Eigenvalue Finite Difference Approximations for Regular and Singular Sturm-Liouville Problems

By Nabil R. Nassif

Abstract. This paper includes two parts. In the first part, general error estimates for "stable" eigenvalue approximations are obtained. These are practical in the sense that they are based on the discretization error of the difference formula over the eigenspace associated with the isolated eigenvalue under consideration. Verification of these general estimates are carried out on two difference schemes: that of Numerov to solve the Schrödinger singular equation and that of the central difference formula for regular Sturm-Liouville problems. In the second part, a sufficient condition for obtaining a "stable" difference scheme is derived. Such a condition (condition (N) of Theorem 2.1) leads to a simple "by hand" verification, when one selects a difference scheme to compute eigenvalues of a differential operator. This condition is checked for one- and two-dimensional problems.

Introduction. In this work, we are concerned with eigenvalue-eigenvector approximation by finite difference methods for differential operators defined on functions with bounded or unbounded domains. Our results will be illustrated in particular for the Schrödinger radial operator whose "energy levels" are obtained numerically using difference schemes. Let

$$(1.1) \qquad L[y] = -y'' + q(x)y, \qquad 0 < x < \infty,$$

and consider the boundary conditions

$$(1.2) \qquad B[y] = cy'(0) + dy(0) = 0$$

and

$$(1.3) \qquad y(x) \quad \text{bounded on} \quad (0, \infty).$$

Let $x_i = ih$, $0 \leqslant i \leqslant N$, $x_0 = 0$, $X = x_N = Nh$, with $\lim_{h \to 0} X = \lim_{h \to 0} N = \infty$.

Optimal error estimates for difference methods will depend on how $X(h)$ and $N(h)$ tend to ∞. For example (see Corollary 2.1), possible choices for $X(h)$ and $N(h)$ are, respectively, m^2 and $2^m m^2$, with $h = 1/2^m$.

The Numerov [8] difference scheme consists in finding $Y = \{Y_i\}_{0 \leqslant i \leqslant N}$, $\lambda_h \in R$, such that

$$(1.4) \qquad \begin{aligned} (-Y_{i-1} + 2Y_i - Y_{i+1})/h^2 + (q_{i-1}Y_{i-1} + 10q_iY_i + q_{i+1}Y_{i+1})/12 \\ = \lambda_h(Y_{i-1} + 10Y_i + Y_{i+1})/12, \end{aligned}$$

$$(1.5) \qquad B_h[Y] = 0,$$

and

(1.6) $Y_N = 0.$

B_h is the difference approximation to B. The choice of B_h should be such that its discretization error with respect to B has the same order as that of L_h with respect to L. When $c = 0$, $d = 1$, the choice of B_h is obvious. When $c \neq 0$, and in the case of Numerov's scheme, one must extend the eigenfunction $y(x)$ on $(-2h, 0)$, and use a difference approximation to $y'(0)$ over the points $-2h$, $-h$, 0, h, and $2h$. It can be verified that, Y_N, Y_0, and Y_k, $k < 0$, can be eliminated, and the system (1.4)–(1.6) is written in the form

(1.7) $-(L_h[Y])_i = \lambda_h[Y_i], \qquad 1 \leqslant i \leqslant N - 1,$

where $L_h: R^{N-1} \to R^{N-1}$.

It is the goal of this paper to present abstract results for the analysis of finite difference methods for eigenvalue problems. The results are sufficiently general, relatively simple, and easily applicable to specific difference methods, such as (1.7). We present stability and convergence estimates involving the "discretization error" of the difference formula over the eigenspace associated with the eigenvalue under consideration. Our results are similar to those obtained by Vainikko [13] for differential operators on bounded domains. The argument used is an adaptation of one introduced by Vainikko and used repeatedly by Osborn [10] for compact operators and by Descloux, Nassif and Rappaz [4] for Galerkin approximations to noncompact operators. It essentially reduces the analysis to that of an algebraic eigenvalue problem. Furthermore, our estimates are general in the sense that they can be applied to operators with functions of several variables. We should mention here results available in the literature. Our results should be compared to the approach of Stummel [12] which is based on the development of a very general framework for the analysis of a variety of approximation processes. It has been our aim to tailor our results to the analysis of difference methods. The results of Kreiss [7] are intimately related to the regularity of the solution, while Grigorieff's results [6] are concerned with compact operators.

The theorems of Part 1 depend directly on "stability conditions" (conditions A1 and A2). In Part 2, we present a general theory based on a condition to be satisfied by the discretization error of the difference formula (condition (N) of Theorem 2.1) on the set $\{ f \mid Lf \in H_h \}$, where H_h is a suitable finite element space.

In each part we have considered two applications: the Numerov scheme (1.4)–(1.6) for the Schrödinger equation and the three-point central difference scheme for regular Sturm-Liouville problems.

Two-dimensional problems can also be treated. The verification of condition (N) for the five-point difference scheme is sketched at the end of Part 2.

Part 1. Convergence Estimates for Isolated Eigenvalues of Finite Multiplicity.

1.1. *Definition and Results.* Let U be a complex Banach space with norm $| \cdot |$ and $\{U_h\}_h$ a sequence of finite-dimensional spaces with norms $| \cdot |_h$. Consider also linear operators $L: U \to U$ with $D(L) \subset U$, $L_h: U_h \to U_h$, $r_h: U \to U_h$. For $u \in D(L)$, we define *the discretization error* associated with u as

$$e_h(u) = r_h L u - L_h r_h u \in U_h.$$

Let $\sigma(L)$ be the spectrum of L and let $\lambda \in \sigma(L)$ be an isolated eigenvalue of finite algebraic multiplicity m. Let Δ be a closed disk with center λ and boundary Γ such that $\Delta \cap \sigma(L) = \{\lambda\}$. Let $\lambda_{h,1}, \ldots, \lambda_{h,m(h)}$ be eigenvalues of L_h, repeated according to their algebraic multiplicities and contained in Δ. We assume that the sequence $\{L_h\}_h$ is such that

(A1) $\exists \varepsilon_0 > 0$, such that $\forall \varepsilon$, $0 < \varepsilon < \varepsilon_0$, $\exists h_0$ such that $\forall h$, $h < h_0$,

$$\sigma(L_h) \cap \{z \mid |z - \lambda| < \varepsilon\}$$

contains exactly m eigenvalues (repeated according to their multiplicities) of L_h. Denote these by $\lambda_{h,1}, \ldots, \lambda_{h,m}$.

For an operator D, $R_z(D) = (z - D)^{-1}$ denotes the resolvent operator. We also assume:

(A2) $\forall K$, compact sets $\subset \zeta(L)$, the resolvent set of L, $\exists h_0 > 0$, such that $\forall h < h_0$, $K \subset \zeta(L_h)$, the resolvent set of L_h; furthermore, $\exists c$ independent of h such that $|R_z(L_h)|_h \leqslant c$, $\forall h < h_0$, $\forall z \in K$.

