also fairly obvious that the improved bounds obtained for Huen's method will also hold for the increment function

\[
\phi(x,\theta;h) = f(x + \frac{h}{2},\theta + \frac{h}{2}f(x,\theta,\lambda),\lambda),
\]

which corresponds to the midpoint rule.

As a further example we consider the classical Runge-Kutta method for which

\[
\phi(x,\theta;h) = \frac{1}{6}(K_1+2K_2+2K_3+K_4),
\]

where

\[
K_1 = f(x,\theta,\lambda)
\]
\[
K_2 = f(x + \frac{h}{2},\theta + \frac{h}{2}K_1,\lambda)
\]
\[
K_3 = f(x + \frac{h}{2},\theta + \frac{h}{2}K_2,\lambda)
\]
\[
K_4 = f(x+h,\theta+hK_3,\lambda).
\]
This obviously corresponds to Simpson's rule.

From Henrici (1962; p.75), the Lipschitz constant satisfies

$$L(\lambda) \leq \left( 1 + \frac{hL_0(\lambda)}{2} + \frac{h^2L_0^2(\lambda)}{6} + \frac{h^3L_0^3(\lambda)}{24} \right) L_0(\lambda)$$

The following bounds are easily verified from the representation of the local truncation error given in Henrici (1962; p.75) together with (2.1.8) and Lemma 2.2.

(a) Prufer phase

$$L_0(\lambda) \leq \|\lambda r - q - \frac{1}{q}\|_{\infty}$$

$$\delta \leq Ch^4\lambda^5$$

$$|e_N| \leq Ch^4\lambda^5E_L(b-a)$$

$$|\lambda_k - \hat{\lambda}_k| \leq Ch^4\lambda^5E_L(b-a), \quad |e_N| \leq \frac{1}{2}\eta^n .$$

(b) Scaled phase

(i) pr ≠ 1

$$L_0(\lambda) \leq \sqrt{\|\lambda - \frac{1}{p} - \frac{r+q}{\lambda}\|_{\infty}}$$

$$\delta \leq Ch^4\lambda^{5/2}$$

$$|e_N| \leq Ch^4\lambda^{5/2}E_L(b-a)$$

$$|\lambda_k - \hat{\lambda}_k| \leq Ch^4\lambda^{5/2}E_L(b-a), \quad |e_N| \leq \frac{1}{2}\eta^n .$$
(ii) $p_r \equiv 1$

\[ L_0(\lambda) = \|q\|_\infty / \sqrt{\lambda} \]

\[ \delta \leq Ch^4 \lambda^{3/2} \]

\[ |e_N| \leq Ch^4 \lambda^{3/2} \]

\[ |\lambda_k - \bar{\lambda}_k| \leq Ch^{4}_k \lambda^{\frac{3}{2}} \kappa_k^2 \rightarrow 0 \quad , \quad |e_N| \leq \frac{1}{2} \gamma \eta \]

\[ \leq Ch^4 k^4 \quad , \quad \sqrt{\bar{\lambda}_k h} \leq C^* \]

for some fixed constant $C^*$.

(c) Modified phase

(i) $(p_r)' \neq 0$

\[ L(\lambda) = \frac{1}{2} \| (p_r)' \|_\infty + C / \lambda \]

\[ \delta \leq Ch^4 \lambda^2 \]

\[ |e_N| \leq Ch^4 \lambda^2 \]

\[ |\lambda_k - \bar{\lambda}_k| \leq Ch^{4}_k \lambda^{2} \kappa_k^2 \rightarrow 0 \quad , \quad |e_N| \leq \frac{1}{2} \gamma \eta \]

\[ \leq Ch^4 k^5 \quad , \quad \sqrt{\bar{\lambda}_k h} \leq C^* \]

(ii) $(p_r)' \equiv 0$

\[ L(\lambda) = C / \lambda \]

\[ \delta \leq Ch^4 \lambda \]

\[ |e_N| \leq Ch^4 \lambda \]

\[ |\lambda_k - \bar{\lambda}_k| \leq Ch^{4}_k \lambda^{2/3} \kappa_k^2 \rightarrow 0 \quad , \quad |e_N| \leq \frac{1}{2} \gamma \eta \]

\[ \leq Ch^4 k^5 \quad , \quad \sqrt{\bar{\lambda}_k h} \leq C^* \]
We now restrict attention to eigenvalue problems which are in Liouville normal form. As noted before, the first step in improving the error bounds for the modified and scaled phase methods is to consider the quadrature error. To do this we define

\[ S_i(f) = \frac{1}{6} \{ f_i + 4f_{i+1/2} + f_{i+1} \}, \]

and

\[ ES_i(f) = \int_{x_i}^{x_{i+1}} f(x)dx - hS_i(f). \]

**Lemma 2.7** Let (1.1.1) - (1.1.3) be in Liouville normal form, and \( q \in C^5[a,b] \). Then, for the modified phase we have

\[ \left| \sum_{i=0}^{N-1} ES_i(f(x, \theta, \lambda)) \right| \leq C h^4 \sqrt{\lambda}, \quad \forall h \leq \frac{\pi}{2}. \]

**Proof** We define \( \phi \) as in §2.4 and set

\[ \varepsilon = \sin 2\theta - \sin 2\phi, \]

\[ g = -q'/4(\lambda-q), \]

and

\[ g_h = \frac{2}{h^2} \{ g_1(x-x_1+\frac{1}{2})(x-x_{1+1}) - 2g_{1+1/2}(x-x_1)(x-x_{1+1}) \]

\[ + g_{i+1}(x-x_i)(x-x_{i+1}) \}, \quad x \in [x_i, x_{i+1}). \]

We also note that

\[ \|d^j\varepsilon/dx^j\|_\infty \leq C\lambda(j-1)/2, \quad j = 0, 1, \ldots, 4. \]  \hspace{1cm} (2.5.1)

From Conte and de Boor (1972; equation (5.28), Theorem 4.3) and (2.5.1), it follows that
\[ |E_{S_1}(f(x, \theta, \lambda)) - ES_1(g_h \sin 2\phi)| \leq |ES_1(\sqrt{\lambda - q})| \]

\[ + |ES_1((g - g_h)\sin 2\phi)| + |ES_1(g_h \epsilon)| \]

\[ \leq C_1h^{\lambda - \frac{1}{2}} + C_2h^{\lambda - 1} + C_3h^{2\sqrt{\lambda}} \]

\[ \leq Ch^{5/\lambda}, \quad (2.5.2) \]

where

\[ ES_1(g_h \sin 2\phi) = h \left[ \sin \frac{\sqrt{\lambda}h}{\sqrt{\lambda}h} - \cos \frac{\sqrt{\lambda}h}{3} - \frac{2}{3} \right] g_{i+\frac{1}{2}} \sin 2\phi_{i+\frac{1}{2}} \]

\[ + h \left[ \sin \frac{\sqrt{\lambda}h}{\sqrt{\lambda}h} - \cos \frac{\sqrt{\lambda}h}{3} \right] \left( g_{i+1} - g_i \right) \cos 2\phi_{i+\frac{1}{2}} \]

\[ + h \left[ - \frac{2 \sin \frac{\sqrt{\lambda}h}{\sqrt{\lambda}h}}{(\sqrt{\lambda}h)^2} + \frac{2 \cos \sqrt{\lambda}h}{(\sqrt{\lambda}h)^2} + \frac{\sin \sqrt{\lambda}h}{\sqrt{\lambda}h} - \frac{\cos \sqrt{\lambda}h}{3} \right] \left( g_{i+1} - 2g_{i+\frac{1}{2}} + g_i \right) \sin 2\phi_{i+\frac{1}{2}} \]

Now

\[ |g_{i+1} - g_i| \leq h \|g\|_{\infty} \]

\[ \leq Ch/\lambda \]

and

\[ |g_{i+1} - 2g_{i+\frac{1}{2}} + g_i| \leq \frac{1}{2}h^2 \|g\|_{\infty} \]

\[ \leq Ch^2/\lambda. \]

Therefore, from the bounds given in Appendix 2,
\[ |E_{1}(g_{h} \sin 2\phi) - h \left[ \frac{\sin \sqrt{\lambda}h}{\sqrt{\lambda}h} - \frac{\cos \sqrt{\lambda}h}{3} - \frac{2}{3} \right] g_{i+\frac{1}{2}} \sin 2\phi_{i+\frac{1}{2}} | \]

\[ \leq h \left( \frac{(\sqrt{\lambda})^{2}}{3} \sin \sqrt{\lambda}h \right) \frac{Ch}{\lambda} \]

\[ + h \left( \frac{\sqrt{\lambda}h}{3} \right) \frac{Ch^{2}}{\lambda} \]

\[ \leq Ch^{5} \sqrt{\lambda} \]

and hence from Lemmas A1.1 and A2.1

\[ | \sum_{i=0}^{N-1} E_{1}(g_{h} \sin 2\phi) | \leq h \left( \frac{\sin \sqrt{\lambda}h}{\sqrt{\lambda}h} - \frac{\cos \sqrt{\lambda}h}{3} - \frac{2}{3} \right) \left| \sum_{i=0}^{N-1} g_{i+\frac{1}{2}} \sin 2\phi_{i+\frac{1}{2}} \right| + Ch^{4} \sqrt{\lambda} \]

\[ \leq h(\sqrt{\lambda})^{3} \sin \sqrt{\lambda}h(g_{\alpha} + (b-a)(g_{\alpha}^{l})) \max_{1 \leq p \leq N} \left| \frac{\sin p\sqrt{\lambda}h}{\sin \sqrt{\lambda}h} \right| + Ch^{4} \sqrt{\lambda} \]

\[ \leq Ch^{4} \sqrt{\lambda} \]

From (2.5.2),

\[ | \sum_{i=0}^{N-1} E_{1}(f(x, 0, \lambda)) | \leq | \sum_{i=0}^{N-1} E_{1}(g_{h} \sin 2\phi) | + Ch^{4} \sqrt{\lambda} \]

and the result then follows.

**LEMMA 2.8** Let \( q \in C^{5}[a, b] \), then

\[ |S_{1}(f(x, 0, \lambda)) - \Phi(x, 0, \lambda; h) | \leq Ch^{4} \right] h/(\lambda \leq \pi \right] \]

when the classical Runge-Kutta method is used to integrate the differential equation for the modified phase.

**Proof** We first give some bounds which will be required in the proof.
The bounds given in (i) are derived from the asymptotic expansion and the differential equation for $\theta$. The remaining bounds are derived in the usual manner from Taylor series expansions together with the bounds given in (i).

We also note that the global error satisfies

$$|e_i| \leq C h^4 \lambda \quad i = 0,1,\ldots,N.$$
\[
S_1(f(x, \theta, \lambda)) - \Phi(x, \bar{\theta}; h) = g_i(\sin 2\theta_i - \sin 2\bar{\theta}_i) 
\]
\[
+ 2 g_{i+\frac{1}{2}}(\sin 2\theta_{i+\frac{1}{2}} - \sin 2\bar{\theta}_{i+\frac{1}{2}} + \frac{h_k}{2}) + 2 g_{i+\frac{3}{2}}(\sin 2\theta_{i+\frac{3}{2}} - \sin 2\bar{\theta}_{i+\frac{3}{2}} + \frac{h_k}{2}) 
\]
\[
+ g_{i+1}(\sin 2\theta_{i+1} - \sin 2\bar{\theta}_{i+1} + \frac{h_k}{2}) .
\]

(2.5.3.)

We now consider each of the terms on the right hand side of (2.5.3) separately:

The first

Since \( \bar{\theta}_i = \theta_i - e_i \), we have

\[
|\sin 2\theta_i - \sin 2\bar{\theta}_i| \leq 2|e_i| \leq Ch^4 \lambda .
\]

The second

Since \( \bar{\theta}_i + \frac{h_k}{2} = \theta_i + \frac{h_k}{2} \), we have

\[
|\left(\theta_{i+\frac{1}{2}} - \frac{1}{2}h^2 \theta_{i+\frac{1}{2}} - \frac{1}{6}h^3 \theta_{i+\frac{1}{2}}\right) - (\bar{\theta}_{i+\frac{1}{2}} + \frac{h_k}{2})| 
\]
\[
\leq |\theta_{i+\frac{1}{2}} - \frac{1}{2}h^2 \theta_{i+\frac{1}{2}} + \frac{1}{6}h^3 \theta_{i+\frac{1}{2}}| 
\]
\[
+ |e_{i+\frac{1}{2}} + \frac{h_k}{2}|\|g\|_{\infty}|\sin 2\theta_i - \sin 2\bar{\theta}_i| 
\]
\[
\leq Ch^4 \lambda + Ch^4 \sqrt{\lambda} + Ch^4 \lambda^{-\frac{1}{2}} 
\]
\[
\leq Ch^4 \lambda .
\]

Therefore
\[
|\sin 2\theta_{1+\frac{1}{2}} - 2\left(\frac{1}{2}\right)^2 \theta''_{1} + \frac{1}{6} \left(\frac{1}{2}\right)^3 \theta'''_{1}\right)\cos 2\theta_{1+\frac{1}{2}} - \sin 2(\bar{\theta}_{1} + \frac{h_{K_{1}}}{2})|
\]
\[
\leq 4\left(\frac{1}{2}\right)^2 \||\theta''\|_{\infty} + \frac{1}{6} \left(\frac{1}{2}\right)^3 \||\theta'''\|_{\infty}\right)^2 + Ch^4\lambda
\]
\[
\leq C_1 h^4 \lambda^{-1} + C_2 h^5 \lambda^{\frac{1}{2}} + C_3 h^6 + Ch^4\lambda
\]
\[
\leq Ch^4\lambda.
\]

The third

Since \( \bar{\theta}_{1} + \frac{h_{K_{2}}}{2} = \theta_{1} + \frac{h_{\theta_{1}}}{2} + e_{1} - \frac{h_{\theta_{1}}}{2} g_{1+\frac{1}{2}}(\sin 2\theta_{1+\frac{1}{2}} - \sin 2(\bar{\theta}_{1} + \frac{h_{K_{1}}}{2})) \),

we have

\[
|\left(\theta_{1+\frac{1}{2}} + \frac{1}{2}\right)^2 \theta''_{1} + \frac{1}{3} \left(\frac{1}{2}\right)^3 \theta'''_{1} - \left(\frac{1}{2}\right)^3 \theta'''_{1+\frac{1}{2}}\cos 2\theta_{1+\frac{1}{2}} - \left(\bar{\theta}_{1} + \frac{h_{K_{2}}}{2}\right)|
\]
\[
\leq \left|\left(\theta_{1+\frac{1}{2}} + \frac{1}{2}\right)^2 \theta''_{1} + \frac{1}{3} \left(\frac{1}{2}\right)^3 \theta'''_{1} - \left(\theta_{1} + \frac{h_{\theta_{1}}}{2}\right)\right|
\]
\[
+ \frac{h_{\theta_{1}}}{2} \|g\|_{\infty} \left|\sin 2\theta_{1+\frac{1}{2}} - 2\left(\frac{1}{2}\right)^2 \theta''_{1} + \frac{1}{6} \left(\frac{1}{2}\right)^3 \theta'''_{1}\right)\cos 2\theta_{1+\frac{1}{2}} - \sin 2(\bar{\theta}_{1} + \frac{h_{K_{1}}}{2})\right|
\]
\[
+ \frac{h_{\theta_{1}}}{2} \|g\|_{\infty} \left|\frac{1}{6} \left(\frac{1}{2}\right)^3 \theta'''_{1}\right| \cos 2\phi_{1+\frac{1}{2}}\right| + |e_{1}|
\]
\[
\leq C_1 h^4 \lambda^{-1} + C_2 h^4 \lambda + \frac{h_{\theta_{1}}}{2} C\lambda^{-1} C_2 h^4 \lambda + \frac{h_{\theta_{1}}}{2} C\lambda^{-1} C_3 h^3 \lambda + C_4 h^4 \lambda
\]
\[
\leq Ch^4\lambda.
\]