For $u_h \in U_h$, X_h and Y_h subspaces of U_h, let

$$\delta_h(u_h, Z_h) = \inf_{z_h \in Z_h} |u_h - z_h|_h,$$

$$\delta_h(Y_h, Z_h) = \sup_{\substack{y_h \in Y_h \\ |y_h|_h = 1}} [\delta_h(y_h, Z_h)],$$

$$\hat{\delta}_h(Y_h, Z_h) = \max[\delta_h(Y_h, Z_h), \delta_h(Z_h, Y_h)].$$

$E = (2\pi i)^{-1} \int_\Gamma R_z(L)\, dz$ is the spectral projector of L relative to λ, and for h small enough

$$F_h = (2\pi i)^{-1} \int_\Gamma R_z(L_h)\, dz$$

is the spectral projector of L_h relative to $\{\lambda_{h,i}\}$, $1 \leqslant i \leqslant m$. $E(U)$ and $F_h(U_h)$ are, respectively, the m-dimensional invariant subspaces of L and L_h corresponding, respectively, to λ and $\{\lambda_{h,i} \mid 1 \leqslant i \leqslant m\}$.

Finally, consider the mapping $r_h^E = r_h|_{E(U)}$: $E(U) \to U_h$ and let $E_h = r_h E(U)$. We assume:

(A3) For h small enough: $\dim(E_h) = m$; furthermore, r_h^E: $E(U) \to E_h$ is a bijection with

$$\left| r_h^E \right|_{U, U_h} = \sup_{\substack{u \in E(U) \\ |u| = 1}} |r_h u|_h \leqslant c_1, \qquad \left| (r_h^E)^{-1} \right|_{U_h, U} = \sup_{\substack{u_h \in E_h \\ |u_h|_h = 1}} \left| (r_h^E)^{-1} u_h \right| \leqslant c_2,$$

with c_1, c_2 constants independent of h.

REMARK 1.1. Note that the assumption on r_h is only local, i.e., uniform boundedness must be satisfied on the invariant subspace $E(U)$ only.

Finally, let us introduce the quantity

$$\gamma_h = \sup_{\substack{u \in E(U) \\ |u| = 1}} |r_h L u - L_h r_h u|_h,$$

and assume

(A4) $\lim_{h \to 0} \gamma_h = 0$.

We now state our results.

Theorem 1.1. *There exists a constant c, independent of h, such that*

$$\delta_h\big(F_h(U_h), r_h E(U)\big) \leqslant c\gamma_h.$$

Eigenvalue estimates are based on the following preliminary argument used by Osborn [10] in a different context.

Introduce the operator $\Lambda_h = F_h r_h|_{E(U)}: E(U) \to F_h(U_h)$. We shall prove that Λ_h is a bijection. Letting $\hat{L} = L|_{E(U)}$ and $\hat{L}_h = \Lambda_h^{-1} L_h \Lambda_h$, one can see that these operators can be considered in $E(U)$, with $\hat{L}$ having the eigenvalue λ of algebraic multiplicity m, and $\hat{L}_h$ the eigenvalues $\lambda_{h,1}, \ldots, \lambda_{h,m}$.

Theorem 1.2. *Under the assumptions* (A1)–(A3), *there exists a constant c independent of h such that*

$$|\hat{L} - \hat{L}_h|_{E(U)} \leqslant c\gamma_h.$$

By the choice of basis in $E(U)$, Theorem 1.2 reduces our original task to a pure matrix problem.

Let f be a holomorphic function defined in the neighborhood of λ. Writing $f(\hat{L})$, $f(\hat{L}_h)$ in terms of Dunford integrals, one verifies that

$$|f(\hat{L}) - f(\hat{L}_h)|_{E(U)} \leqslant c|\hat{L} - \hat{L}_h|_{E(U)}.$$

Using the classical properties of traces and determinants, one obtains Theorem 1.3a, b; Theorem 1.3c, d is a direct application of results quoted in Wilkinson [14, pp. 80–81]. Here, α is the ascent of the eigenvalue λ of L and β the number of Jordan blocks of the canonical form of $\hat{L}$.

Theorem 1.3. *There exists a constant c independent of h such that for h small enough,*

(a) $|f(\lambda) - (1/m)\sum_{i=1}^{m} f(\lambda_{h,i})| \leqslant c\gamma_h$,

(b) $|f^m(\lambda) - \prod_{i=1}^{m} f(\lambda_{h,i})| \leqslant c\gamma_h$,

(c) $\max_{1 \leqslant i \leqslant m} |\lambda - \lambda_{h,i}| \leqslant c(\gamma_h)^{1/\alpha}$,

(d) $\min_{1 \leqslant i \leqslant m} |\lambda - \lambda_{h,i}| \leqslant c(\gamma_h)^{\beta/m}$.

1.2. Proofs. To obtain the above results, we need the following lemmas; throughout, c is a generic constant. (A2) leads to

Lemma 1.1. *There exists $h_0 > 0$ such that $|F_h|_h \leqslant c, \forall h < h_0$.*

Proof. One has for $u_h \in U_h$, $|u_h|_h = 1$,

$$F_h u_h = \frac{1}{2\pi i} \int_\Gamma R_z(L_h) u_h \, dz,$$

and by using (A2), with K replaced by Γ, one obtains,

$$|F_h|_h \leqslant \frac{c}{2\pi} \operatorname{meas}(\Gamma). \quad \square$$

Lemma 1.2. *There holds*

$$\sup_{\substack{u \in E(U) \\ |u| = 1}} |r_h E_h u - F_h r_h u|_h \leqslant c\gamma_h.$$

Proof. We write

$$r_h Eu - F_h r_h u = \frac{1}{2\pi i} \int_\Gamma \left[r_h R_z(L) - R_z(L_h) r_h \right] u \, dz.$$

Now use the following identities,

$$z \in \Gamma: \; r_h R_z(L) - R_z(L_h) r_h = R_z(L_h)\left[(z - L_h) r_h - r_h(z - L) \right] R_z(L)$$
$$= R_z(L_h)\left[r_h L - L_h r_h \right] R_z(L),$$

to get

$$r_h Eu - F_h r_h u = \int_\Gamma (2\pi i)^{-1} R_z(L_h) \left[r_h L - L_h r_h \right] R_z(L) u \, dz.$$

Clearly, since $R_z(L)u \in E(U)$, and using (A2) with K replaced by (Γ), this implies

$$\left| r_h Eu - F_h r_h u \right|_h \leqslant (1/2\pi) \int_\Gamma \left| R_z(L_h) \right|_h c\gamma_h \left| R_z(L) \right| |u| \, dz,$$

which proves the result. □

Using assumption (A3) and Lemma 1.2, one easily deduces

LEMMA 1.3. *One has*

$$\delta_h\left(r_h E(U), F_h(U_h) \right) \leqslant c\gamma_h.$$

We omit also the proof of the following elementary result.

LEMMA 1.4. *Let Y_h and Z_h be two subspaces of U_h with the same finite dimension. Let $P_h: Y_h \to Z_h$ be a linear operator such that*

$$\left| P_h y - y \right|_h \leqslant .5 |y|_h, \qquad y \in U_h.$$

Then P_h is a bijection and $\left| P_h^{-1} z \right| \leqslant 2|z|$, $z \in Z_h$. Furthermore,

$$\sup_{\substack{z \in Z_h \\ |z|_h = 1}} \left| P_h^{-1} z - z \right|_h \leqslant 2 \sup_{\substack{y \in Y_h \\ |y|_h = 1}} \left| P_h y - y \right|_h.$$

Proof of Theorem 1.1. Let $\theta_h = F_h |_{E_h}: E_h \to F_h(U_h)$ (recall $E_h = r_h E(U)$); for h small enough, E_h and $F_h(U_h)$ have the same finite dimension m; on the other hand, (A4) implies $\lim_{h \to 0} \gamma_h = 0$. Using Lemmas 1.2 and 1.4, θ_h^{-1} exists for h small enough and is such that

(1.8) $$\sup_{\substack{y \in F_h(U_h) \\ |y_h|_h = 1}} \left| \theta_h^{-1} y \right|_h \leqslant c.$$

Furthermore,

$$\sup_{\substack{y \in F_h(U_h) \\ |y|_h = 1}} \left| \theta_h^{-1} y - y \right|_h \leqslant c\gamma_h,$$

i.e., $\delta_h(F_h(U_h), r_h E(U)) \leqslant c\gamma_h$. □

Proof of Theorem 1.2. Note that

$$\hat{L} - \hat{L}_h = \hat{L} - \Lambda_h^{-1} L_h \Lambda_h = \Lambda_h^{-1} \Lambda_h \hat{L} - \Lambda_h^{-1} L_h \Lambda_h,$$

and for $u \in E(U)$, using $\Lambda_h = \theta_h = \theta_h r_h^E$ and $\Lambda_h^{-1} = (r_h^E)^{-1}(\theta_h)^{-1}$, we have for $u \in E(U)$ such that $|u| = 1$,

$$\hat{L} u = \hat{L}_h u = \Lambda_h^{-1}\left[\Lambda_h \hat{L} u - L_h \Lambda_h u \right].$$

From (A3) and (1.8) one sees that $|\hat{L}u - \hat{L}_h u| \leqslant c|\Lambda_h Lu - L_h \Lambda_h u|_h$. Note that $L_h \Lambda_h = L_h F_h r_h = F_h L_h r_h$, so that $\Lambda_h Lu - L_h \Lambda_h u = F_h r_h Lu - F_h L_h r_h u$. Using the uniform boundedness of F_h on U_h, we obtain immediately our result. □

Remark 1.2. Note that the estimates depend solely on the discretization error of the difference scheme over the invariant subspace, i.e., γ_h.

Remark 1.3. In the selfadjoint case, since $\alpha = 1$ and $\beta = m$, note from Theorem 1.3(b) and (c) that every eigenvalue $\lambda_{h,i}$ converges to λ with the same rate. This can be checked by a simple algebraic manipulation which we omit here (see [5]).

1.3. *Application to Numerov's Scheme for the Schrödinger Operator.* We let $U = L^2(0, \infty)$; $U_h = R^{N-1}$; on $q(x)$ we make the following assumption:

(Q)
$$(1) \quad q \in C^\infty(0, \infty) \cap C[0, \infty], \, q \to 0 \quad \text{as } x \to \infty,$$
$$(2) \quad \alpha = \inf_{x \in R_+} q(x) < 0, \qquad M = \sup_{x \in R_+} |q(x)|,$$
$$(3) \quad q \text{ Lipschitz continuous on } (0, \infty).$$

In case of $c = 0$, $d = 1$ in (1.2), there exists an infinite sequence $\{\lambda_k\}_k$ of isolated eigenvalues of multiplicity 1 such that for all k, $\alpha < \lambda_k < 0$, with $\lim_{k \to \infty} \lambda_k = 0$. Furthermore, each corresponding eigenfunction has exactly $k - 1$ positive zeros and tends exponentially to zero as $x \to \infty$. The eigenfunctions are in $C^\infty(0, \infty)$.

For $f \in U$, set $|f| = \{ \int_0^\infty |f(x)|^2 \, dx \}^{1/2}$, and for $f_h \in U_h$, $f_h = \{f_{h,i}\}_i$, set

$$|f_h|_h = \left\{ \sum_{i=1}^{N-1} h |f_{h,i}|^2 \right\}^{1/2}.$$

Under the assumptions (Q)(1)–(Q)(3), (A1) and (A2) will be verified in the second part of the paper. We turn now to the verification of (A3). For that purpose, introduce $H_h = \{ \psi \in C(0, X) \mid \psi(0) = \psi(X) = 0, \, \psi \text{ linear on } (x_{i-1}, x_i), \, i = 1, \ldots, N \}$. Note that H_h is isomorphic to U_h. Furthermore, if $\psi_h = \{\psi(x_i) \mid 1 \leqslant i \leqslant N - 1\}$, then there exist two constants c_1, c_2 independent of h such that

$$(1.9) \qquad c_2 |\psi_h|_h \leqslant |\psi| \leqslant c_1 |\psi_h|_h, \quad \forall \psi \in U_h.$$

Also, for a function $f \in C(0, \infty)$ with $f(0) = 0$, let $I_h f \in H_h$ be its interpolant satisfying $(I_h f)(x_i) = f(x_i)$, $1 \leqslant i \leqslant N - 1$.

We now prove the following

LEMMA 1.4. *Let E_k be the invariant subspace corresponding to the eigenvalue λ_k, $1 \leqslant k$. Then under the assumptions (Q)(1)–(Q)(2), there exists a sequence $\{\varepsilon_h\}$ such that $\lim_{h \to 0} \varepsilon_h = 0$ and*

$$|f - I_h f| \leqslant \varepsilon_h |f|, \qquad f \in E_k.$$

Proof. We prove the assertion with $|f| = 1$. Choose h sufficiently small so that the interval $(0, X - h)$ includes the $k - 1$ zeros of every eigenfunction; thus, on $(X - h, \infty)$, $f(x)$, and consequently $I_h f$, keeps a constant sign.