Therefore

\[
|\sin 2\theta_{1+\frac{1}{2}} + 2\left(\frac{1}{2}\right)^2 \theta''_{1} + \frac{1}{6} \left(\frac{1}{2}\right)^3 \theta'''_{1}\right)\cos 2\theta_{1+\frac{1}{2}} - \sin 2(\bar{\theta}_{1} + \frac{h_{K_{2}}}{2})|
\]
\[
\leq 4\left(\frac{1}{2}\right)^2 \||\theta''\|_{\infty} + \frac{1}{6} \left(\frac{1}{2}\right)^3 \||\theta'''\|_{\infty}\right)^2 + \frac{h_{\theta_{1}}}{2} \|g\|_{\infty} \||\theta''\|_{\infty} + \frac{h_{\theta_{1}}}{2} \|g\|_{\infty} \||\theta'''\|_{\infty}\right) + C_2 h^4\lambda
\]
\[
\leq C_1 h^4 + C_2 h^4\lambda
\]
\[
\leq Ch^4\lambda.
\]
The fourth

Since \( \tilde{\theta}_i + \hbar \kappa_3 = \theta_i + \hbar \theta'_i \frac{1}{2} - e_i - \hbar g_{i+\frac{1}{2}} (\sin 2\theta_{i+\frac{1}{2}} - \sin (\tilde{\theta}_i + \frac{\hbar}{2} \kappa_3)) \),

we have

\[
| (\theta_{i+1} + \frac{1}{3} (\frac{\hbar}{2})^3 \theta''')_{i+1} + 2g_{i+\frac{1}{2}} (\frac{\hbar}{2})^3 \theta''_{i+1} \cos 2\theta_{i+\frac{1}{2}} - (\tilde{\theta}_i + \hbar \kappa_3) |
\]

\[
\leq | \theta_{i+1} - \frac{1}{3} (\frac{\hbar}{2})^3 \theta'''_{i+1} - (\tilde{\theta}_i + \hbar \theta'_i \frac{1}{2}) |
\]

\[
+ \h ||g|| \| \sin 2\theta_{i+\frac{1}{2}} + 2 (\frac{1}{3} (\frac{\hbar}{2})^2 \theta''_{i+1} + \frac{1}{3} (\frac{\hbar}{2})^3 \theta'''_{i+1} - (\frac{\hbar}{2})^3 g_{i+\frac{1}{2}} \theta''_{i+1} \cos 2\theta_{i+\frac{1}{2}} \cos 2\theta_{i+\frac{1}{2}} - \sin (\tilde{\theta}_i + \frac{\hbar}{2} \kappa_3) |
\]

\[
+ \h ||g|| \| (\frac{1}{3} (\frac{\hbar}{2})^3 \theta''')_{i+1} - (\frac{\hbar}{2})^3 g_{i+\frac{1}{2}} \theta''_{i+1} \cos 2\theta_{i+\frac{1}{2}} \cos 2\theta_{i+\frac{1}{2}} | + | e_i |
\]

\[
\leq C_1 h^4 \sqrt{\lambda} + Ch^4 \sqrt{\lambda} + Ch^{-1} C_2 h^4 \sqrt{\lambda} + Ch^{-1} (C_3 h^3 + C_4 h^3 \lambda^{-\frac{3}{2}}) + C_5 h^4 \lambda
\]

\[
\leq Ch^4 \lambda
\]

Therefore

\[
| \sin 2\theta_{i+1} + 2 (\frac{1}{3} (\frac{\hbar}{2})^3 \theta''')_{i+1} + 2g_{i+\frac{1}{2}} (\frac{\hbar}{2})^3 \theta''_{i+1} \cos 2\theta_{i+\frac{1}{2}} \cos 2\theta_{i+\frac{1}{2}} - \sin (\tilde{\theta}_i + \hbar \kappa_3) |
\]

\[
\leq 4 (\frac{1}{3} (\frac{\hbar}{2})^3 \| \theta'''' \|_\infty + 2 ||g|| (\frac{\hbar}{2})^3 \| \theta'''' \|_\infty )^2 + Ch^4 \lambda
\]

\[
\leq C_1 h^6 + Ch^4 \lambda
\]

\[
\leq Ch^4 \lambda
\]
Substituting these bounds in (2.5.3), we obtain

\[ |S_i(f(x, \theta, \lambda)) - \Phi(x_i, \bar{\theta}_i; h)| \]

\[ \leq \frac{1}{6} \left\{ 2\|g\|_\infty C_1 h^4/\lambda + 2g_{i+\frac{1}{2}} \left( \frac{h}{2} \right)^2 \theta''_i + \frac{1}{3} (\frac{h}{2})^3 \theta'''_i \right\} \cos 2\theta_{i+\frac{1}{2}} \]

\[ + 2g_{i+\frac{1}{2}} \left( \frac{h}{2} \right)^2 \theta''_i + \frac{2}{3} (\frac{h}{2})^3 \theta'''_i \cos 2\theta_{i+\frac{1}{2}} \cos \theta_{i+1} \]

\[ + g_{i+1} \left( \frac{h}{2} \right)^3 \theta''''_i - 4 (\frac{h}{2})^3 g_{i+\frac{1}{2}} \cos 2\theta_{i+\frac{1}{2}} \cos \theta_{i+1} \]

\[ + 2\|g\|_\infty C_2 h^4/\lambda + 2\|g\|_\infty C_3 h^4/\lambda + \|g\|_\infty C_4 h^4/\lambda \} \]

\[ \leq C_5 h^4 + \frac{1}{6} \left\{ \left( \frac{2}{3} \right)^3 \theta''''_i - 4 (\frac{h}{2})^3 g_{i+\frac{1}{2}} \cos 2\theta_{i+\frac{1}{2}} \right\} \right\} \}

\[ \leq C_5 h^4 + \frac{1}{6} \left\{ \left( \frac{2}{3} \right)^3 \theta''''_i - 4 (\frac{h}{2})^3 \|g\|_\infty \left\{ \frac{h}{2} \right\} g'(\xi_1) \cos 2\theta_{i+1} \right\} \]

\[ + h |g_{i+\frac{1}{2}} \theta'(\xi_2) \sin 2\theta(\xi_2)| \right\} \xi_1, \xi_2 \in (x_i, x_{i+1}) \]

\[ \leq C_5 h^4 + \{C_7 \lambda^{-1} + C_8 \lambda^{-\frac{1}{2}} \}

\leq C h^4 .

From these two results we derive

**LEMMA 2.9**  
Let \( q \in C^5[a, b] \), then

\[ |e_N| \leq Ch^4/\lambda \quad \text{when } h/\lambda < \frac{\pi}{2} \]

when the classical Runge-Kutta method is used to integrate the differential equation for the modified phase.
Proof Since

\[
e_i + 1 - e_i = (\theta_{i+1} - \theta_i) - (\tilde{\theta}_{i+1} - \tilde{\theta}_i)
\]

\[
= \int_{x_i}^{x_{i+1}} f(x, \theta, \lambda) \, dx - h \phi(x_i, \tilde{\theta}_i; h)
\]

\[
= i \sum_{i=0}^{N-1} (f(x, \theta, \lambda)) + h(S_i(f(x, \theta, \lambda)) - \phi(x_i, \tilde{\theta}_i; h))
\]

we have from Lemmas 2.7 and 2.8

\[
|e_N| = \left| \sum_{i=0}^{N-1} (e_{i+1} - e_i) \right|
\]

\[
\leq \left| \sum_{i=0}^{N-1} ES_i(f(x, \theta, \lambda)) \right| + \left| \sum_{i=0}^{N-1} h(S_i(f(x, \theta, \lambda)) - \phi(x_i, \tilde{\theta}_i; h)) \right|
\]

\[
\leq C_1 h^4 \sqrt{\lambda} + C_2 h^4 \sum_{i=0}^{N-1} h
\]

\[
\leq Ch^4 \sqrt{\lambda}
\]

provided \( h \sqrt{\lambda} \leq \frac{\pi}{2} \).

With this improved global error bound we obtain

THEOREM 2.4 Let \( q \in C^5[a, b] \). Then there is an \( h_0 > 0 \) such that whenever \( h < h_0 \), the eigenvalue estimates satisfy

\[
|\lambda_k - \tilde{\lambda}_k| \leq C h^4 k^2 , \quad \sqrt{\tilde{\lambda}_k} h \leq \frac{\pi}{2}
\]

(2.5.4)

when the classical Runge-Kutta method is used to integrate the differential equation for the modified phase.
Proof. Since $|e_N| \leq Ch^4\lambda$, it is clear that there is an $h_0$ such that whenever $h < h_0$ the conditions of Lemma 2.2 will be satisfied. Applying Lemmas 2.9 and 2.2 then yields the bound

$$|\lambda_k - \tilde{\lambda}_k| \leq C_1 h^{\frac{1}{2}} \sqrt{\lambda_k}$$

whenever $h < h_0$ and $\sqrt{\lambda_k} h \leq \frac{\pi}{2}$. The stated result then follows from (1.1.4).

Finally, if we make the obvious changes to Lemmas 2.7, 2.8 and 2.9, we also have

**Theorem 2.5.** Let $q \in C^5[a,b]$. Then there is an $h_0 > 0$ such that whenever $h < h_0$, the eigenvalue estimates satisfy

$$|\lambda_k - \tilde{\lambda}_k| \leq Ch^4 h^2,$$

$$\sqrt{\lambda_k} h \leq \frac{\pi}{2}$$

(2.5.5)

when the classical Runge-Kutta method is used to integrate the differential equation for the scaled phase.

To investigate the agreement between these bounds and the numerical results we approximate the eigenvalues of (2.3.1) - (2.3.2) using the classical Runge-Kutta method with $N = 40$. The eigenvalue errors for the modified phase are given in figure 2.7 and those for the scaled phase are given in figure 2.8.

It is not obvious for this example that the errors observed are in agreement with the predicted bounds for either of these methods. However, if we consider the individual terms which comprise the error bound we see that for both methods the error can be expressed as
\[ |\lambda_k - \tilde{\lambda}_k| \leq \frac{C_1 h}{\sqrt{\lambda}} \left| \cot \frac{\sqrt{\lambda} h}{3} + \frac{2}{3} \csc \sqrt{\lambda} h - \frac{1}{\sqrt{\lambda} h} \right| + C_2 h^4 \sqrt{\lambda} . \]

Since \[ \left| \frac{\cot x}{3} + \frac{2}{3} \csc x - \frac{1}{x} \right| \leq 10^{-2} x^3 \text{ for } x \leq \frac{\pi}{2} , \] the dominant term will be \( C_2 h^4 \sqrt{\lambda} \) unless \( C_1 \sqrt{\lambda} >> C_2 \). Thus, although the predicted \( k^2 \) growth of the eigenvalue error will not always be observed, (2.5.4) and (2.5.5) are in fact the best bounds of this form which can be given.
Figure 2.7  Eigenvalue error in using the classical Runge-Kutta method to integrate the modified phase for (2.3.1) - (2.3.2).
Figure 2.8  Eigenvalue error in using the classical Runge-Kutta method to integrate the scaled phase for (2.3.1) - (2.3.2).
CHAPTER 3

APPROXIMATION OF THE DIFFERENTIAL EQUATION

3.1 Introduction

In this chapter we examine the estimates of the eigenvalues of (1.1.1) - (1.1.3) obtained by replacing the coefficients \( p, q \) and \( r \) with piecewise constant approximations. We restrict attention to such approximations because it is only in this case that we can construct computationally tractable schemes which avoid the need for piecewise polynomial approximations of the eigenfunction.

Since it is known that a bounded symmetric perturbation of a self-adjoint operator results in a uniformly bounded perturbation of the spectrum (see for example, Kato (1966; p.291)) we begin by considering eigenvalue problems that are in Liouville normal form.

3.2 Approximation of Differential Equations in Normal Form

In this section we consider eigenvalue problems of the form

\[
- \ddot{z} + sz = \lambda z , \quad z \in D , \quad \dot{z} = \frac{dz}{dt}
\]

(3.2.1)

where \( s \) is a continuous function and \( D = \{ z \in L^2[0,T] : \dot{z} , z \text{ are absolutely continuous, } \dot{z} \in L^2[0,T] , \sigma_1 z(0) + \dot{z}(0) = 0 , \sigma_2 z(T) - \dot{z}(T) = 0 \} \).

We further consider approximating problems of the form

\[
- \ddot{z} + \tilde{s}z = \lambda z , \quad z \in D
\]

(3.2.2)

where \( \tilde{s} \) is a piecewise continuous function.
Let \( \{\lambda_k\}_{k=1}^\infty \), \( \{\tilde{\lambda}_k\}_{k=1}^\infty \) be the eigenvalues of (3.2.1) and (3.2.2) respectively, arranged in ascending order, and \( \{z_k\}_{k=1}^\infty \), \( \{\tilde{z}_k\}_{k=1}^\infty \) be the corresponding eigenfunctions, scaled so that

\[ \|z_k\|_2 = \|\tilde{z}_k\|_2 = 1 \]

and

\[ (z_k, \tilde{z}_k) \geq 0. \]

Then we have the following results.

**Theorem 3.1** Let \( \rho := \frac{1}{2} \min_k |\lambda_{k+1} - \lambda_k| > 0 \) and \( \tilde{s} \) be such that \( \|s-\tilde{s}\|_{\infty} < \frac{\rho}{2} \).

Then

(i) \[ |\lambda_k - \tilde{\lambda}_k| \leq \|s-\tilde{s}\|_{\infty}, \quad k = 1,2,\ldots \]

(ii) \[ \|z_k - \tilde{z}_k\|_2 \leq \frac{4}{\rho} \|s-\tilde{s}\|_{\infty}, \quad k = 1,2,\ldots . \]

**Proof**

(i) The first assertion follows from a result of Kato (1966; p.291) which states that if \( T \) is a self-adjoint operator and \( B \) a bounded symmetric operator both acting in a Hilbert space \( H \), then \( T + B \) is self-adjoint, and

\[ \text{dist}[\Sigma(T), \Sigma(T+B)] \leq \|B\| \]

where \( \Sigma(T) \), \( \Sigma(T+B) \) are the spectra of the operators \( T \) and \( T + B \) respectively, and

\[ \text{dist}[X,Y] = \max \{\sup_{x \in X} \inf_{y \in Y} |x-y|, \ \sup_{y \in Y} \inf_{x \in X} |x-y|\} \]

for any two sets \( X \) and \( Y \) contained in \( \mathbb{C} \).
Now if we define the operators \( L \) and \( \tilde{L} \) by

\[
Lz = -\dot{z} + sz, \quad z \in \mathbb{D}
\]
\[
\tilde{L}z = -\dot{z} + \tilde{sz}, \quad z \in \mathbb{D}
\]

then it is clear that \( \tilde{L} = L - B \) where \( B \) is the bounded symmetric operator defined by

\[
Bz = (s-\tilde{s})z.
\]

From Stone (1932; Theorem 10.18) \( L \) is self-adjoint. Since \( D \subset L^2([0,T]) \), the conditions of Kato's theorem are satisfied and hence,

\[
\text{dist}[\Sigma(L), \Sigma(\tilde{L})] \leq \|B\|_2.
\]

The ordering of the spectra and the bound on \( \|s-\tilde{s}\|_\infty \) then imply

\[
|\lambda_k - \tilde{\lambda}_k| \leq \|s-\tilde{s}\|_\infty, \quad k = 1, 2, \ldots.
\]

(ii) Let

\[
\Gamma_k = \{\lambda \in \mathbb{C} : |\lambda - \lambda_k| = \rho\}, \quad k = 1, 2, \ldots.
\]

As \( \lambda_k \) and \( \tilde{\lambda}_k \) are the only eigenvalues of \( L \) and \( \tilde{L} \) respectively on the disc bounded by \( \Gamma_k \), and both eigenvalues are interior points of \( \Gamma_k \), the projection operators

\[
P_k := -\frac{1}{2\pi i} \oint_{\Gamma_k} (L-\lambda I)^{-1} d\lambda \quad (3.2.3)
\]

and

\[
\tilde{P}_k := -\frac{1}{2\pi i} \oint_{\Gamma_k} (\tilde{L}-\lambda I)^{-1} d\lambda \quad (3.2.4)
\]
are well defined and

\[ P_k f = (z_k, f) z_k \] \tag{3.2.5} \\
\[ \tilde{P}_k f = (z_k, f) \tilde{z}_k \] \tag{3.2.6}

for any \( f \in L^2[0, T] \).

Furthermore, it is easily verified that for \( \lambda \in \Gamma_k \)

\[ (\tilde{L} - \lambda I)^{-1} = (L - \lambda I)^{-1} + (\tilde{L} - \lambda I)^{-1} B (L - \lambda I)^{-1} \]

and hence, from (3.2.6) with \( f = z_k \) and (3.2.4),

\[ (\tilde{z}_k, z_k) \tilde{z}_k = \tilde{P}_k z_k \]

\[ = P_k z_k + R_k z_k \]

where

\[ R_k = - \frac{1}{2\pi i} \oint_{\Gamma_k} (\tilde{L} - \lambda I)^{-1} B (L - \lambda I)^{-1} d\lambda \]

i.e. using (3.2.5) in the above,

\[ (\tilde{z}_k, z_k) \tilde{z}_k = z_k + R_k z_k \] \tag{3.2.7}

From Kato (1966; p.291) and the bound on \( \| s - \tilde{s} \|_\infty \) we find that

\[ \| R_k \|_2 \leq \frac{2}{\rho} \| s - \tilde{s} \|_\infty < 1 \] \tag{3.2.8}

and from (3.2.7)

\[ \| R_k \|_2 \geq 1 - (\tilde{z}_k, z_k) \geq 0 \]

But, also from (3.2.7)
and so,

$$\|	ilde{z}_k - z_k\|_2 \leq 2\|R_k\|_2$$

$$\leq \frac{4}{\rho}||s-\tilde{s}||_\infty.$$ 

From these basic results it is also possible to derive a refined estimate of the eigenvalue perturbation which will be useful for obtaining higher order convergence results in the next section. This result is

**THEOREM 3.2** If $||s-\tilde{s}||_\infty < \frac{\rho}{2}$ where $\rho$ is as defined in Theorem 3.1, then

$$|\lambda_k - \tilde{\lambda}_k| - \int_0^T (s-\tilde{s}) z_k^2 dt \leq \frac{4}{\rho}||s-\tilde{s}||^2_\infty, \quad k = 1, 2, \ldots$$

**Proof** Let $k$ be a given integer. From (3.2.7) we have, since $\|R_k\|_2 < 1$ implies that $(\tilde{z}_k, z_k) \neq 0$,

$$\tilde{z}_k = (z_k + R_k z_k)/(\tilde{z}_k, z_k) \quad (3.2.9)$$

where $z_k$ and $\tilde{z}_k$ are the eigenfunctions of (3.2.1) and (3.2.2) respectively, corresponding to the eigenvalues $\lambda_k$ and $\tilde{\lambda}_k$.

Applying $\tilde{L}$ to $\tilde{z}_k$ and using (3.2.2) and (3.2.9) yields

$$\tilde{L}\tilde{z}_k = \tilde{\lambda}_k (z_k + R_k z_k)/(\tilde{z}_k, z_k)$$

but since $\tilde{L} = L - B$, we also have

$$\tilde{L}\tilde{z}_k = (\lambda_k z_k - B z_k + LR_k z_k)/(\tilde{z}_k, z_k).$$

Hence
and on taking the inner product of both sides with $z_k$ and noting that $(z_k, z_k) = 1$,

$$\left(\lambda_k - \tilde{\lambda}_k\right) z_k - B z_k = - (L - \tilde{\lambda}_k I) R_k z_k$$

But, since $(L - \tilde{\lambda}_k I)$ is self-adjoint,

$$\left(\lambda_k - \tilde{\lambda}_k\right) - \int_0^T (s - \tilde{s}) z_k^2 dt = - (z_k, (L - \tilde{\lambda}_k I) R_k z_k) .$$

Theorem 3.1 and the inequality (3.2.8) then yield the desired result.

### 3.3 Convergence Results for Problems in Normal Form

From the preceding results it is a simple matter to obtain results analogous to those of Pruess (1973) when $s$ is approximated by a piecewise polynomial. However, due to the inherent difficulties in solving the approximate problem for the general case, we shall restrict attention to the case of piecewise constant approximation. That is, $\tilde{s}$ is of the form

$$\tilde{s}(t) = \tilde{s}_i, \quad t \in (t_i, t_{i+1}) \quad i = 0, 1, \ldots, N-1$$

where $\tilde{s}_i$ is some constant, and $\Delta_N$ is some partition of $[0, T]$.

For such approximations, we have from Theorem 3.1,

**Corollary 3.1** Let $s \in C^1[0, T]$, $\Delta_N$ be a partition of $[0, T]$ and $\tilde{s}_i$ interpolate $s$ at some point in $[t_i, t_{i+1}]$ for each $i$. Then there is an $h_0 > 0$ such that for each partition $\Delta_N$ with $h < h_0$
If we define \( h_0 = \frac{1}{\|S\|_\infty} \), then the result follows from Theorem 3.1 since \( \|S - \tilde{S}\|_\infty \leq h\|\tilde{S}\|_\infty \).

Similarly, if \( s \in C^2[0,T] \) and \( \tilde{S} \) is given by midpoint interpolation, then Ixaru's (1972) result follows from Theorem 3.2 by using any standard result on the error of midpoint product integration. However, initial computational results indicated that for midpoint interpolation on a uniform grid, this bound can be improved. Before giving this improved bound, the following definitions and lemma are required:

On the uniform partition \( \Delta_N \) of \([0,T]\) define \( s^* \) to be the piecewise constant approximation determined by the rule

\[
s^*(t) = s_{i+\frac{1}{2}}, \quad t \in (t_i, t_{i+1}).
\]

**Lemma 3.1** Let \( s \in C^2[0,T] \), \( f \in C^1[0,T] \) and \( \Delta_N \) be a uniform partition of \([0,T]\). Then

\[
\left| \int_0^T (s - s^*)f dt \right| \leq T \left\{ \frac{1}{4}\|\tilde{S}\|_\infty\|\tilde{F}\|_\infty + \frac{1}{8}\|\tilde{S}\|_\infty\|\tilde{F}\|_\infty \right\} h^2.
\]
Proof

\[
\left| \int_0^T (s - s^*) f(t) dt \right| \leq \sum_{i=0}^{N-1} \left| \int_{t_i}^{t_{i+1}} [s(t) - s_{i+1/2}] f(t) dt \right|
\]

\[
\leq \sum_{i=0}^{N-1} \left| \int_{t_i}^{t_{i+1}} s_{i+1/2} (t - t_{i+1/2}) f_{i+1/2} dt \right|
\]

\[
+ \sum_{i=0}^{N-1} \left| \int_{t_i}^{t_{i+1}} [s(t) - s_{i+1/2} - s_{i+1/2} (t - t_{i+1/2})] f(t) dt \right|
\]

Using the inequalities

\[
|s(t) - s_{i+1/2} - s_{i+1/2} (t - t_{i+1/2})| \leq \frac{1}{8} \| \ddot{s} \|_\infty h^2, \quad t \in [t_i, t_{i+1}]
\]

and

\[
|f(t) - f_{i+1/2}| \leq \frac{1}{2} \| \dot{f} \|_\infty h, \quad t \in [t_i, t_{i+1}]
\]

it is easy to verify that

\[
\left| \int_0^T (s - s^*) f(t) dt \right| \leq T \left( \frac{1}{4} \| \ddot{s} \|_\infty \| \dot{f} \|_\infty + \frac{1}{8} \| \ddot{s} \|_\infty \| f \|_\infty \right) h^2.
\]

If we now define \( \{ \lambda_k \}_k=1^\infty \) and \( \{ z_k \}_k=1^\infty \) to be the eigenvalues and eigenfunctions of (3.2.2) with \( \ddot{s} = s^* \), and \( \{ \mu_k \}_k=1^\infty \) and \( \{ v_k \}_k=1^\infty \) the eigenvalues and eigenfunctions defined in section 1.1, we have

**Theorem 3.3** Let \( s \in C^2[0,T] \). Then there is an \( h_0 > 0 \) such that for each uniform partition \( N \) with \( h < h_0 \),

|\lambda_k - \lambda_k^*| \leq \begin{cases} 
\frac{C_1}{h_k} \left| \sin \frac{\mu_k h}{h_k^2} \right| \left[ \max_{1 \leq p \leq N-1} \left| \sin \frac{p \mu_k h}{h_k^2} \right| \right] h^2 + C_2 h^2, \sin \frac{\mu_k h}{h_k} \neq 0 \\
Ch, \sin \frac{\mu_k h}{h_k} = 0
\end{cases}

\textbf{Proof} \quad \text{Let } h_0 = \rho/\|s\|_\infty \text{ and } \Delta_N \text{ be a uniform partition with } h < h_0, \text{ then the conditions of Theorem 3.2 are satisfied since}

\|s - s^*\|_\infty \leq \frac{1}{2} h \|\dot{s}\|_\infty < \rho/2.

Using the identity

\[ z_k^2 = \nu_k^2 + 2(\nu_k - v_k)\nu_k + (\nu_k - v_k)^2 \]

in Theorem 3.2, we find

\[ |\lambda_k - \lambda_k^*| \leq \int_0^T (s - s^*)\nu_k^2 dt + 2 \int_0^T (s - s^*)(\nu_k - v_k)\nu_k dt \]

\[ + \int_0^T (s - s^*)(\nu_k - v_k)^2 dt + \frac{4}{\rho}\|\dot{s}\|_\infty^2 h^2 \]

Estimating the last two integrals through the application of Lemma 3.1 together with the bounds (1.1.5) - (1.1.6) and (1.1.17) - (1.1.18), then yields

\[ |\lambda_k - \lambda_k^*| \leq \int_0^T (s - s^*)\nu_k^2 dt + Ch^2. \quad (3.3.1) \]

If on each of the intervals \((t_i, t_{i+1})\) we replace \((s - s^*)\) by a Taylor's series expanded about \(t_{i+\frac{1}{2}}\),
\[ |\int_0^T (s-s^*) v_k^2 dt| \leq \sum_{i=0}^{N-1} e^{s_{i+\frac{1}{2}}} (t-t_{i+\frac{1}{2}}) v_k^2 dt \]
\[ + \frac{1}{8h^2} \|\tilde{s}\|_\infty \int_0^T v_k^2 dt \]

and, since \( v_k = A_k \sin(\sqrt{\mu_k} t + \phi_k) \), we can integrate the above to give

\[ |\int_0^T (s-s^*) v_k^2 dt| \leq \sum_{i=0}^{N-1} e^{s_{i+\frac{1}{2}}} (t-t_{i+\frac{1}{2}}) v_k^2 dt \]

\[ + \frac{1}{8h^2} \|\tilde{s}\|_\infty \int_0^T v_k^2 dt \]

If we now use Lemma A1.1 to bound the above summation, the stated result then follows from (3.3.1).

From Appendix 2, it is clear that the bound given in Theorem 3.3 can be written

\[ |\lambda_k - \lambda^*_k| \leq C h^2, \quad \sqrt{\mu_k} h \leq \frac{\pi}{2}. \]

But as \( \sqrt{\mu_k} h \) increases above \( \frac{\pi}{2} \) the constant \( C \) will increase and the error will become less uniform. Thus to obtain uniform eigenvalue estimates we need to improve the estimates for those values of \( k \) for which \( \sqrt{\mu_k} h > \frac{\pi}{2} \). This can be done in one of two ways.

From (1.1.19)

\[ |\lambda_k - \lambda^*_k| \leq \frac{1}{T} \int_0^T s dt \leq C/\mu_k \]  \hspace{1cm} (3.3.2)

and so this expansion will provide uniform \( 0(h^2) \) estimates when \( \sqrt{\mu_k} h > \frac{\pi}{2} \).

However, as we noted in Chapter 1, this expansion may only give accurate estimate when \( k \) is very large. One alternative to using (3.3.2)
is to use the information derived in the proof of Theorem 3.3 to correct the eigenvalue estimate \( \lambda_k^* \).

If we define

\[
\bar{s}_h(t) = (t_{t_i} + t) \frac{(s_i + 1 - s_i)}{h} \quad t \in (t_i, t_i+1)
\]

and note that

\[
|s - s^* - s_h| \leq \frac{1}{4} \|\bar{s}\|_\infty h^2,
\]

and

\[
\left| \int_0^T (s - s^*) dt \right| \leq \frac{1}{12} h^2 \|\bar{s}\|_\infty
\]

then

\[
\left| \int_0^T (s - s^*) v_k^2 dt + \frac{A_k^2}{2} \int_0^T s_h \cos 2(\nu_k t + \phi_k) dt \right|
\]

\[
\leq \frac{A_k^2}{2} \left| \int_0^T (s - s^*) dt \right| + \frac{A_k^2}{2} \left| \int_0^T (s - s^*) \cos 2(\nu_k t + \phi_k) dt \right|
\]

\[
\leq C h^2.
\]

Therefore, from Theorem 3.2 and Theorem 3.3

\[
|\lambda_k - \lambda_k^* + \frac{A_k^2}{2} \int_0^T s_h \cos 2(\nu_k t + \phi_k) dt|
\]

\[
\leq |\lambda_k - \lambda_k^*| \left| \int_0^T (s - s^*) z_k^2 dt \right| + \left| \int_0^T (s - s^*) (z_k^2 - v_k^2) dt \right|
\]

\[
+ \left| \int_0^T (s - s^*) v_k^2 dt + \frac{A_k^2}{2} \int_0^T s_h \cos 2(\nu_k t + 2\phi_k) dt \right|
\]

\[
\leq C h^2.
\]

(3.3.3)
Since $A_k$, $\phi_k$ and $\mu_k$ can be easily computed and

$$\int_0^T s_h \cos 2(\sqrt{\mu_k} t + \phi_k) dt$$

$$= \frac{h}{2} \left( \frac{\cos \sqrt{\mu_k} h}{\sqrt{\mu_k} h} - \sin \sqrt{\mu_k} h \right) \sum_{i=0}^{N-1} (s_{i+1} - s_i) \sin 2(\sqrt{\mu_k} t_{i+1} + \phi_k)$$

this gives us a means for correcting the eigenvalue estimates to obtain uniform $O(h^2)$ approximations of the exact eigenvalues.

### 3.4 Approximation of Differential Equations not in Normal Form

Although the technique of approximating the coefficients of the differential equation by piecewise constant functions provides a uniform approximation to the eigenvalues when the problem is in normal form, it can be shown that when this technique is applied to the general case (1.1.1) - (1.1.3), Pruess' error bounds are sharp.

This suggests that when the problem is not in normal form, we should use the Liouville transformation to transform (1.1.1) - (1.1.3) into normal form (1.1.10) - (1.1.12). We can then use the previously outlined method to obtain uniform approximations to the eigenvalues of this transformed problem and hence of the original problem.