We have the trivial inequality

$$|f - I_h f|^2 \leqslant \int_0^{X-h} [f(x) - (I_h f)(x)]^2 \, dx + 2 \int_{X-h}^\infty [f(x)]^2 \, dx.$$

As $f(x)$ decays exponentially to zero, h is also chosen so that on $(X - h, \infty)$, $|f(x)| \leqslant c_k \exp(-d_k x)$, c_k and d_k depending on f and E_k only. Since f is C^∞, it is well known that

$$\left\{ \int_0^{X-h} [f(x) - (I_h f)(x)]^2 \, dx \right\}^{1/2} \leqslant ch^2 \left\{ \int_0^{X-h} [f''(x)]^2 \, dx \right\}^{1/2},$$

with c independent of h and X. Furthermore, since

$$-f''(x) + q(x)f(x) = \lambda_k f(x), \qquad 0 < x < \infty,$$

one obtains, using (Q)(2),

$$\left\{ \int_0^{X-h} |f(x) - (I_h f)(x)|^2 \, dx \right\}^{1/2} \leqslant ch^2 \big[|\lambda_k| + M \big].$$

Turning to the second term, $2 \int_{X-h}^\infty |f(x)|^2 \, dx$, it is bounded by $\delta_h = 2(c_k^2 / d_k) \exp\{ -2d_k(X - h) \}$. Letting $\varepsilon_h^2 = \max\{ \delta_h, c^2 h^4 (|\lambda_k| + M)^2 \}$, we conclude the result. $\square$

If we write now $f_h = r_h f = \{ f(x_i) \}$, $1 \leqslant i \leqslant N - 1$, we have the following

LEMMA 1.5. *Let E_k be the invariant subspace corresponding to the eigenvalue λ_k, $1 \leqslant k$. Let also $E_{k,h} = r_h E_k$, and $r_h^E \colon E_k \to E_{k,h}$. Then for h small enough, $E_{k,h}$ and r_h^E satisfy condition* (A3).

Proof. From the identity $f_h = r_h f = r_h I_h f$, and (1.9), we have

$$(1.10) \qquad c_2 |f_h|_h \leqslant |I_h f| \leqslant c_1 |f_h|_h.$$

Thus, for $|f| = 1$, using Lemma 1.3, we may write

$$c_2 |f_h|_h \leqslant |I_h f| \leqslant |f| + |f - I_h f| \leqslant 1 + \varepsilon_h,$$

thus giving $|r_h^E|_{U, U_h} \leqslant c_1$. As h is chosen so that $(0, X)$ includes the $k - 1$ zeros of every eigenfunction, one concludes that r_h^E is bijective and $\dim(E_{k,h}) = 1$.

Finally, consider $f_h \in U_h$ such that $|f_h|_h = 1$, and $f \in E_k$ such that $f_h = r_h^E f$; from $|f| \leqslant |I_h f| + |f - I_h f| \leqslant |I_h f| + \varepsilon_h |f|$, one concludes for h sufficiently small (as $\varepsilon_h \to 0$) that $(1 - \varepsilon_h)|f| \leqslant |I_h f|$. Using again (1.10), one obtains

$$\left| \left(r_h^E \right)^{-1} \right|_{U_h, U} \leqslant c_2. \quad \square$$

We turn finally to the estimation of the discretization error over the subspace E_k, $\gamma_h = \sup_{f \in E_k; |f| = 1} |r_h Lf - L_h r_h f|_h$. We have the following

LEMMA 1.6. *Let E_k be the invariant subspace corresponding to the eigenvalue λ_k, $k \geqslant 1$. Under the assumptions* (Q)(1)–(Q)(3), *and assuming q', q'', q''', $q^{(4)}$ are bounded on $(0, \infty)$, the following inequality is valid for h sufficiently small:*

$$\gamma_h \leqslant 3h^4 \big(C_1 + h^{-13/2} |f(X)| \big).$$

Proof. We take f such that $|f| = 1$. Let $\sigma_h = r_h Lf - L_h r_h f \in R^{N-1}$. Let also R_h be the linear transformation in R^{N-1}, represented by the tridiagonal matrix

$$
\frac{1}{12}
\begin{pmatrix}
10 & 1 & & & & & \\
1 & 10 & 1 & & & & \\
 & 1 & & 1 & & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & \ddots & & & \\
 & & & & & 10 & 1 \\
 & & & & & 1 & 10
\end{pmatrix}.
$$

Note that

$$
(R_h \sigma_h)_i = \left(f''_{i-1} + 10 f''_i + f''_{i+1} \right)/12 + \left(f_{i-1} - 2 f_i + f_{i+1} \right)/h
$$
$$
+ \delta_{i,N-1}\left(f''(X)/12 - f(X)/h^2 \right), \qquad 1 \leqslant i \leqslant N-1,
$$

where $\delta_{i,k}$ is the Kronecker delta. The assumptions on q permit the use of the Taylor expansion to obtain

$$
(R_h \sigma_h)_i = \frac{1}{120 h^2}\left[\int_{x_i}^{x_{i+1}} (x - x_i)^5 f^{(6)}(x)\, dx + \int_{x_i}^{x_{i-1}} (x - x_i)^5 f^{(6)}(x)\, dx \right]
$$
$$
+ \frac{1}{72}\left[\int_{x_i}^{x_{i+1}} (x - x_i)^3 f^{(6)}(x)\, dx + \int_{x_i}^{x_{i-1}} (x - x_i)^3 f^{(6)}(x)\, dx \right]
$$
$$
+ \delta_{i,N-1}\left(f''(X)/12 - f(X)/h^2 \right)
$$

and

$$
(R_h \sigma_h)_i \leqslant e h^{4 - 1/2}\left[\left\{ \int_{x_i}^{x_{i+1}} |f^{(6)}(x)|^2\, dx \right\}^{1/2} + \left\{ \int_{x_{i-1}}^{x_i} |f^{(6)}(x)|^2\, dx \right\}^{1/2} \right]
$$
$$
+ \delta_{i,N-1}|f''(X)/12 - f(X)/h^2| \qquad (e \cong 7.7 \times 10^{-3}).
$$

This implies

$$
\left[\sum_{i=1}^{N-1} h |(R_h \sigma_h)_i|^2 \right]^{1/2} \leqslant 2 e h^4 \left(\int_0^X |f^{(6)}(x)|^2\, dx \right)^{1/2} + \sqrt{h}\, |f''(X)/12 - f(X)/h^2|.
$$