In some cases however it may not be possible to carry out this transformation explicitly. Thus to obtain uniform estimates it is necessary to also approximate the transformation.

From the form of the exactly transformed problem (1.1.10) - (1.1.12), it can be seen that the transformed interval length $T$, the function $s$, and the boundary condition coefficients $\sigma_1^*$ and $\sigma_2^*$ all need to be
evaluated. Let us therefore consider how we should approximate them.

Since a perturbation of $T$ will produce a perturbation of the
eigenvalue which is proportional to the size of the eigenvalue, it is clear
that $T$ needs to be accurately approximated. However this causes no
difficulty in practice because the integral defining $T$ (i.e. (1.1.8))
may be evaluated with sufficient accuracy so that any non-uniformity will
not be apparent in the range of eigenvalues which are of interest.

The next problem is the evaluation of the function $s$. If the
required derivatives of $p$ and $r$ are not available, it becomes necessary
to use differences to approximate them. This raises the problem of choosing
a partition on which to apply the differences. To apply Theorem 3.3 we
require either the values $s_{i+\frac{1}{2}}$, $i = 0,1,\ldots,N-1$ or (since
$$|s_{i+\frac{1}{2}} - \frac{1}{2}(s_i + s_{i+1})| \leq \frac{1}{16} h^2 \|s\|_\infty$$
$s_i$, $i = 0,1,\ldots,N$ on the uniform partition
of the transformed interval $[0,T]$. Thus we require a partition of $[a,b]$
for which

$$t(x_{i+1}) - t(x_i) = h = T/N \quad i = 0,1,\ldots,N-1.$$ 

However the non-linearity of $t(x)$ makes it difficult to obtain such a
partition.

A simpler approach is to approximate $s$ on the partition defined by

$$t_i = t(x_i), \quad x_i = a + i\frac{(b-a)}{N} \quad i = 0,1,\ldots,N.$$

This approach will still give the desired estimates of $s_{i+\frac{1}{2}}$ although the
resulting partition of $[0,T]$ will no longer satisfy the conditions of
Theorem 3.3. Nevertheless it is clear that the same argument as that used
in Theorem 2.6 can be used to obtain the eigenvalue error bound
The final problem is the evaluation of $\sigma_1^*$ and $\sigma_2^*$. If these values cannot be found exactly, the conditions of Kato's theorem are no longer satisfied. The effect of perturbations in $\sigma_1^*$ and $\sigma_2^*$ is investigated in the following theorem.

**THEOREM 3.4** Let \( \{\lambda_k(\sigma, \eta)\}_{k=1}^\infty \) be the ordered eigenvalues and \( \{z_k(t, \sigma, \eta)\}_{k=1}^\infty \) be the corresponding normalised eigenfunctions of

\[
-\ddot{z} + s z = \lambda z , \quad z \in (0,T)
\]

\[
\sigma z(0) + \dot{z}(0) = 0
\]

\[
\eta z(T) - \dot{z}(T) = 0
\]

where \( s \in C[0,T] \). Then

\[
|\lambda_k - \lambda_k^*| \leq Ch^2 , \quad \sqrt{\mu_k} h \leq \frac{\pi}{2}.
\]

Proof. It is clearly sufficient to show that the derivatives of \( \lambda_k(\sigma, \eta) \) with respect to \( \sigma \) and \( \eta \) exist and are continuous. To do this we note that from Courant and Hilbert (1953; p.419) \( \lambda_k(\sigma, \eta) \) is a continuous function of \( \sigma \) and \( \eta \), and from Coddington and Levinson (1955; p.58) \( z_k(t, \sigma, \eta) \) depends continuously on \( \sigma \) and \( \eta \).

Let \( z = z_k(t, \sigma, \eta) \) and \( \ddot{z} = \ddot{z}_k(t, \sigma, \eta) \), then

\[
-\ddot{z} + sz = \lambda_k(\sigma, \eta) z
\]

and
Therefore

\[ -\dddot{z} + s\dddot{z} = \lambda_k(\bar{\sigma}, \bar{\eta})\dddot{z}. \]

We find on integrating (3.4.1)

\[
\left[ \lambda_k(\sigma, \eta) - \lambda_k(\bar{\sigma}, \bar{\eta}) \right] \int_0^T \dddot{z} \, dt = -\dddot{z}(0)(\sigma-\bar{\sigma}) - \dddot{z}(T)(\eta-\bar{\eta}).
\]

Now, since \( z \) depends continuously on \( \sigma \) and \( \eta \), there is a \( \delta = \delta(k) \) such that

\[
\int_0^T \dddot{z} \, dx > 0
\]

whenever \( (\bar{\sigma}, \bar{\eta}) \in N_\delta(\sigma, \eta) = \{(x, y) : (x-\sigma)^2 + (y-\eta)^2 < \delta^2\} \). Hence from (3.4.2)

\[
\left[ \lambda_k(\sigma, \eta) - \lambda_k(\bar{\sigma}, \bar{\eta}) \right] = -\frac{z(0)\ddot{z}(0)(\sigma-\bar{\sigma}) - z(T)\ddot{z}(T)(\eta-\bar{\eta})}{\int_0^T \dddot{z} \, dt}
\]

whenever \( (\bar{\sigma}, \bar{\eta}) \in N_\delta(\sigma, \eta) \).

On taking the relevant limits and noting that

\[
\lim_{\bar{\sigma} \to \sigma} \int_0^T \dddot{z} \, dt = \lim_{\bar{\eta} \to \eta} \int_0^T \dddot{z} \, dt = \|z_k\|_2^2 = 1
\]
we find that the derivatives of \( \lambda_k \) with respect to \( \sigma \) and \( \eta \) exist, and

\[
\frac{3\lambda_k}{3\sigma}(\sigma, \eta) = - z_k^2(0, \sigma, \eta)
\]

and

\[
\frac{3\lambda_k}{3\eta}(\sigma, \eta) = - z_k^2(T, \sigma, \eta).
\]

Thus the derivatives are continuous and bounded by \( \|z_k^2\|_\infty \). The result then follows from the eigenfunction bound (1.1.5).

Using these bounds in a standard mean value theorem shows that the perturbation of the eigenvalues is of the same order as the perturbations in \( \sigma_1^* \) and \( \sigma_2^* \). Thus, if \( \sigma_1 \) and \( \sigma_2 \) are approximated sufficiently well, the desired properties of the eigenvalue approximations will not be lost.

3.5 Numerical Schemes for Piecewise Constant Approximation

When \( \tilde{s} \) is chosen as a piecewise constant function, the solution of (3.2.2) for a given value of \( \lambda \) is

\[
v_\lambda(t) = \begin{cases} 
        A_0 F_0(t, \lambda) + B_0 G_0(t, \lambda) , & t \in [t_0, t_1] \\
        \vdots & \vdots \\
        \vdots & \vdots \\
        A_{N-1} F_{N-1}(t, \lambda) + B_{N-1} G_{N-1}(t, \lambda) , & t \in [t_{N-1}, t_N]
\end{cases}
\]

where \( F_i(t, \lambda) \) and \( G_i(t, \lambda) \) are the fundamental solutions of

\[- v + \tilde{s}_i v = \lambda v , \quad t \in (t_i, t_{i+1})\]

which were chosen as
The constants \( \{ A_i, B_i \}_{i=0}^{N-1} \) are determined up to an arbitrary multiple by the additional requirement that \( v_{\lambda} \in \mathbb{D} \).

The determination of the eigenvalues of (3.2.2) thus becomes that of finding the values of \( \lambda \) for which \( \{ A_i \}_{i=0}^{N-1} \) and \( \{ B_i \}_{i=0}^{N-1} \) are not identically zero. To do this, we note that the requirement \( v_{\lambda} \in \mathbb{D} \) yields a system of equations involving the unknowns \( A_i, B_i, v_{\lambda}(t_i), \dot{v}_{\lambda}(t_i) \) and the known values \( F_i(t_{i+1}, \lambda), G_i(t_{i+1}, \lambda) \). We can then proceed in a number of ways. Canosa (1970) uses these relations to eliminate the unknowns \( \{ v_{\lambda}(t_i), \dot{v}_{\lambda}(t_i) \}_{i=0}^{N-1} \) and obtains a system of equations in \( \{ A_i, B_i \}_{i=0}^{N-1} \). The eigenvalues are then simply the zeros of the determinant of this system. However, if these relations are used to eliminate the unknowns \( \{ A_i, B_i \}_{i=0}^{N-1} \) and \( \{ \dot{v}_{\lambda}(t_i) \}_{i=0}^{N-1} \) from the continuity conditions, we obtain

\[
G_{i+1}(t_{i+2}, \lambda)v_{\lambda}(t_i)
- \left[ F_i(t_{i+1}, \lambda)G_{i+1}(t_{i+2}, \lambda) + F_{i+1}(t_{i+2}, \lambda)G_i(t_{i+1}, \lambda) \right]v_{\lambda}(t_{i+1})
+ G_{i+1}(t_{i+1}, \lambda)v_{\lambda}(t_{i+2}) = 0 , \quad i = 0, 1, \ldots, N-2 .
\]
These relations, together with the equations

\[(F_0(t_1, \lambda) - \sigma_1 G_0(t_1, \lambda)) \nu_0(t_0) - \nu_1(t_1) = 0\]

and

\[- \nu_1(t_{N-1}) + (F_{N-1}(t_N, \lambda) - \sigma_2 G_{N-1}(t_N, \lambda)) \nu_1(t_N) = 0\]

which are obtained in a similar fashion from the boundary conditions, yield a system of equations of the form

\[D(\lambda) \nu = 0\]

where

\[\nu^T = (\nu_0(t_0), \nu_1(t_1), \ldots, \nu_N(t_N))\]

and \(D(\lambda)\) is a tridiagonal matrix.

This approach provides a simpler procedure for finding the eigenvalues of (3.2.2) and also yields a simple direct method for evaluating the eigenfunction at the knots of the partition. Unfortunately, there is the difficulty that not all zeros of the determinant are necessarily eigenvalues. To illustrate this, consider the problem

\[- \ddot{\nu} = \lambda \nu\]

\[\dot{\nu}(0) = 0 = \nu(\pi)\]

the exact eigenvalues of which are \(\lambda_k = (k + \frac{1}{2})^2\), \(k = 1, 2, \ldots\).

Now for the partition \(\{0, \frac{\pi}{2}, \pi\}\)
and so, $\det(D(\lambda)) = -\frac{1}{\sqrt{\lambda}} \sin \frac{\sqrt{\lambda} \pi}{2} \cos \sqrt{\lambda} \pi$. Therefore $\det(D(\lambda))$ is zero whenever $\lambda$ is an eigenvalue, but it is also zero when $\lambda = 4p^2$, $p = 1, 2, \ldots$ which are not eigenvalues.

Although there does not appear to be any simple analytical means for removing these extraneous zeros, it should be noted that they are an artifact introduced by the elimination of the values \( \{v_\lambda(t_i)\}_{i=0}^{N-1} \) and that they only arise non-trivially when $G_i(t_{i+1}, \lambda)$ and $G_{i+1}(t_{i+2}, \lambda)$ both vanish for some value of $\lambda$. This can only occur when $\lambda \geq \pi^2/h^2 - \|s\|_\infty$. Thus, for most problems this difficulty will either not occur or will occur in a range for which the asymptotic expansion rather than the approximation method will be used.

An alternative approach has been proposed by Pruess (1973). If we treat (3.2.2) as an initial value problem and define

$$\mathbf{v}_i^T = (v_\lambda(t_i), \dot{v}_\lambda(t_i))$$

and

$$M_i(\lambda) = \begin{bmatrix}
F_i(t_{i+1}, \lambda) & G_i(t_{i+1}, \lambda) \\
-(\lambda-s_i)G_i(t_{i+1}, \lambda) & F_i(t_{i+1}, \lambda)
\end{bmatrix}$$

then

$$v_{i+1} = M_i(\lambda)v_i$$

$$i = 0, 1, \ldots, N-1$$

(3.5.1)
where \( v_0^T = (1, -\sigma_1^*) \). Clearly \( \lambda \) will be an eigenvalue of (3.2.2) when 

\[
(1, \sigma_2^*) v_N = 0.
\]

Since \( v_N = \prod_{i=0}^{N-1} M_i(\lambda) \left( \begin{array}{c} 1 \\ -\sigma_1^* \end{array} \right) \) this gives a very simple and efficient means for locating the eigenvalues of (3.2.2). Also the values of the eigenfunction and its derivative at the knots of the partition are obtained as a by-product of the calculation.

One possible disadvantage of this method is the numerical instability which occurs when the eigenfunction, or its derivative, has rapid changes in magnitude (see e.g. Canosa (1970) and Pruess (1973)). This instability can be avoided by using some stable matrix routine to evaluate the determinant of the matrix

\[
D(\lambda) = \begin{pmatrix}
\sigma_1^* & 1 & & & & \\
M_0(\lambda) & -I & & & \\
& M_1(\lambda) & -I & & \\
& & \ddots & \ddots & \\
& & & \ddots & \ddots \\
0 & & & & \sigma_2^* -1
\end{pmatrix}
\]

The eigenvalues are then found by iterating on \( \lambda \) until \(|D(\lambda)| = 0\).

One such scheme can be constructed on noting that only the direction of \( v_N \) (and not its magnitude) is required to locate the eigenvalues. Thus the recurrence
\[ \lambda_0^T = (1, -\sigma_1^*) \]

\[ \hat{\lambda}_{i+1} = \frac{M_i(\lambda) \hat{\nu}_i}{\|M_i(\lambda) \hat{\nu}_i\|} \quad i = 0, 1, \ldots, N-1 \]

where \( \| \cdot \| \) is any vector norm, will be simple and efficient and will not suffer from the numerical instabilities of (3.5.1).

### 3.6 Numerical Examples

To provide numerical confirmation of the preceding results, the method outlined in §3.5 was implemented in a computer program. The zeroes of \( \omega(\lambda) = \nu_{\lambda}(t_N) - \sigma_2^* \hat{\nu}(t_N) \) were found using a modified secant method, the starting values for which were found by a fixed step search based on an initial prediction provided by an asymptotic expansion for the eigenvalues.

The first problem considered was

\[ -\ddot{u} + e^t u = \lambda u , \quad t \in (0, 1) \quad (3.6.1) \]

\[ u(0) = 0 = u(1) . \quad (3.6.2) \]

The approximating problem was chosen to be that given by approximating \( s \) using midpoint approximation on the uniform portion of \([0,1]\). The first forty eigenvalues of this approximating problem for \( N = 16 \) were found and an estimate of the error was obtained by comparing these values with the accurate estimates generated for chapter 2. The errors, given in figure 3.1, are in good agreement with the bound given in theorem 3.3.

Although these eigenvalue errors will decrease uniformly if we decrease \( h \), a better strategy is to apply the correction (3.3.3) or to switch over to the asymptotic expansion for suitably large values of \( k \),
Figure 3.1  Eigenvalue error for (3.6.1) - (3.6.2) obtained by approximating the differential equation.
or alternatively to use a higher order method such as that proposed by Pruess (1975).

The error in the estimates obtained by switching over to the asymptotic expansion for the above example (again with \( N = 16 \)) is given in figure 3.2. In figure 3.3 we give the error in using (3.3.3) to correct the eigenvalue estimates, and the eigenvalue errors in using the \( 0(h^4) \) method proposed by Pruess (1975) are given in figure 3.4.

Clearly the \( 0(h^4) \) method gives the best approximations of the smaller eigenvalues. However the error in the estimates grows rapidly with \( k \) and for \( k > \frac{N}{2} \) becomes almost identical with that of the simpler \( 0(h^2) \) method given in figure 3.1. Thus when a large number of eigenvalues are required it is better to use the simpler \( 0(h^2) \) method in conjunction with either the correction (3.3.3) or the asymptotic expansion.

The next problem considered was

\[
- \frac{d}{dx} \left( x \frac{du}{dx} \right) + u = \frac{\lambda}{x} u, \quad x \in (1,e) \quad (3.6.3)
\]

\[
u(1) = 0 = u(e) \quad (3.6.4)
\]

which was obtained from the first problem via the transformation \( x = e^t \). This was solved using the approximate transformation technique outlined in the previous section.

The method used was to firstly partition the \( x \)-interval, and then use Simpson's rule to approximate the transformation. This yields a partition of the \( t \)-interval and an approximation of the parameter \( T \) (which in this case was evaluated to an accuracy of \( 1.0 \times 10^{-6} \)). The final step was to approximate \( s \) by the use of centred finite difference approximations on the previously obtained partition of the \( t \)-interval. The method
Figure 3.2  Eigenvalue error for (3.6.1) - (3.6.2) using approximation of the differential equation together with the asymptotic expansion.
Figure 3.3 Eigenvalue error in using (3.3.3) to correct the eigenvalue estimates.
Figure 3.4  Eigenvalue error for (3.6.1) - (3.6.2) using Pruess' 0(h^4) method.
outlined previously for problems in normal form was then used to obtain the
eigenvalues of this approximating problem.

This procedure was carried out for two partitions of the x-interval. The first was a uniform partition. The errors obtained, given in figure 3.5, show that uniform approximations are in fact obtained for those values of k for which $\sqrt{\mu_k}h \leq \frac{\pi}{2}$.

The second partition used was that which yields a uniform partition of the transformed interval $[0,1]$. The results obtained for this partition did not differ significantly from those obtained for the exactly transformed problem.
Figure 3.5  Eigenvalue error for (3.6.3) - (3.6.4) using the approximate transformation.
CHAPTER 4
CORRECTION OF FINITE DIFFERENCE EIGENVALUE ESTIMATES

4.1 Introduction

When the coefficients are suitably smooth and \( \sigma_1 = \sigma_2 = \infty \), the study of the Sturm-Liouville eigenvalue problem (1.1.1) - (1.1.3) can be reduced to a study of the Liouville normal form

\[
\begin{align*}
- \ddot{z} + qz &= \lambda z \\
\dot{z}(0) &= 0 = z(\pi) \\
\end{align*}
\] (4.1.1)

We assume \( \int_0^\pi q \, dt = 0 \), since otherwise \( \int_0^\pi q \, dt \) \( z \) can be subtracted from both sides of (4.1.1) without changing its basic form. We also assume throughout this chapter that \( q \in C^2[0,\pi] \).

The ordered eigenvalues of (4.1.1) - (4.1.2) are denoted by \( \{\lambda_k\}_{k=1}^\infty \) and the corresponding eigenfunctions \( \{z_k\}_{k=1}^\infty \) are normalised so that \( z_k(0) = k \). When \( q(t) \equiv 0 \) we note that

\[
\lambda_k = k^2 ,
\]

and

\[
z_k(t) = \sin kt .
\]

On using the standard central difference formula to approximate \( \ddot{z} \) on the uniform partition \( \Delta_N \) of \([0,\pi]\), the differential eigenvalue problem (4.1.1) - (4.1.2) is approximated by the algebraic problem

\[
- A\ddot{u} + Qu = \tilde{\lambda}u 
\] (4.1.3)

where
\[ u^T = (u_1, u_2, \ldots, u_{N-1}) , \]
\[ Q = \text{diag} \{ q_1, q_2, \ldots, q_{N-1} \} \]

and
\[
A = \frac{1}{h^2} \begin{pmatrix}
    -2 & 1 & 0 \\
    1 & -2 & 1 \\
    & \ddots & \ddots & 1 \\
    0 & & 1 & -2 
\end{pmatrix}.
\]

We use \( \{ \tilde{\lambda}_k \}_{k=1}^{N-1} \) to denote the ordered eigenvalues of (4.1.3) and \( \{ u_k \}_{k=1}^{N-1} \) to denote the corresponding eigenvectors. When \( q(t) \equiv 0 \) the eigenvalue problem (4.1.3) reduces to
\[ -Au = \tilde{\mu}u , \]
which has the eigenvalues
\[ \tilde{\mu}_k = \frac{2}{h^2} (1 - \cos kh) , \quad k = 1, 2, \ldots, N-1 \]
and eigenvectors \( \tilde{\mu}_k^T = (s_{k,1}, \ldots, s_{k,N-1}) \) where
\[ s_{k,j} = \sin kt_j , \quad j = 1, 2, \ldots, N-1 . \]

It is easily verified when \( q(t) \equiv 0 \) that the eigenvalues \( \{ \tilde{\mu}_k \}_{k=1}^{N-1} \) satisfy
\[ \frac{h^2 k^4}{20} \leq |k^2 - \tilde{\mu}_k| \leq \frac{h^2 k^4}{12} , \quad k = 1, 2, \ldots, N-1 . \]

Also when \( q(t) \not\equiv 0 \), it follows from Keller (1968; Theorem 5.3.3) that
\[ |\lambda_k - \tilde{\lambda}_k| \leq Ch^2 k^4 , \quad 1 \leq k \leq \alpha N , \]
for some $\alpha < 1$ which is independent of $N$. Thus it is obvious that this method will only give reasonable estimates of a small number of eigenvalues.

The use of $h^2$-extrapolation helps in obtaining a larger number of reasonable estimates. However, since the error in the extrapolated values is $O(h^4k^6)$ when $q(t) \equiv 0$, it is clear that reasonable estimates will only be obtained when $k \ll N$.

In chapter 3 we used the asymptotic behaviour of the eigenvalues and eigenfunctions to correct the eigenvalue estimates. In this chapter we apply a similar strategy which enables us to reduce the growth in the eigenvalue error. In fact, we will show that the error $(k^2 - \tilde{\nu}_k)$ yields an accurate estimate of the asymptotic behaviour of $(\lambda_k - \tilde{\lambda}_k)$ and that the corrected eigenvalue estimates

$$\hat{\lambda}_k = \tilde{\lambda}_k + (k^2 - \tilde{\nu}_k), \quad k = 1, 2, \ldots, N-1,$$

satisfy

$$|\lambda_k - \hat{\lambda}_k| \leq Chk^2 \quad 1 \leq k \leq \alpha N$$

for some $\alpha < 1$ which is independent of $N$. The obvious motivation for this correction is that it gives the exact eigenvalues when $q(t) \equiv 0$.

4.2 Preliminaries

We initially derive some results on the asymptotic behaviour of $\lambda_k$ and $z_k$.

**Theorem 4.1** The eigenvalues $\{\lambda_k\}_{k=1}^{\infty}$ of (4.1.1) - (4.1.2) satisfy

$$|\lambda_k - k^2| \leq Ck^{-2}, \quad k = 1, 2, \ldots \quad (4.2.1)$$
Also the eigenfunctions \( \{z_k\}_{k=1}^{\infty} \) satisfy

\[
z_k(t) = \sin kt + e(t) , \quad k = 1, 2, \ldots \tag{4.2.2}
\]

where

\[
e(t) = \frac{1}{k}\nu(t) + \frac{1}{k^2}\omega(t) , \tag{4.2.3}
\]

and

\[
\nu(t) = \int_0^t q(x)\sin kx \sin k(t-x)dx \tag{4.2.4}
\]

\[
e(0) = e(\pi) = e^{(2)}(0) = e^{(2)}(\pi) = 0
\]

\[
e^{(l+1)}(t) = 0(k^l) , \quad \nu^{(l)}(t) = 0(k^l) , \quad \omega^{(l)}(t) = 0(k^l) , \quad l = 0, 1, 2, \ldots
\]

(the superscript "(l)" denotes l'th order differentiation with respect to t).

**Proof** From Fix (1967; Corollary 3)

\[
\lambda_k = k^2 + \frac{1}{\pi} \int_0^\pi q(x)dx + 0(k^{-2})
\]

and the first result follows immediately from the assumption that

\[
\int_0^\pi q(t)dt = 0 .
\]

It is well known (see Courant and Hilbert (1953; equation (10), p.285)) that a particular solution of

\[
\ddot{z} + \lambda z = f , \quad z(0) = \dot{z}(0) = 0
\]

is given by

\[
z(t) = \frac{1}{\sqrt{\lambda}} \int_0^t f(x)\sin \sqrt{\lambda}(t-x)dx .
\]
Applying this result to
\[ \ddot{z} + k^2 z = (k^2 - \lambda + q)z , \quad z(0) = \dot{z}(0) = 0 \]
yields
\[ z(t) = \sin kt + \frac{1}{k} \int_0^t (k^2 - \lambda + q) \sin k(t-x)z(x)dx \]
as the general solution of (4.1.1) with the initial conditions \( z(0) = 0 \), \( \dot{z}(0) = k \). Applying the Picard iteration method (i.e. the method of successive substitutions) to this equation with initial iterate \( \sin kt \) and using (4.2.1), we obtain the required (4.2.2) and (4.2.3).

We now turn to the construction of a discrete analogue of (4.2.2). To obtain an explicit characterization of the behaviour of \( \tilde{\lambda}_k \) and \( u_k \), we require the following two lemmas.

**Lemma 4.1**

\[ \exp(-i\beta \lambda) \sum_{r=0}^L \exp(2i\beta r) = \frac{\sin((\lambda+1)\beta)}{\sin \beta} , \quad \beta \neq 0, \pi, 2\pi, \ldots \]

**Proof**

\[ \sum_{r=0}^L \exp(2i\beta r) = \frac{\exp(2i(L+1)\beta)-1}{\exp(2i\beta)-1} \]
\[ = \exp(i\beta \lambda) \frac{\sin((\lambda+1)\beta)}{\sin \beta} \]
and the result follows on multiplying both sides by \( \exp(-i\beta \lambda) \).
**Lemma 4.2** For $\beta \neq p\pi$, $p = 0, 1, 2, \ldots$, a particular solution of the difference equations

$$u_{j+1} - 2\cos \beta u_j + u_{j-1} = f_j, \quad j = 1, 2, \ldots, N-1 \tag{4.2.5}$$

which satisfies $u_0 = u_1 = 0$ is given by

$$u_j = \left\{ \sum_{m=1}^{j} \sin \beta(j-m)f_m \right\} / \sin \beta$$

**Proof** Writing $a = \exp(i\beta)$ and $b = \exp(-i\beta)$ and setting

$$z_j = u_j - bu_{j-1} \tag{4.2.6}$$

(4.2.5) becomes

$$z_{j+1} - az_j = f_j, \quad j = 1, 2, \ldots, N-1$$

where $z_1 = 0$. As an immediate consequence it follows that

$$z_{j+1} = \sum_{m=1}^{j} a^{j-m} f_m, \quad j = 1, 2, \ldots, N-1$$

and, from (4.2.6),

$$u_{j+1} = \sum_{m=1}^{j} b^{j-m} \sum_{r=1}^{m} a^{m-r} f_r.$$

Interchanging the order of summation, this gives

$$u_{j+1} = \sum_{r=1}^{j} f_r \sum_{m=1}^{j} a^{m-r} b^{j-m}$$

$$= \sum_{r=1}^{j} f_r \sum_{m=0}^{j-r} a^m b^{j-r-m}$$

$$= \sum_{r=1}^{j} f_r \left\{ b^{j-r} \sum_{m=0}^{j-r} a^m b^{-m} \right\}.$$
Since $a = \exp(i\beta)$ and $b = \exp(-i\beta)$ it now follows from Lemma 4.1 that

$$u_{j+1} = \left\{ \sum_{r=1}^{j} f_r \sin(j+1-r)\beta \right\} / \sin \beta$$

$$= \left\{ \sum_{r=1}^{j+1} f_r \sin(j+1-r)\beta \right\} / \sin \beta .$$

We are now in a position to prove

**THEOREM 4.2** For $k \leq N-1$, \n
$$|\tilde{\chi}_k - \tilde{u}_k| \leq \|q\|_\infty$$ \n
(4.2.7) \n
and

$$u_{k,j} = \sin kx_j + \frac{h^2}{\sin kh} \sum_{m=1}^{j} (\tilde{\mu}_k - \tilde{\lambda}_k + q_m) \sin k(x_j - x_m) u_{k,m} .$$ \n
(4.2.8)

**Proof** The result (4.2.7) is an immediate consequence of the perturbation theory for the eigenvalues of symmetric matrices (see Wilkinson (1965; Chapter 2, p.101)).

To prove (4.2.8) we first observe that from (4.1.3)

$$u_{k,j+1} - 2u_{k,j} + u_{k,j-1} = h^2(-\tilde{\lambda}_k + q_j)u_{k,j}$$

and hence, on adding $h^2 \tilde{\mu}_k u_{k,j}$ to both sides of this equation,

$$u_{k,j+1} - 2 \cos kh u_{k,j} + u_{k,j-1} = h^2(\tilde{\mu}_k - \tilde{\lambda}_k + q_j)u_{k,j} .$$ \n
(4.2.9)

Since the boundary conditions (4.1.2) imply that $u_{k,0} = u_{k,N} = 0$, it follows that the homogeneous solution associated with the left hand side of (4.2.9) is $\sin kt$. Hence, on applying Lemma 4.2 to (4.2.9) we obtain (4.2.8) as the general solution.
COROLLARY 4.1  If \( kh \leq \alpha r, \alpha < 1, \) then

\[
u_k - \nu_k = s_k + \xi
\]

where

\[
\|\xi\|_\infty \leq C/k.
\]

Proof  From (4.2.7) and (4.2.8) we have

\[
|u_{k,j}| \leq 1 + \frac{h^2}{\sin kh} \sum_{m=1}^{j-1} 2\|q\|_\infty |u_{k,m}|
\]

\[
\leq 1 + 2\|q\|_\infty h \sum_{m=1}^{j-1} |u_{k,m}|.
\]

Since \(|u_{k,1}| \leq 1\) and \(|u_{k,2}| \leq (1+2\|q\|_\infty h)\), we have by induction

\[
|u_{k,j}| \leq (1+2\|q\|_\infty h)^{j-1}
\]

and hence

\[
|u_{k,j}| \leq \exp(2\|q\|_\infty x_{j-1}).
\]

Therefore since

\[
\frac{h}{\sin kh} \leq \frac{C(\alpha)}{k}
\]

and

\[
\xi_j = \frac{h^2}{\sin kh} \sum_{m=1}^{j} (\bar{u}_{k,m} - \tilde{\lambda}_k + q_m) \sin k(x_j - x_m) u_{k,m}
\]

we have
\[ |\varepsilon_j| \leq \frac{\hbar^2}{\sin k h} \sum_{m=1}^{j-1} 2\|q\|_\infty |u_{k,m}| \]
\[ \leq \frac{2\|q\|_\infty \hbar^2(j-1)}{\sin k h} \|u_k\|_\infty \]
\[ \leq C/k. \]

4.3 Error estimate for \( \tilde{\lambda}_k \)

Before giving the major result for this chapter it is necessary to examine in some detail the asymptotic behaviour of \( \tilde{\lambda}_k \). For each of the eigenfunctions \( z_k \) of (4.1.1) - (4.1.2) we define

\[ \tilde{z}_k^T = (z_{k,1}, z_{k,2}, \ldots, z_{k,N-1}), \]

and

\[ \tilde{\tilde{z}}_k^T = (\tilde{z}_{k,1}, \tilde{z}_{k,2}, \ldots, \tilde{z}_{k,N-1}), \]

where

\[ z_{k,j} = z_k(t_j), \quad \tilde{z}_{k,j} = \tilde{z}_k(t_j) \quad j = 1, 2, \ldots, N-1. \]

If we observe that

\[ u_{-k}^T \tilde{A} u_{-k} = u_{-k}^T \tilde{Q} - \tilde{\lambda}_k u_{-k}^T \]

and

\[ \tilde{z}_k = Qz_k - \tilde{\lambda}_k z_k \]

then we have

\[ \lambda_k - \tilde{\lambda}_k = \frac{(u_{-k}^T \tilde{A} z_k - u_{-k}^T \tilde{z}_k z_k) / u_{-k}^T \tilde{z}_k z_k}{u_{-k}^T z_k z_k}. \]

(4.3.1)

Also, since \( u_{-k} = s_{-k} + \varepsilon \) and \( z_{-k} = s_{-k} + \varepsilon \), it follows that

\[ u_{-k}^T \tilde{A} z_{-k} - u_{-k}^T \tilde{z}_{-k} = (k^2 - \tilde{\mu}_k) u_{-k}^T s_{-k} + \varepsilon^T (Ae - \varepsilon) + \varepsilon^T (\tilde{A}e - \tilde{\varepsilon}) \]

(4.3.2)

We now obtain estimates for the last two terms on the right hand side of this relation.
We consider the third term first:

**LEMMA 4.3**  
For $k \leq N-1$

$$\|Av-v-(k^2-\bar{\nu}_k)v\|_{\infty} \leq Ch^2k^3$$

where $v$ is as defined in Theorem 4.1.