Consider now the equation $-f''(x) + q(x)f(x) = \lambda_k f(x)$; multiplication by f and integration from 0 to ∞ yields

$$
\int_0^\infty f'^2(x)\, dx + \int_0^\infty q(x) f^2(x)\, dx = \lambda_k \int_0^\infty f^2(x)\, dx,
$$

and therefore $|f'|^2 \leqslant M_k |f|^2$, where $M_k = \sup_{x \in (0,\infty)}|\lambda_k - q(x)|$. Successive differentiation of the above equation allows us to obtain $|f^{(j)}| \leqslant A_j |f|$, $2 \leqslant j \leqslant 6$. Since $|f| = 1$, one obtains for h sufficiently small

$$
\left\{ \sum_{i=1}^{N-1} h |(R_h \sigma_h)_i|^2 \right\}^{1/2} \leqslant 2 e h^4 A_6 + 2 h^{-5/2}|f(X)|,
$$
$$
|R_h \sigma_h|_h \leqslant 2 h^4 \left(e A_6 + h^{-13/2}|f(X)| \right).
$$

From $|R_h \sigma_h|_h \geqslant \tfrac{2}{3}|\sigma_h|_h$ one obtains the result. $\square$

From the above, one clearly deduces

COROLLARY 1.1. *There exist choices for h, $X(h)$ such that for the system* (1.1)–(1.3) *Numerov's scheme yields a discretization error of order $O(h^4)$ over E_k, the invariant subspace corresponding to the eigenvalue λ_k.*

Proof. Since $|f(x)| \leqslant c_k \exp(-d_k x)$ for x sufficiently large, any choice for which $X(h) = O(h^{-m})$, $m > 0$, will make $h^{-13/2}|f(X)|$ bounded as $h \to 0$. For example, $h = 1/n$, $X(h) = n$, $N(h) = n^2$, is a trivial choice. A more practical one for computer use is $h = 1/2m$, $X(h) = m^i$, $i > 1$, $N(h) = 2^m m^i$, which also yields the required result.

Remark. In the last choice, note that if one uses $i = 1$, then $h^{-13/2}|f(X)| \to \infty$ as $h \to 0$.

We state finally a last theorem based on Theorems 1.1 and 1.2.

THEOREM 1.3. *Under the assumptions of Lemma 1.6, for every isolated eigenvalue λ_k, $k \geqslant 1$, with multiplicity 1 of the operator L in* (1.1)–(1.3), *the Numerov scheme yields a sequence of operators L_h: $R^{N-1} \to R^{N-1}$, and a sequence of isolated eigenvalues $\lambda_{k,h}$ of L_h, with the same multiplicity as λ_k, such that for some choices of $\{h, X(h)\}$ one has*

$$|\lambda_k - \lambda_{k,h}| \leqslant ch^4, \qquad \hat{\delta}_h(r_h E_k, F_{k,h}) \leqslant ch^4.$$

($F_{k,h}$ in R^{N-1} is the invariant subspace corresponding to $\lambda_{k,h}$.)

1.4. *Application to Regular Sturm-Liouville Problems.* Consider the eigenvalue problem

$$(1.11) \qquad -\frac{d}{dx}\left[q(x)\frac{dy}{dx}\right] + s(x)y = \lambda p(x)y, \qquad a < x < b,$$

$$y(a) = y(b) = 0,$$

where

(C1) p, q and s are continuous and positive on $[a, b]$.

It is well known [9] that under the assumption (C1) there exists an increasing sequence of eigenvalues $\lambda_1 < \lambda_2 < \cdots < \lambda_n < \cdots$ that approach ∞, each having multiplicity 1. The eigenfunction corresponding to λ_n has exactly $n - 1$ zeros in the open interval (a, b).

Furthermore, we assume sufficient regularity on p, q and s, so that $y \in C^4(a, b)$; for example,

(C2) $q \in C^3(a, b)$; $p, s \in C^2(a, b)$.

Consider a partition $x = a + ih$, $0 \leqslant i \leqslant N$, with $Nh = b - a$, and a discretization of (1.11) based on the central difference formula,

$$\delta_{h/2}y(x) = (y(x + h/2) - y(x - h/2))/h,$$

$$(1.12) \qquad -\delta_{h/2}(q_i\delta_{h/2}Y_i) + s_iY_i = \lambda_h p_iY_i, \qquad 0 < i < N,$$

$$(1.13) \qquad Y_0 = Y_N = 0.$$

To abide by our original notation, L and L_h are defined by

$$Ly = (-(q(x)y')' + s(x)y)/p(x),$$

$$(L_hY)_i = (-\delta_{h/2}(q_i\delta_{h/2}Y_i) + s_iY_i)/p_i, \qquad 0 < i < N,$$

where $Y \in R^{N-1}$.

As in Subsection 1.3, we let $U = L^2(a, b)$, $U_h = R^{N-1}$, with respective norms

$$|y| = \left\{ \int_a^b [y(x)]^2 \, dx \right\}^{1/2} \quad \text{and} \quad |Y|_h = \left\{ \sum_{i=1}^{N-1} h Y_i^2 \right\}^{1/2}, \qquad y \in U, \, Y \in U_h.$$

(A1) and (A2) will be verified in the second part of this paper. The verification of (A3) is similar to that of the Numerov scheme in Subsection 1.3, i.e., one introduces the subspace $H_h = \{ \psi \in C(a, b) \,|\, \psi(a) = \psi(b) = 0, \, \psi \text{ linear on } (x_i, x_{i+1}), \, i = 0, \ldots, N-1 \}$, and obtains analogues of Lemmas 1.4 and 1.5 in the newly introduced norms.

Let finally λ_k be an isolated eigenvalue of L, with E_k its invariant subspace, and $\gamma_h = \sup_{f \in E_k : |f| = 1} |r_h L f - L_h r_h f|_h$. The estimation of γ_h is based on the formula

$$\begin{aligned}
\delta_{h/2}(q_i \delta_{h/2} y_i) = {} & (q(x) y'(x))' + \frac{1}{2h} \int_{x_{i-1/2}}^{x_{i+1/2}} (x - x_i)^2 (qy')''' \, dx \\
& + \frac{q_{i+1/2}}{6h^2} \int_{x_i}^{x_{i+1}} (x - x_{i+1/2})^3 y^{(4)}(x) \, dx \\
& + \frac{q_{i-1/2}}{6h^2} \int_{x_{i-1}}^{x_i} (x - x_{i-1/2})^3 y^{(4)}(x) \, dx + \frac{h}{24} \int_{x_{i-1/2}}^{x_{i+1/2}} (qy''')' \, dx,
\end{aligned}$$

(1.14)

which allows us to prove

LEMMA 1.7. *Let E_k be the invariant subspace corresponding to the eigenvalue λ_k, $k \geq 1$. Then under the assumption* (C2), *the following inequality is valid:*

$$|r_h L f - L_h r_h f|_h \leq \frac{h^2}{\sqrt{80}\, \underline{p}} \left(|(qf')'''|^2 + \bar{q}^2 |f^{(4)}|^2 + |(qf''')'|^2 \right)^{1/2}, \qquad f \in E_k,$$

with $\underline{p} = \inf_x p(x)$ and $\bar{q} = \sup_x |q(x)|$.