**Proof**  
Let

$$\alpha(t,h) = \int_t^{t+h} q(x)\sin kx\sin k(t+h-x)\,dx$$

$$= h \int_0^1 q(t+hx)\sin k(t+hx)\sin kh(1-x)\,dx.$$ 

Clearly (using the notation $\alpha^{(p)}(t,h) = \frac{\partial^p \alpha}{\partial h^p}(t,h)$)

$$\alpha(t,0) = \alpha^{(1)}(t,0) = 0,$$

$$\alpha^{(2)}(t,0) = kq(t)\sin kt,$$

and

$$\alpha^{(p)}(t,h) = 0(k^{p-1}).$$

Therefore

$$(A\alpha)_j = (\alpha(t_j,h)-2\alpha(t_j,0)+\alpha(t_j,-h))/h^2$$

$$= \alpha^{(2)}(t_j,0) + \frac{h^2}{12} \alpha^{(4)}(t_j,h^*)$$

for some $h^* \in (-h,h)$, and hence

$$|(A\alpha)_j - kq_j s_k, j| \leq Ch^2k^3. \quad (4.3.3)$$
From (4.2.4) it follows that

\[ (A_{v})_{j} = \frac{1}{h^{2}} \int_{0}^{\tau_{j}} q(x) \sin k\{ \sin(k(t_{j+1} - x)) - 2 \sin(k(t_{j} - x)) + \sin(k(t_{j-1} - x)) \} dx + (A_{\tilde{\omega}})_{j}, \]

which, on noting that

\[
\sin(k(t_{j+1} - x)) - 2 \sin(k(t_{j} - x)) + \sin(k(t_{j-1} - x)) \\
= -2(1 - \cos kh) \sin(k(t_{j} - x)) \\
= -h^{2}\tilde{\mu}_{k} \sin(k(t_{j} - x))
\]
yields

\[ (A_{v})_{j} + \tilde{\mu}_{k} v_{j} - (A_{\tilde{\omega}})_{j} = 0. \]

Since \( \ddot{v}(t) = kq(t) \sin kt - k^{2}v(t) \), this equality together with (4.3.3) shows that

\[ |(A_{v})_{j} - \ddot{v}_{j} - (k^{2} - \tilde{\mu}_{k})v_{j}| \leq Ch^{2}k^{3}. \]

**Lemma 4.4** For \( k \leq N-1 \)

\[ \|A_{\tilde{\omega}} - (k^{2} - \tilde{\mu}_{k})e - \bar{e}\|_{\infty} \leq Ch^{2}k^{2}. \]

**Proof** From (4.2.3)

\[ A_{\tilde{\omega}} = \frac{1}{k^2}A_{\tilde{\omega}} + \frac{1}{k^2}A_{\omega}. \]

On interpreting \( (A_{\omega})_{j} \) as the central difference approximation of \( \tilde{w}_{j} \),

this gives the bound
\[(A\varepsilon)_{j} - \frac{1}{k}(A\varepsilon)_{j} - \frac{1}{k^{2}}w_{j} \] \[\leq Ch^{2}k^{2}\]

Therefore, by Lemma 4.3

\[\left|(A\varepsilon)_{j} - \frac{1}{k}v_{j} - \frac{1}{k}(k^{2} - \bar{\mu}_{k})v_{j} - \frac{1}{k^{2}}w_{j}\right| \leq Ch^{2}k^{2}\]

and hence

\[\left|(A\varepsilon)_{j} - \ddot{\varepsilon}_{j} - (k^{2} - \bar{\mu}_{k})e_{j}\right| \leq \left|\frac{1}{k^{2}}(k^{2} - \bar{\mu}_{k}w_{j}\right| + Ch^{2}k^{2}\]

\[\leq Ch^{2}k^{2}\] #

As a direct consequence of this lemma, we obtain the required estimate of the third term:

\[\text{COROLLARY 4.2} \quad \text{Let } \alpha < 1. \text{ Then for } k \leq \alpha N,\]

\[\|e\|_{\infty} \leq C/k. \quad (4.3.4)\]

\[\text{Proof} \quad \text{It is only necessary to recall that }\]

If we now observe that

\[s_{k}^{T}(A\varepsilon - \ddot{\varepsilon}) = (k^{2} - \bar{\mu}_{k})s_{k}^{T}e_{k} - s_{k}^{T}(\ddot{\varepsilon} + k^{2}e)\]

and

\[(\ddot{\varepsilon} + k^{2}e)_{j} = (k^{2} - \lambda_{k} + q_{j})z_{k},j\]

then we have

\[\text{LEMMA 4.5} \quad \text{For } k \leq N-1\]

\[\left|s_{k}^{T}(A\varepsilon - \ddot{\varepsilon}) - (k^{2} - \bar{\mu}_{k})s_{k}^{T}e_{k}\right| \leq C_{1}h + C_{2}\left|\cot kh - \frac{1}{kh}\right|. \quad (4.3.5)\]
Proof  Now

\[
\sum_{k} T_{-k}^{T} (\tilde{z} + k^2 \tilde{e}) = \sum_{m=1}^{N-1} (k^2 - \lambda_k + q_m) \sin k t z_{m+k,m} .
\]

(4.3.6)

Therefore, on noting that

\[
(-1)^{k+1} k e(\pi) = \int_{0}^{\pi} (k^2 - \lambda_k + q(t)) \sin k t z_{k}(t) dt
\]

\[= 0
\]

and defining (as in chapter 2)

\[
E_{J}(f) = \int_{t_j}^{t_{j+1}} f(t) dt - \frac{h}{2}(f(t_{j+1}) + f(t_j)) ,
\]

(4.3.6) yields

\[
|s_{N}^{T} \tilde{T} (\tilde{z} + k^2 \tilde{e})| = \left| \sum_{j=0}^{N-1} E_{J}((k^2 - \lambda_k + q(t)) \sin k t z_{k}(t)) \right|
\]

\[\leq |k^2 - \lambda_k| \sum_{j=0}^{N-1} \left| E_{J}(\sin k t z_{k}(t)) \right|
\]

\[\quad + \sum_{j=0}^{N-1} \left| E_{J}(q \sin k t e) \right| + \frac{1}{2} \sum_{j=0}^{N-1} \left| E_{J}(q) \right|
\]

\[\quad + \frac{1}{2} \sum_{j=0}^{N-1} \left| E_{J}(q \cos 2kt) \right|
\]

(4.3.7)

since \( z_{k}(t) = \sin kt + e(t) \) and \( \sin^2 kt = \frac{1}{2}(1 - \cos 2kt) \).

On noting that

\[
\left\| \frac{d^p}{dt^p}(q \tilde{e}) \right\|_{\infty} \leq C k^{p-1} \quad p = 0, 1, 2,
\]

and
we have, from (2.4.2),

\[ |ET_j(\sin kt z_k(t))| \leq Ch^3k^2, \]

\[ |ET_j(q \sin kt e)| \leq Ch^3k, \]

and

\[ |ET_j(q)| \leq Ch^3. \]

Also, from the proof of Lemma 2.3, it follows that

\[
| \sum_{j=0}^{N-1} ET_j(q \cos 2kt) | \leq C_1h^2k + \frac{h}{2} \left| \frac{\sin kh}{kh} - \cos kh \right| + \frac{h}{2} \left| \sum_{j=0}^{N-1} q_{j+\frac{1}{2}} \cos 2kt_j + \frac{1}{2} \right| \\
\leq C_1h^2k + C_2h|\cot kh - \frac{1}{kh}|. 
\]

The result then follows on substituting these bounds in (4.3.7).

We are now in a position to give the main result of this chapter.

**THEOREM 4.3** Let

\[
\hat{\lambda}_k = \tilde{\lambda}_k + k^2 - \tilde{\mu}_k \quad k = 1,2,\ldots,N-1 \quad (4.3.8)
\]

and assume that \( kh \leq \alpha \pi, \alpha < 1 \). Then there is a \( k_0 \), bounded independently of \( N \), such that

\[
|\lambda_k - \hat{\lambda}_k| \leq Ch^2k \quad k_0 \leq k < \alpha N .
\]

**Proof** When \( kh \leq \alpha \pi \),
\[ |\cot kh - \frac{1}{kh}| \leq Chh. \]

Therefore, from (4.3.2), (4.3.4) and (4.3.5)

\[ |u^T_k A z_k - u^T_k \tilde{z}_k - (k^2 - \tilde{\mu}_k) u^T_k \tilde{z}_k| \leq Ch. \]

In addition, it follows from Theorem 4.1 and Lemma 4.1 that

\[ \left| \frac{u^T_k z_k - N}{2} \right| \leq \frac{C_N}{k}. \]

Hence there is a \( k_0 \) such that

\[ u^T_k z_k \geq CN \quad k \geq k_0. \]

Combining these results with (4.3.1) then yields the desired result. #

The situation when \( k < k_0 \) does not pose any problem. From Keller (1968; Theorem 5.3.3) we have

\[ |\lambda_k - \lambda_k| \leq |\lambda_k - \lambda_k| + |\tilde{\mu}_k - k^2| \]

\[ \leq C_1h^2k_0^4 + C_2h^2k_0^4 \quad k < k_0 \]

\[ \leq Ch^2 \quad k < k_0. \]

This bound in conjunction with the above theorem guarantees that the corrected eigenvalues \( \{\lambda_k\}_{k=1}^{\alpha N} \) will at least yield uniform \( 0(h) \) approximations of the exact eigenvalues.
4.4 Numerical Examples

The errors in the standard and corrected eigenvalue estimates for the first ten eigenvalues of

\[
- \ddot{z} + e^t z = \lambda z
\]

\[z(0) = 0 = z(1)\]

obtained using the centred difference scheme (4.1.3) with \( N = 40 \), are given in Table 4.1. It is clear from these results that the corrected estimates are greatly superior to the original ones. In fact the estimates are so good that the structure of the error cannot be seen due to the effects of rounding error.

| TABLE 4.1 | Error in the standard and corrected finite difference eigenvalue estimates for (4.4.1) - (4.4.2) |
|---|---|---|
| \( k \) | \( \lambda_k \) | \( \hat{\lambda}_k - \lambda_k \) | \( \hat{\lambda}_k - \lambda_k \) |
| 1 | 11.5424 | .0057 | .0006 |
| 2 | 41.1867 | .0813 | .0002 |
| 3 | 90.5404 | .4106 | .0004 |
| 4 | 159.6296 | 1.2954 | .0007 |
| 5 | 248.4569 | 3.1544 | -.0002 |
| 6 | 357.0230 | 6.5261 | -.0006 |
| 7 | 485.3281 | 12.0593 | .0001 |
| 8 | 633.3724 | 20.5083 | -.0007 |
| 9 | 801.1558 | 32.7373 | .0002 |
| 10 | 988.6783 | 49.7023 | .0001 |

A clearer illustration of the behaviour of the eigenvalue error can be obtained if we instead consider the eigenvalue problem
\[-z' + e^t z = \lambda z\]  \hspace{1cm} (4.4.3)

\[z(0) = 0 = z(\pi).\] \hspace{1cm} (4.4.4)

The errors in the standard and corrected eigenvalue estimates using \(N = 40\) are given in Table 4.2. For the standard estimates, the error is obviously in close agreement with predicted \(k^4\) growth. Also the growth in the error for the corrected estimates, displayed in Figure 4.1, appears to be consistent with that predicted by Theorem 4.3.

<table>
<thead>
<tr>
<th>(k)</th>
<th>(\lambda_k)</th>
<th>(\tilde{\lambda}_k - \lambda_k)</th>
<th>(\tilde{\lambda}_k - \lambda_k) (k^4)</th>
<th>(\check{\lambda}_k - \lambda_k)</th>
<th>(\check{\lambda}_k - \lambda_k) (k)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4.89667</td>
<td>0.0029</td>
<td>0.0029</td>
<td>0.0024</td>
<td>0.0024</td>
</tr>
<tr>
<td>2</td>
<td>10.04519</td>
<td>0.0172</td>
<td>0.0011</td>
<td>0.0091</td>
<td>0.0045</td>
</tr>
<tr>
<td>3</td>
<td>16.01927</td>
<td>0.0546</td>
<td>0.0007</td>
<td>0.0131</td>
<td>0.0043</td>
</tr>
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<td>0.0006</td>
<td>0.0124</td>
<td>0.0031</td>
</tr>
<tr>
<td>5</td>
<td>32.26371</td>
<td>0.3308</td>
<td>0.0005</td>
<td>0.0113</td>
<td>0.0023</td>
</tr>
<tr>
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<td>0.0015</td>
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<td>0.0005</td>
<td>0.0110</td>
<td>0.0014</td>
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<td>0.0124</td>
<td>0.0011</td>
</tr>
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</tr>
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<td>13</td>
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<td>14.1947</td>
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<td>0.0140</td>
<td>0.0011</td>
</tr>
<tr>
<td>14</td>
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<td>0.0150</td>
<td>0.0011</td>
</tr>
<tr>
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<td>0.0011</td>
</tr>
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<td>0.0005</td>
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<td>0.0011</td>
</tr>
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<td>62.2331</td>
<td>0.0005</td>
<td>0.0224</td>
<td>0.0012</td>
</tr>
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<td>75.7968</td>
<td>0.0005</td>
<td>0.0245</td>
<td>0.0012</td>
</tr>
</tbody>
</table>
Figure 4.1  Error in the corrected finite difference eigenvalue estimates for (4.4.3) - (4.4.4)
To further investigate the behaviour of the error in the corrected eigenvalue estimates, the eigenvalue errors for the first twenty eigenvalues of (4.4.3) - (4.4.4) for a sequence of values of \( N \) are given in Table 4.3. If we consider the errors for a fixed value of \( k \) then it is clear that the predicted second order convergence is obtained as \( h \to 0 \). However if we consider the errors for a fixed value of \( N \) it can be seen that, although the error tends to increase with \( k \), the rate of growth is not as great as that predicted by Theorem 4.3. Another indication that the bound may not be the best possible is given in Table 4.4 which gives the error in the corrected eigenvalue estimates for the first twenty eigenvalues of the almost singular problem.

\[
- \ddot{z} + (t+0.1)^{-2} z = \lambda z \tag{4.4.5}
\]

\[
z(0) = 0 = z(\pi) \tag{4.4.6}
\]

Although these results indicate that the bound given in theorem 4.3 is not sharp, it is not clear how the preceding analysis could be improved.