Proof. We take $f \in E_k$ such that $|f| = 1$. Let $\sigma_h = r_h L f - L_h r_h f \in R^{N-1}$. Note that

$$\sigma_{h,i} = \left(-(q(x) f'(x))'_{x=x_i} + \delta_{h/2}(q_i \delta_{h/2} f_i) \right) / p_i, \qquad 0 < i < N.$$

Using (1.14), one bounds $\sigma_{h,i}$ as follows:

$$\begin{aligned}
p_i |\sigma_{h,i}| \leq {} & \frac{1}{8\sqrt{5}} h^{2-1/2} \left\{ \int_{x_{i-1/2}}^{x_{i+1/2}} |(qf')'''|^2 \, dx \right\}^{1/2} \\
& + \frac{q_{i+1/2}}{48\sqrt{7}} h^{2-1/2} \left\{ \int_{x_i}^{x_{i+1}} |f^{(4)}(x)|^2 \, dx \right\}^{1/2} \\
& + \frac{q_{i-1/2} h^{2-1/2}}{48\sqrt{7}} k \left\{ \int_{x_{i-1}}^{x_i} |f^{(4)}(x)|^2 \, dx \right\}^{1/2} \\
& + \frac{h^{2-1/2}}{24} \left\{ \int_{x_{i-1/2}}^{x_{i+1/2}} |(qf''')'|^2 \, dx \right\}.
\end{aligned}$$

Thus, if $\bar{q} = \sup_{x \in (a,b)} |q(x)|$ and $\underline{p} = \inf_{x \in (a,b)} p(x)$,

$$p_i^2 h |\sigma_{h,i}|^2 \leqslant \frac{1}{80} h^4 \int_{x_{i-1/2}}^{x_{i+1/2}} |(qf')'''|^2 \, dx + \frac{\bar{q}^2 h^4}{4032} \int_{x_{i-1}}^{x_{i+1}} |f^{(4)}(x)|^2 \, dx$$

$$+ \frac{h^4}{576} \int_{x_{i-1/2}}^{x_{i+1/2}} |(qf''')'|^2 \, dx,$$

and therefore

$$\sum_{i=1}^{N-1} h |\sigma_{h,i}|^2 \leqslant \frac{h^4}{\underline{p}^2} \left(\frac{1}{80} |(qf')'''|^2 + \frac{\bar{q}^2}{2016} |f^{(4)}|^2 + \frac{1}{576} |(qf''')'|^2 \right),$$

which proves our lemma. $\square$

To obtain final eigenvalue-eigenvector estimates, we note first that, when multiplying (1.11) by $y(x)$ and integrating by parts from a to b,

$$\int_a^b q(x) f'^2 \, dx + \int_a^b s(x) f^2 \, dx = \lambda_k \int_a^b p(x) f^2 \, dx, \qquad f \in E_k,$$

which yields

$$(1.15) \qquad \underline{q} |f'|^2 \leqslant \left(\sup_{x \in (a,b)} |\lambda_k p - s| \right) |f|^2 = M |f|^2,$$

where $\underline{q}$ is $\inf_{x \in (a,b)} |q|$. Using again (1.11), one bounds $|(qf')'|$ and $|f''|$ in terms of $|f|$; specifically,

$$(1.16) \qquad |(qf')'| \leqslant M |f| \qquad (M \text{ defined as in } (1.15)),$$

$$(1.17) \qquad |f''| \leqslant \frac{1}{\underline{q}} \left(M + \bar{q}' \sqrt{\frac{M}{\underline{q}}} \right) |f| \qquad \left(\bar{q}' = \sup_x |q'(x)| \right).$$

Successive differentiation allows us to bound f''', $f^{(4)}$, and $(qf')'''$ in terms of $|f|$, which, together with Lemma 1.7, gives $\gamma_h \leqslant ch^2$, and hence the following theorem.

THEOREM 1.4. *Let E_k be the invariant subspace associated with λ_k, an eigenvalue of the regular Sturm-Liouville operator defined in (1.11). Then under the assumption (C2), the three-point central difference formula (1.12)–(1.13) yields a sequence of eigenvalues $\lambda_{k,h}$ with corresponding eigenspaces $E_{k,h} \subset R^{N-1}$ such that for all h,*

$$|\lambda_k - \lambda_{k,h}| \leqslant ch^2, \qquad \hat{\delta}_h(r_h E_k, F_{k,h}) \leqslant ch^2.$$

Part 2. A Sufficient Condition for Stability.

2.1. *Definition and Results.* In this part we show that conditions (A1) and (A2) follow from an analysis of the discretization error of the difference formula over a suitable subspace. Specifically, consider the system (1.1)–(1.3), whose eigenvalues are approximated using a difference method such as the Numerov scheme, and define the sequence of operators $\{L_X\}_h$ by

$$(2.1) \qquad L_X y = -y'' + q(x) y, \qquad 0 < x < X,$$

$$(2.2) \qquad cy'(0) + dy(0) = 0,$$

$$(2.3) \qquad y(X) = 0.$$

Note that (1.7) discretizes (1.1)–(1.3) as well as (2.1)–(2.3).

In (1.2) we considered without loss of generality the case $c = 0$. Let $H_h = \{\psi \in C(0, X) \mid \psi$ linear in (x_i, x_{i+1}), $0 \leqslant i \leqslant N - 1, \psi(0) = \psi(X) = 0\}$. Let $\gamma > 0$ be such that $(-\infty, 0) \in \zeta(L_X + \gamma)$, the resolvent set of $L_X + \gamma$; for every $\psi \in H_h$, let $z = A_X \psi \in C^2(0, X)$ be uniquely defined by

$$(L_X + \gamma)z = \psi, \qquad z(0) = z(X) = 0.$$

As in Part 1, we introduce the notations

$$f \in L^2(0, \infty), \quad |f| = \left\{ \int_0^\infty |f(x)|^2 \, dx \right\}^{1/2},$$

$$f \in H^1(0, \infty), \quad \|f\| = \left\{ |f|^2 + |f'|^2 \right\}^{1/2}.$$

Also between R^{N-1} and H_h we consider the mappings r_h: $H_h \to R^{N-1}$ and p_h: $R^{N-1} \to H_h$, where, if $\{w_{h,i}(x)\}_i$ is the usual "hat" functions basis in H_h, and $c \in R^{N-1}$, $\psi = p_h c = \sum_{i=1}^{N-1} c_i w_{h,i}(x)$, and $c = r_h \psi$.

We may therefore consider the discrete norms on H_h or R^{N-1},

$$\psi \in H_h, \quad |\psi|_h = \left\{ \sum_{i=1}^{N-1} h |(r_h \psi)_i|^2 \right\}^{1/2},$$

$$\psi \in H_h, \quad \|\psi\|_h = \left\{ |\psi|_h^2 + |\psi'|^2 \right\}^{1/2}.$$

$|\cdot|_h$ shall be used without distinction on H_h and R^{N-1}. One proves the existence of two constants c_1, c_2 independent of h such that

(2.4) $c_2 |\psi| \leqslant |\psi|_h \leqslant c_1 |\psi|, \qquad c_2 \|\psi\| \leqslant \|\psi\|_h \leqslant c_1 \|\psi\|.$

Furthermore, one has naturally $|\psi|_h \leqslant \|\psi\|_h$, $\forall \psi \in H_h$. Note that (1.7) as a general difference scheme can be easily transformed to a mapping in H_h, by considering the mapping $p_h L_h r_h$: $H_h \to H_h$.

Our main result is as follows.

THEOREM 2.1. *Assume the difference operator* L_h *is selected for the numerical approximation of the spectrum of* L. *If* L_h *and* L *satisfy the condition*

(N) $\lim_{\substack{h \to 0}} \sup_{\substack{\psi \in H_h \\ \|\psi\| = 1 \\ z = A_X \psi}} |r_h L_X z - L_h r_h z|_h = 0,$

then L_h *satisfies properties* (A1), (A2).

To prove this theorem, we need to introduce additional notations. Let

$$[\psi, \phi]_h = \sum_{i=1}^{N-1} h(r_h \psi)_i (r_h \bar{\phi})_i \quad (\bar{\phi}: \text{complex conjugate}),$$

$$(\psi, \phi)_h = \int_0^x \psi'(x) \bar{\phi}'(x) \, dx + [\psi, \phi]_h, \qquad \psi, \phi \in H_h.$$

One then defines the sesquilinear form a_h on $H_h \times H_h$ by

$$a_h(\psi, \phi) = [p_h(L_h + \gamma)\psi, \phi]_h$$

and assumes the existence of constants γ_0, $\gamma_1 > 0$ independent of h such that

(2.5) $a_h(\psi, \psi) \geqslant \gamma_0 \|\psi\|_h^2, \qquad |a_h(\phi, \psi)| \leqslant \gamma_1 \|\phi\|_h \|\psi\|_h.$

This allows the use of the Lax-Milgram theorem to define the sequence of operators $\{B_h\}_h$: $H_h \to H_h$ by the relation $a_h(B_h\psi, \phi) = [\psi, \phi]_h$, $\forall \psi$, $\phi \in H_h$. Note also that

$$(2.6) \qquad \|B_h\psi\|_h \leqslant c|\psi|_h, \quad \forall \psi \in H_h \ (c \text{ independent of } h).$$

The analysis of the spectrum of L_h: $R^{N-1} \to R^{N-1}$ is equivalent to the analysis of the spectrum of B_h: $H_h \to H_h$. For condition (A1), this is straightforward; condition (A2) is obtained below using $\| \cdot \|_h$, but the following lemma shows that this implies (A2) in $| \cdot |_h$.

LEMMA 2.1. *For h sufficiently small, $z \neq -\gamma$ and $z \in \zeta(L_h)$ if and only if $z_1 = 1/(z + \gamma) \in \zeta(L_h)$. Furthermore, $\|(B_h - z_1)\psi\|_h \geqslant c_0\|\psi\|_h$, $\forall \psi \in H_h$ (c_0 independent of h) implies $|(L_h - z)f|_h \geqslant c|f|_h$, $\forall f \in R^{N-1}$ (c independent of h).*

Proof. The first part of this lemma can easily be seen from the identity

$$\left[(p_h L_h r_h - z_1)\psi, \phi\right]_h = (z + \gamma)a_h((z_1 - B_h)\psi, \phi), \quad \forall \phi, \psi \in H_h.$$

As for the second part, note that for $f \in R^{N-1}$, $p_h f = \psi \in H_h$, one has

$$(L_h - z)f_h = \sup_{\substack{\psi \in H_h \\ |\psi|_h = 1}} \left|\left[(p_h L_h r_h - z)\psi, \phi\right]_h\right| \geqslant \sup_{\substack{\phi \in H_h \\ |\phi|_h = 1}} \left|a_h((B_h - z_1)\psi, \phi)\right|.$$

Taking $\phi = (B_h - z_1)\psi/|(B_h - z_1)\psi|_h$, and using (2.5), we get

$$|(L_h - z)f|_h \geqslant \gamma_0|z + \gamma|\|(B_h - z_1)\phi\|_h^2/|(B_h - z_1)\phi|_h.$$

One then has

$$|(L_h - z)f|_h \geqslant \gamma_0|z + \gamma|\|(B_h - z_1)\psi\|_h \geqslant \gamma_0 c_0|z + \gamma|\|\phi\|_h.$$

Using (2.4), one obtains the result. $\square$

The proof of Theorem 2.1 is based on a perturbation theory result.

THEOREM 2.2. *Let A_h^1, A_h^2: $H_h \to H_h$ be such that*

$$(P) \qquad \lim_{h \to 0} \sup_{\substack{\psi \in H_h \\ \|\psi\| = 1}} \left\|(A_h^1 - A_h^2)\psi\right\| = 0.$$

Then A_h^1 satisfies (A1) and (A2) if and only if A_h^2 satisfies (A1) and (A2).

Proof. Assume A_h^1 satisfies (A1) and (A2).

(i) To show that A_h^2 satisfies (A2), assume there exists $\{h_i\}$ and, correspondingly, $\psi_i \in H_{h_i}$, $\|\psi_i\| = 1$ such that $\lim_{h_i \to 0}\|(A_{h_i}^2 - \mu)\psi_i\| = 0$. Note

$$\left\|(A_{h_i}^1 - \mu)\psi\right\| \leqslant \left\|(A_{h_i}^1 - A_{h_i}^2)\psi\right\| + \left\|(A_{h_i}^2 - \mu)\psi\right\|.$$

Thus, $\lim_{h_i \to 0}\|(A_{h_i}^1 - \mu)\psi\| = 0$ and $\mu \notin \zeta(A_{h_i}^1)$, which contradicts (A2) for A_h^1.