4.5 Extensions

Although we will not generalize the convergence bound given in Theorem 4.3 it is worthwhile noting that the technique of correcting the eigenvalue estimates can also be extended to the more general eigenvalue problem

\[
- \ddot{z} + qz = \lambda z \tag{4.5.1}
\]

\[
\sigma_1 z(0) + \dot{z}(0) = 0 \tag{4.5.2}
\]

\[
\sigma_2 z(\pi) - \dot{z}(\pi) = 0 \tag{4.5.3}
\]
### TABLE 4.3
Eigenvalue errors for the corrected finite difference eigenvalue estimates for (4.4.3) - (4.4.4)

<table>
<thead>
<tr>
<th>k</th>
<th>$\lambda_k$</th>
<th>$\hat{\lambda}_k - \lambda_k$</th>
</tr>
</thead>
<tbody>
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<td></td>
<td>$N = 20$</td>
</tr>
<tr>
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<td>.0095</td>
</tr>
<tr>
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<td>$\hat{\lambda}_k - \lambda_k$</td>
</tr>
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<td>-------------</td>
<td>---------------------</td>
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<td>$N = 40$</td>
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<tr>
<td>20</td>
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On using the standard central difference formula to approximate $\ddot{z}$ on the uniform partition $\Delta_N$ of $[0,\pi]$ and the usual divided difference to approximate $\dot{z}$, the differential eigenvalue problem (4.5.2) - (4.5.3) is approximated by the algebraic problem

$$- A^* u + Qu = \tilde{\lambda} u$$

(4.5.4)

where $u$ and $Q$ are as in (4.1.3), and

$$A^* = \frac{1}{h^2} \begin{pmatrix}
-2 + \frac{1}{1-h\sigma_1} & 1 & 0 \\
1 & -2 & 1 & \\
& \ddots & \ddots & \ddots \\
0 & 1 & -2 & 1 \\
1 - 2 + \frac{1}{1-h\sigma_2} & & & & 
\end{pmatrix}$$

With the ordered eigenvalues of (4.5.4) denoted by $\{\tilde{\lambda}_k\}_{k=1}^N$, the corrected eigenvalue estimates are given by

$$\hat{\lambda}_k = \tilde{\lambda}_k + \mu_k - \bar{\mu}_k$$

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

where $\{\mu_k\}_{k=1}^\infty$ are the eigenvalues of (4.5.1) - (4.5.3) with $q(t) \equiv 0$ and $\{\bar{\mu}_k\}_{k=1}^{N-1}$ are the eigenvalues of (4.5.4) with $Q \equiv 0$.

If we apply this technique with $N = 40$ to the eigenvalue problem

$$- \ddot{u} + e^T u = \lambda u$$

(4.5.5)

$$u(0) = 0 = \dot{u}(\pi)$$

(4.5.6)
then the results given in Table 4.4 show that the errors in the corrected estimates are again generally superior to the original estimates. In fact the error in the corrected estimates appears to be uniformly bounded for the values of k given. This behaviour is also evident in the errors given in Figure 4.2 for N = 40, 80, 160. However these results also indicate that the derivative terms in the boundary conditions causes the second order convergence of the corrected eigenvalue estimates to be reduced to first order.

We also note that the eigenvalue estimates \( \{ \hat{\lambda}_k \}_{k=1}^{N-1} \) obtained by applying the standard finite difference method to (1.1.1) - (1.1.3) on the partition \( \Delta_N \) of \([a,b]\) can be corrected once the parameters \( T, \sigma_1^* \) and \( \sigma_2^* \) in the equivalent Liouville normal form (1.1.10) - (1.1.12) and the image \( \Delta_N \) of the partition \( \Delta_N \) under the transformation

\[
t = t(x) = \int_a^X \left( \frac{r}{p} \right)^{\frac{r}{p}} dx
\]

are known. The corrected eigenvalue estimates are given by

\[
\hat{\lambda}_k = \tilde{\lambda}_k + \mu_k - \check{\mu}_k \quad \quad k = 1, 2, \ldots, N-1
\]

where \( \{ \mu_k \}_{k=1}^{\infty} \) are the ordered eigenvalues of the eigenvalue problem

\[
- \ddot{z} = \mu z \quad \quad (4.5.7)
\]

\[
\sigma_1^* z(0) + \dot{z}(0) = 0 \quad \quad (4.5.8)
\]

\[
\sigma_2^* z(T) - \dot{z}(T) = 0 \quad \quad (4.5.9)
\]

and \( \{ \check{\mu}_k \}_{k=1}^{N-1} \) are the eigenvalues of the finite difference approximation to (4.5.7) - (4.5.9) on the partition \( \pi_N \) of \([0,T]\).
<table>
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TABLE 4.4  Error in standard and corrected eigenvalue estimates for (4.5.5) - (4.5.6)
Figure 4.2  Error in the corrected finite difference estimates for (4.5.5) - (4.5.6):

- $\times$ - $N = 40$
- $\diamond$ - $N = 80$
- $\uparrow$ - $N = 160$. 

124
As a final point we note that the eigenvalue estimates generated by a finite element method could also be improved if they are corrected in the same manner as above. All that is required is the exact eigenvalue \( \{ \lambda_k \}_{k=1}^{\infty} \) of (4.5.7) - (4.5.9) and the estimates \( \{ \tilde{\lambda}_k \}_{k=1}^{N-1} \) of these eigenvalues generated by applying the numerical method to this reduced problem. For example if we use the standard linear elements on a uniform partition of \([0,\pi]\) to approximate the eigenvalues of (4.1.1) - (4.1.2), then we have
\[
\mu_k = k^2 \quad \text{and} \quad \tilde{\mu}_k = \frac{6(1-\cos kh)}{2(2+\cos kh)} , \quad k = 1,2,\ldots,N-1 .
\]
The eigenvalue estimates \( \{ \tilde{\lambda}_k \}_{k=1}^{N-1} \) can then be corrected as before.
APPENDIX 1

Let \( \Delta_N = \{ x_i \}_{i=0}^{N} \) be the uniform partition of \([a,b]\), and denote

\[
f_{\frac{j}{2} + \frac{1}{2}} = f(x_{\frac{j}{2} + \frac{1}{2}}) = f\left(\frac{1}{2}(x_{\frac{j}{2} + \frac{1}{2}} + x_{\frac{j}{2} + 1})\right) \quad i = 0,1,\ldots,N-1
\]

for any function \( f \) defined on \([a,b]\). Then we have

**LEMMA A1.1** Let \( \phi(x,\lambda) = \phi_0 + \sqrt{\lambda}(x-a) \) and \( g \in C^1\{a,b\} \). Then for \( j = 1,2,\ldots,N \),

\[
\left| \sum_{k=0}^{j-1} g_{\frac{k}{2} + 1} \sin 2\phi_{\frac{k}{2} + 1/2} \right| \leq \left\{ \begin{array}{ll}
\left( \left\| g \right\|_\infty + (b-a) \left\| g \right\|_\infty \right) \max_{1 \leq p \leq j} \left| \frac{\sin p\sqrt{\lambda}h}{\sin \sqrt{\lambda}h} \right|, & \sin \sqrt{\lambda}h \neq 0 \\
\left( \left\| g \right\|_\infty + (b-a) \left\| g \right\|_\infty \right) j, & \sin \sqrt{\lambda}h = 0.
\end{array} \right.
\]

**Proof** On summing by parts

\[
\sum_{k=0}^{j-1} g_{\frac{k}{2} + 1} \sin 2\phi_{\frac{k}{2} + 1/2} = g_{\frac{j}{2}} \sin 2\phi_{\frac{j}{2} + 1/2} - \sum_{k=1}^{j-1} \left( g_{\frac{k}{2} + 1/2} - g_{\frac{k}{2}} \right) \sum_{k=0}^{\frac{j-1}{2}} \sin 2\phi_{\frac{k}{2} + 1/2}.
\]

Now, if \( \sin \sqrt{\lambda}h \neq 0 \),

\[
\sum_{k=0}^{\frac{j-1}{2}} \sin 2\phi_{\frac{k}{2} + 1/2} = \sum_{k=0}^{\frac{j-1}{2}} \sin 2(\phi_0 + \sqrt{\lambda}(x_{\frac{k}{2} + 1/2} - a))
\]

\[
= \text{Im} \left\{ \sum_{k=0}^{\frac{j-1}{2}} e^{i(2\phi_0 + \sqrt{\lambda}(k+\frac{1}{2})h))} \right\}
\]

\[
= \text{Im} \left\{ e^{i(2\phi_0 + \sqrt{\lambda}h)} \sum_{k=0}^{\frac{j-1}{2}} (e^{i\sqrt{\lambda}h})^k \right\}
\]

\[
= \text{Im} \left\{ e^{i(2\phi_0 + \sqrt{\lambda}h)} \frac{\sin \frac{j}{2}\sqrt{\lambda}h}{\sin \sqrt{\lambda}h} \right\}
\]

\[
= \sin (2\phi_0 + \sqrt{\lambda}h) \frac{\sin \frac{j}{2}\sqrt{\lambda}h}{\sin \sqrt{\lambda}h}.
\]
Also

\[ |g_{\ell+\frac{1}{2}} - g_{\ell-\frac{1}{2}}| \leq h\|g\|_\infty. \]

Therefore

\[ \left| \sum_{\ell=0}^{j-1} g_{\ell+\frac{1}{2}} \sin 2\phi_{k+\frac{1}{2}} \right| \leq \|g\|_\infty \left| \frac{\sin j\sqrt{\lambda} h}{\sin \sqrt{\lambda} h} \right| + (b-a) \|g\|_\infty \max_{1 \leq p \leq j-1} \left| \frac{\sin p\sqrt{\lambda} h}{\sin \sqrt{\lambda} h} \right| \]

\[ \leq (\|g\|_\infty + (b-a)\|g\|_\infty) \max_{1 \leq p \leq j} \left| \frac{\sin p\sqrt{\lambda} h}{\sin \sqrt{\lambda} h} \right|. \]

On the other hand, if \( \sin \sqrt{\lambda} h = 0 \),

\[ \left| \sum_{k=0}^{\ell-1} \sin 2\phi_{k+\frac{1}{2}} \right| = \left| \sum_{k=0}^{\ell-1} \sin (2\phi_0 + \sqrt{\lambda} h) \cos 2k\sqrt{\lambda} h \right| \]

\[ = \ell |\sin (2\phi_0 + \sqrt{\lambda} h)|. \]

Hence

\[ \left| \sum_{\ell=0}^{j-1} g_{\ell+\frac{1}{2}} \sin 2\phi_{k+\frac{1}{2}} \right| \leq j\|g\|_\infty + \sum_{\ell=0}^{j-1} h\|g\|_\ell \]

\[ \leq j(\|g\|_\infty + (b-a)\|g\|_\infty). \]

For the next lemma we restrict attention to the scaled phase associated with an eigenvalue problem in Liouville normal form (1.1.10) - (1.1.12).

**Lemma A1.2** Let \( \phi(x, \lambda) = \theta(a, \lambda) + \sqrt{\lambda}(x-a) \) and \( q \in C^3[a, b] \). Also let \( \mu \) be an eigenvalue of (1.1.10) - (1.1.12) and \( \hat{\gamma} \) and \( \hat{\eta} \) be as defined in Lemma 2.2. If in addition \( \lambda \) satisfies \( |\lambda - \mu| \leq \frac{1}{2} \hat{\gamma} \hat{\eta} \) and \( \lambda > \frac{1}{4} \hat{\gamma} \hat{\eta} \), then
\[(i) \quad |\sin 2\phi_0| \leq C/\sqrt{\lambda}, \]

\[(ii) \quad |\sin 2\phi_n| \leq C/\sqrt{\lambda}, \]

and

\[(iii) \quad \left| \sum_{k=0}^{N-1} q_{\ell}^k \cos 2\phi_{\ell}^k \right| \leq \frac{C_1 (||q||_{\infty} + ||q||_{\infty})}{\lambda \sin \sqrt{\lambda h}} + \frac{C_2}{\sin \sqrt{\lambda h}} + \frac{h (||q||_{\infty} + (b-a) ||q||_{\infty})}{\sin^2 \sqrt{\lambda h}}. \]

**Proof**

(i) From (1.1.2) and the definition of the scaled phase

\[|\sin 2\phi_0| = |\sin 2\theta(a,\lambda)|\]

\[= 2 \left| \frac{\tan \theta(a,\lambda)}{\sec^2 (a,\lambda)} \right| \]

\[= 2 \left| \frac{-\sigma_{1} \sqrt{\lambda}}{\lambda + \sigma_{1}^2} \right| \]

\[\leq C/\sqrt{\lambda}. \]

(ii) Since \(|\lambda - \mu| \leq \frac{1}{2} \sqrt{\gamma} \) and \(\lambda \geq \frac{1}{4} \sqrt{\gamma} \), it follows that

\[|\sqrt{\lambda} - \sqrt{\mu}| \leq 2 \sqrt{\lambda - \mu} \]

\[\leq \sqrt{\gamma} \sqrt{\lambda} \]

\[\leq C/\sqrt{\lambda}. \]

Also from (2.4.6)

\[|\phi(b,\lambda) - \theta(b,\lambda)| \leq C/\sqrt{\lambda}. \]

Therefore
\[ |\sin 2\phi_n| = |\sin 2(\theta(a,\lambda)+(b-a)\sqrt{\mu})| \]
\[ \leq |\sin 2(\theta(a,\mu)+(b-a)\sqrt{\mu})| \]
\[ + |\sin 2(\theta(a,\lambda)-(b-a)\sqrt{\mu})-\sin 2(\theta(a,\mu)+(b-a)\sqrt{\mu})| \]
\[ \leq |\sin \theta(b,\mu)| + |\sin 2\phi(b,\mu)-\sin \theta(b,\mu)| \]
\[ + 2 \left| \theta(a,\lambda)-\theta(a,\mu) \right| + 2(b-a)|\sqrt{\lambda}-\sqrt{\mu}| \]
\[ \leq \frac{2}{\mu + \sigma^2} \frac{C_1}{\sqrt{\mu}} + \frac{C_2}{\sqrt{\lambda}} \]
\[ \leq C/\sqrt{\lambda} . \]

(iii) Before deriving the remaining bound we note that

\[ \sum_{k=0}^{j-1} \cos 2\phi_{k+\frac{1}{2}} = \sum_{k=0}^{j-1} \cos(2\phi_0+(2k+1)\lambda h) \]
\[ = \cos(2\phi_0+j\lambda h) \sin j\sqrt{\lambda h} / \sin \sqrt{\lambda h} \]
\[ = \frac{(\sin 2\phi_j-\sin 2\phi_0)}{2 \sin \sqrt{\lambda h}} , \]
\[ \sum_{k=1}^{j-1} \sin 2\phi_k = \sum_{k=1}^{j-1} \sin(2\phi_0+2k\sqrt{\lambda h}) \]
\[ = \sin(2\phi_0+j\sqrt{\lambda h}) \frac{\sin(j-1)\sqrt{\lambda h}}{\sin \sqrt{\lambda h} , \]

and

\[ |q_{\ell+\frac{1}{2}}-q_{\ell-\frac{1}{2}}-hq_{\ell}'| \leq C \|q\|_\infty . \]
On summing by parts,
\[
\sum_{\ell=0}^{N-1} q_{\ell+\frac{1}{2}} \cos 2\phi_{\ell+\frac{1}{2}} = q_{N-\frac{1}{2}} \sum_{k=0}^{N-1} \cos 2\phi_{k+\frac{1}{2}}
\]
\[
- \sum_{\ell=1}^{N-1} (q_{\ell+\frac{1}{2}} - q_{N-\frac{1}{2}}) \sum_{k=0}^{\ell-1} \cos 2\phi_{k+\frac{1}{2}}
\]
and
\[
\sum_{\ell=1}^{N-1} q_{\ell} \sin 2\phi_{\ell} = q_{N-1} \sum_{k=1}^{N-1} \sin 2\phi_{k}
\]
\[
- \sum_{\ell=2}^{N-1} (q_{\ell} - q_{\ell-1}) \sum_{k=1}^{\ell-1} \sin 2\phi_{k}
\]

Therefore
\[
\left| \sum_{\ell=0}^{N-1} q_{\ell+\frac{1}{2}} \cos 2\phi_{\ell+\frac{1}{2}} \right| \leq |q_{N-\frac{1}{2}}| \frac{|\sin 2\phi_{N} - \sin 2\phi_{0}|}{2 \sin \sqrt{\lambda} h}
\]
\[
+ \sum_{\ell=1}^{N-1} \left| q_{\ell+\frac{1}{2}} - q_{N-\frac{1}{2}} \right| \frac{|\sin 2\phi_{\ell} - \sin 2\phi_{0}|}{2 \sin \sqrt{\lambda} h}
\]
\[
+ \sum_{\ell=1}^{N-1} h |q_{\ell}| \frac{|\sin 2\phi_{0}|}{2 \sin \sqrt{\lambda} h} + \sum_{\ell=1}^{N-1} \frac{|h q_{\ell}'|}{2 \sin 2\sqrt{\lambda} h}
\]
\[
\leq \frac{C_{1} \|q\|_{\infty}}{\sqrt{\lambda} \sin \sqrt{\lambda} h} + \frac{C_{2} \|q''\|_{\infty}}{\sin \sqrt{\lambda} h} + \frac{C_{3} \|q''\|_{\infty}}{\sqrt{\lambda} \sin \sqrt{\lambda} h}
\]
\[
+ \frac{h}{2 \sin \sqrt{\lambda} h} \left\{ \frac{|q_{N-1}'}{\sin \sqrt{\lambda} h} + \sum_{\ell=1}^{N-1} \frac{|q_{\ell}' - q_{\ell-1}'|}{\sin \sqrt{\lambda} h} \right\}
\]
In the next lemma we derive an analogue of Lemma A1.1 for the general eigenvalue problem (1.1.1) - (1.1.3). For $x \in [a, b]$ define $t \in [0, T]$ by

$$t = t(x) = \int_a^x \left( \frac{x}{p} \right)^{1/2} dx; \quad T = \int_a^b \left( \frac{x}{p} \right)^{1/2} dx.$$  

The image of the uniform partition $\Lambda_N = \{x_i\}_{i=0}^N$ of $[a, b]$ under this transformation is the partition $\Pi_N = \{t_i, i = 0, 1, \ldots, N \mid t_{i+1} - t_i = \delta_i > 0, \ t_0 = 0, \ t_N = T\}$, where

$$\delta_i = \int_{x_i}^{x_{i+1}} \left( \frac{x}{p} \right)^{1/2} dx.$$  

Where necessary, we set

$$t_{i+\frac{1}{2}} = (t_i + t_{i+1})/2.$$  

When $(\frac{x}{p}) \in C^2[a, b]$ it is readily verified that

$$mh \leq \delta_i \leq Mh \quad i = 0, 1, \ldots, N-1$$  

and

$$|\delta_{i+1} - \delta_i| \leq Ch^2 \quad i = 0, 1, \ldots, N-1$$
where

\[ m = \min_{x \in [a,b]} \left( \frac{p}{p} \right)^{\frac{1}{2}} , \]

\[ M = \max_{x \in [a,b]} \left( \frac{p}{p} \right)^{\frac{1}{2}} , \]

and

\[ C = 2 \left\| \frac{d}{dx} \left( \frac{p}{p} \right)^{\frac{1}{2}} \right\|_{\infty} . \]

If we define

\[ \psi(\tau) = \sin \tau - \tau \cos \tau , \]

then we have

**Lemma A1.3** \( \text{Let } \phi(t,\lambda) = \phi_0(\lambda) + \sqrt{\lambda} t , \quad g \in C^1[0,T] \text{ and } (\frac{p}{p}) \in C^2[a,b] . \)

Then for \( j = 1,2,\ldots,N-1 \),

\[ \left| \sum_{i=0}^{j} \psi(\sqrt{\lambda} \delta_i) g_{i+\frac{1}{2}} \sin 2\phi_{i+\frac{1}{2}} \right| \leq Ch^2\lambda(\|g\|_{\infty} + \|\dot{g}\|_{\infty}) , \quad \sqrt{\lambda} h \leq \frac{\pi}{2\left\| \frac{p}{p} \right\|_{\infty}} . \]

**Proof** On summing by parts

\[ \sum_{i=0}^{j} \psi(\sqrt{\lambda} \delta_i) g_{i+\frac{1}{2}} \sin 2\phi_{i+\frac{1}{2}} = \psi(\sqrt{\lambda} \delta_j) g_{j+\frac{1}{2}} \sum_{i=0}^{j} \sin 2\phi_{i+\frac{1}{2}} \]

\[ - \sum_{i=1}^{j-1} (\psi(\sqrt{\lambda} \delta_i) g_{i+\frac{1}{2}} - \psi(\sqrt{\lambda} \delta_{i-1}) g_{i-\frac{1}{2}}) \sum_{k=0}^{i-1} \sin 2\phi_k+\frac{1}{2} . \]

In addition
\[
\sum_{k=0}^{i-1} \sin 2\phi_{k+\frac{1}{2}} = \sum_{k=0}^{i-1} \sin 2(\phi_0 + \sqrt{\lambda} t_{k+\frac{1}{2}})
\]

\[
= - \sum_{k=0}^{i-1} \left( \frac{\cos 2\phi_{k+1} - \cos 2\phi_k}{2 \sin \sqrt{\lambda} \delta_k} \right)
\]

\[
= - \frac{\cos 2\phi_i - \cos 2\phi_0}{2 \sin \sqrt{\lambda} \delta_{i-1}} + \frac{\cos 2\phi_0}{2 \sin \sqrt{\lambda} \delta_0}
\]

\[
+ \sum_{k=1}^{i-1} \cos 2\phi_k \left( \frac{1}{\sin \sqrt{\lambda} \delta_k} - \frac{1}{\sin \sqrt{\lambda} \delta_{k+1}} \right).
\]

But

\[
\left| \frac{1}{\sin \sqrt{\lambda} \delta_k} - \frac{1}{\sin \sqrt{\lambda} \delta_{k-1}} \right| = \left| \frac{\cos \frac{\sqrt{\lambda}}{2} (\delta_k + \delta_{k-1}) \sin \frac{\sqrt{\lambda}}{2} (\delta_k - \delta_{k-1})}{\sin \sqrt{\lambda} \delta_k \sin \sqrt{\lambda} \delta_{k-1}} \right|
\]

\[
\leq \frac{\sqrt{\lambda} |\delta_k - \delta_{k-1}|}{2 \sin^2 m/\sqrt{\lambda} h}
\]

\[
\leq \frac{\sqrt{\lambda} Ch^2}{2 \sin m/\sqrt{\lambda} h} \frac{2 m/\sqrt{\lambda} h}{\pi}
\]

\[
\leq C_1 h / \sin m/\sqrt{\lambda} h.
\]

Hence

\[
\left| \sum_{k=0}^{i-1} \sin 2\phi_{k+\frac{1}{2}} \right| \leq \frac{1}{\sin m/\sqrt{\lambda} h} + \frac{C_1}{\sin m/\sqrt{\lambda} h} \sum_{k=0}^{i-1} h
\]

\[
\leq \frac{1 + C_1 (b-a)}{\sin m/\sqrt{\lambda} h}
\]

\[
= \frac{C_2}{\sin m/\sqrt{\lambda} h}.
\]
Since \( \psi'(\tau) = \tau \sin \tau \) is a monotonically increasing function of \( \tau \) on \([0, \pi/2]\), we obtain
\[
|\psi(\sqrt{\lambda} \delta_i) - \psi(\sqrt{\lambda} \delta_{i-1})| = |\sqrt{\lambda} (\delta_i - \delta_{i-1}) \psi'(\xi)|, \quad \xi_i \in [m\lambda h, M\lambda h]
\]
\[
\leq C h^2 \sqrt{\lambda} M\lambda h \sin M\lambda h.
\]
Similarly
\[
|\psi(\sqrt{\lambda} \delta_i)| = |\sqrt{\lambda} \delta_i \psi'(\xi_i)|, \quad \xi_i \in [m\lambda h, M\lambda h]
\]
\[
\leq M^2 h^2 \sqrt{\lambda} \sin M\lambda h.
\]
Hence
\[
|\psi(\sqrt{\lambda} \delta_i) g_{1+\epsilon} - \psi(\sqrt{\lambda} \delta_{i-1}) g_{1-\epsilon}|
\]
\[
\leq |g_{1+\epsilon} - g_{1-\epsilon}| |\psi(\sqrt{\lambda} \delta_i)| + |g_{1-1} - g_{1-1-\epsilon}| |\psi(\sqrt{\lambda} \delta_{i-1}) - \psi(\sqrt{\lambda} \delta_{i-1})|
\]
\[
\leq \frac{1}{2} (\delta_{i-1} + \delta_i) \|g\| M^2 h^2 \sqrt{\lambda} \sin M\lambda h + \|g\| C M h^3 \sqrt{\lambda} \sin M\lambda h
\]
\[
\leq C_3 h^3 \sqrt{\lambda} \sin M\lambda h (\|g\|_\infty + \|\tilde{g}\|_\infty).
\]
Therefore
\[
\left| \sum_{i=0}^{j} \psi(\sqrt{\lambda} \delta^i) g_{1+\frac{i}{2}} \sin 2\psi_{1+\frac{i}{2}} \right| \leq C_2 M^2 h^2 \lambda \frac{\sin M\sqrt{\lambda} h}{\sin m\sqrt{\lambda} h} ||g||_\infty \\
\quad + \sum_{i=1}^{j} C_2 C_3 h^3 \lambda \frac{\sin M\sqrt{\lambda} h}{\sin m\sqrt{\lambda} h} (||g||_\infty + ||\dot{g}||_\infty) \\
\leq C_4 (||g||_\infty + ||\dot{g}||_\infty) h^2 \lambda \frac{\sin M\sqrt{\lambda} h}{\sin m\sqrt{\lambda} h} \\
\leq C_4 (||g||_\infty + ||\dot{g}||_\infty) h^2 \lambda \frac{\pi}{\frac{2}{2} M\sqrt{\lambda} h} \frac{2}{m\sqrt{\lambda} h} \\
\leq C_5 (||g||_\infty + ||\dot{g}||_\infty) h^2 \lambda .
\]
APPENDIX 2

LEMMA A2.1  When \( \tau \in (0, \frac{\pi}{2}] \),

(i) \[
\left| \frac{\sin \tau}{\tau^2} - \frac{\cos \tau}{\tau} \right| \leq \sin \tau
\]

(ii) \[
\left| \frac{\sin \tau}{\tau^2} - \frac{\cos \tau}{\tau} - \frac{\sin \tau}{3} \right| \leq \frac{1}{3\tau^2} \sin \tau
\]

(iii) \[
\left| \frac{-\cos \tau}{3} + \frac{\sin \tau}{\tau} + \frac{2\cos \tau}{\tau^2} - \frac{2\sin \tau}{3} \right| \leq \frac{1}{3\tau} \sin \tau
\]

(iv) \[
\left| \frac{\sin \tau}{\tau} - \frac{\cos \tau}{3} - \frac{2}{3} \right| \leq \frac{1}{6\tau^3} \sin \tau
\]

Proof

(i) Let \( \psi(\tau) = \sin \tau - \tau \cos \tau \), then

\[
\psi'(\tau) = \tau \sin \tau.
\]

Expanding \( \psi \) about \( \tau = 0 \), we have

\[
\psi(\tau) = \psi(0) + \tau \psi'(\xi) \quad \xi \in (0, \tau).
\]

Now \( \psi'(\tau) \) is a monotonically increasing function for \( \tau \in [0, \frac{\pi}{2}] \), so for \( \tau \in [0, \frac{\pi}{2}] \)

\[
|\psi(\tau)| \leq \tau |\psi'(\xi)|
\]

\[
\leq \tau |\psi'(\tau)|
\]

\[
= \tau^2 \sin \tau.
\]

Therefore
\[
\left| \frac{\sin \tau}{\tau^2} - \frac{\cos \tau}{\tau} \right| = \frac{1}{\tau^2} |\psi(\tau)| \\
\leq \sin \tau .
\]

(ii) Let
\[\psi(\tau) = \sin \tau - \tau \cos \tau - \frac{1}{3} \tau^2 \sin \tau .\]

Then
\[\psi'(\tau) = -\frac{1}{3} \tau^2 \cos \tau + \frac{1}{3} \tau \sin \tau ,\]

and
\[\psi''(\tau) = \frac{1}{3} \tau^2 \sin \tau + \frac{1}{3} (\sin \tau - \tau \cos \tau) .\]

Now
\[\psi(\tau) = \psi(0) + \tau \psi'(0) + \frac{1}{2} \tau^2 \psi''(\xi) \quad \xi \in (0, \tau) = \frac{1}{2} \tau^2 \psi''(\xi) .\]

But, from (i),
\[|\psi(\tau)| \leq \frac{1}{2} \tau^2 |\psi''(\xi)| \leq \frac{1}{2} \tau^2 \left( \frac{1}{3} |\xi^2 \sin \xi| + \frac{1}{3} |\sin \xi - \xi \cos \xi| \right) \leq \frac{1}{2} \tau^2 \left( \frac{1}{3} \tau^2 \sin \tau + \frac{1}{3} \tau^2 \sin \tau \right) = \frac{1}{3} \tau^4 \sin \tau ,\]

and the stated bound follows as before.
(iii) Let \( \psi(\tau) = -\frac{1}{3}\tau^3 \cos \tau + \tau^2 \sin \tau + 2\tau \cos \tau - 2 \sin \tau \),
then
\[
\psi'(\tau) = \frac{1}{3}\tau^3 \sin \tau ,
\]
and hence
\[
|\psi(\tau)| \leq |\psi(0)| + \tau |\psi'(\xi)| \quad \xi \in (0, \tau)
\leq \frac{1}{3}\tau^3 \sin \tau .
\]
The bound then follows as for (i).

(iv) Let \( \psi(\tau) = -\frac{1}{3}\tau \cos \tau - \frac{2}{3} + \sin \tau \),
then
\[
\psi'(\tau) = \frac{2}{3} \cos \tau - \frac{2}{3} + \frac{1}{3} \tau \sin \tau ,
\]
and
\[
\psi''(\tau) = \frac{1}{3}(\tau \cos \tau - \sin \tau) .
\]
Hence, by (i),
\[
|\psi(\tau)| \leq |\psi(0)| + \tau |\psi'(0)| + \frac{1}{2}\tau^2 |\psi''(\xi)| \quad \xi \in (0, \tau)
= \frac{1}{2}\tau^2 . \frac{1}{3}|\xi \cos \xi - \sin \xi|
\leq \frac{1}{6}\tau^2 \xi^2 \sin \xi
\leq \frac{1}{6}\tau^4 \sin \tau .
\]
The stated bound then follows as before.
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