(ii) For (A1), let λ be an isolated eigenvalue of finite algebraic multiplicity m, and Δ a disc centered at λ, with boundary Γ such that for all h sufficiently small, Δ contains m eigenvalues of A_h^1 (repeated according to their multiplicities) converging to λ; $E_h^1 = (2\pi i)^{-1}\int_\Gamma R_z(A_h^1)\,dz$ is the spectral projector corresponding to A_h^1 and $E_h^1(H_h)$, its invariant subspace. Similarly, $E_h^2 = (2\pi i)^{-1}\int_\Gamma R_z(A_h^2)\,dz$, and one notes that

$$(2.7) \qquad \lim_{h \to 0} \sup_{\substack{\psi \in H_h \\ \|\psi\| = 1}} \left\|(E_h^1 - E_h^2)\psi\right\| = 0.$$

This can be seen from the identity

$$E_h^1 - E_h^2 = (2\pi i)^{-1} \int_\Gamma R_z(A_h^1)(A_h^2 - A_h^1) R_z(A_h^2)\, dz.$$

Using the first part of the theorem and (P), one obtains (2.7). Consider now the mapping $\bar{E}_h^2 = E_h^2|_{E_h^1(H_h)}: E_h^1(H_h) \to E_h^2(H_h)$. For $\psi \in H_h$ such that $\|\psi\| = 1$, one has from (2.7) that $\lim_{h \to 0}\|\psi - \bar{E}_h^2\psi\| = 0$, which obviously shows that for h sufficiently small, $\bar{E}_h^2$ is injective. Hence $\dim(E_h^1(H_h)) \leqslant \dim(E_h^2(H_h))$. A similar argument on $\bar{E}_h^1 = E_h^1|_{E_h^2(H_h)}: E_h^2(H_h) \to E_h^1(H_h)$ shows that $\dim(E_h^2(H_h)) \leqslant \dim(E_h^1(H_h))$, and therefore $\dim(E_h^1(H_h)) = \dim(E_h^2(H_h))$. $\square$

2.2. *Proof of Theorem* 2.1. To obtain Theorem 2.1, we now relate the "difference operator" B_h to the interpolation operator $C_h = I_h A_X|_{H_h}$. This is done in

LEMMA 2.2. *The difference approximation B_h and the "interpolatory" approximation $I_h A_X|_{H_h}$ satisfy the inequality*

$$\|(B_h - I_h A_X)\psi\| \leqslant c|r_h L_X z - L_h r_h z|_h \quad (c \text{ independent of } h).$$

Proof. To obtain the result, let $e_h = B_h\psi - I_h A_X\psi$. With $z = A_X\psi$, consider $\sigma_h = r_h L_X z - L_h r_h z$, the discretization error associated with z, which can be written as $r_h(L_X - 2\alpha)z - (L_h - 2\alpha)r_h z$. Clearly, from $\sigma_h \in R^{N-1}$ one writes

$$[p_h \sigma_h, \phi]_h = [p_h r_h(L_X - 2\alpha)z, \phi]_h - [p_h(L_h - 2\alpha)r_h z, \phi]_h,$$

and therefore, using $z = A_X\psi$ and the definition of B_h,

$$[\psi, \phi]_h - a_h(p_h r_h z, \phi) = [p_h \sigma_h, \phi]_h, \qquad a_h(B_h\psi - I_h A_X\psi, \phi) = [p_h \sigma_h, \phi]_h.$$

Letting $\phi = e_h$ and using inequalities (2.4), one obtains the result. $\square$

Hence, if the discretization error is such that

$$\text{(N)} \qquad\qquad \lim_{h \to 0} \sup_{\substack{\psi \in H_h \\ \|\psi\| = 1 \\ z = A_X\psi}} |r_h L_X z - L_h r_h z|_h = 0,$$

then B_h and C_h satisfy property (P), demonstrating clearly that Theorem 2.1 is a consequence of Theorem 2.2 and Lemma 2.2. The analysis of the convergence of $\sigma(L_h)$ depends on a well-known result of approximation theory.

LEMMA 2.3. *Assume q satisfies* (Q)(2) *(see Part* 1); *then*

$$\|A_X\psi - I_h A_X\psi\|_X \leqslant ch|\psi|.$$

Here c is a constant independent of h and X. $(\| \cdot \|_X$ *here is the $H^1(0, X)$-norm.)*

Proof. One knows that $\|A_X\psi - I_h A_X\psi\|_X$ is bounded by

$$ch\left[\int_0^X |z''(x)|^2 dx\right]^{1/2}, \quad \text{with } c \text{ independent of } h \text{ and } X.$$

Furthermore, using trivial energy inequalities directly related to the equation $-z'' + q(x)z = \psi(x)$, one finds

$$\left\{\int_0^X |z''(x)|^2 dx\right\}^{1/2} \leqslant c(M, \alpha)\left\{\int_0^X |\psi|^2 dx\right\}^{1/2},$$

which yields the result. $\square$

2.3. *Corollaries for Bounded and Unbounded Domains.* For bounded domains $X = a$, note that $A_X = A$; $L_X = L$. $\sigma(A)$ includes only isolated eigenvalues of finite algebraic multiplicity. Furthermore, A is compact in $L^2(0, a)$. In this case, Lemma 2.3 yields

$$(2.8) \qquad \|(A - C_h)\psi\| \leqslant ch\|\psi\|, \qquad \psi \in H_h.$$

Moreover, H_h is dense in $H^1(0, a)$; together with (2.8), this is sufficient, according to Descloux, Nassif and Rappaz [4], to have $\sigma(C_h)$ satisfy (A1) and (A2). This immediately yields

COROLLARY 2.1. *Assume a difference operator L_h is chosen to compute the eigenvalues of a differential operator L defined by $Ly = -y'' + q(x)y$, $0 < x < a$, $y(0) = y(a) = 0$; then a sufficient condition for $\sigma(L_h)$ to satisfy properties* (A1) *and* (A2) *is that*

$$\lim_{h \to 0} \sup_{\substack{\psi \in H_h \\ \|\psi\| = 1 \\ z = A\psi}} |r_h Lz - L_h r_h z|_h = 0.$$

Furthermore, property (A1) *is satisfied for every isolated eigenvalue of L.*

For unbounded domains, our findings are based on Galerkin finite element approximation. Define first $\pi\colon H^1(0, \infty) \to H_h$, the a-projector, by the relation

$$a(f, \psi) = a(\pi_h f, \psi), \quad \forall \psi \in H_h.$$

Then

$$A_h = \pi_h A \,|_{H_h}\colon H_h \to H_h$$

is the Galerkin approximation.

The following lemma is fundamental.

LEMMA 2.4. *The Galerkin approximation $A_h = \pi_h A|_{H_h}$ and the interpolatory approximation $C_h = I_h A_X|_{H_h}$ satisfy property* (P).

Proof. From the relation

$$a((A_h - C_h)\psi, \phi) = a_h(A_X\psi - I_h A_X\psi, \phi), \quad \forall \psi, \phi \in H_h,$$

one obtains

$$\|(A_h - C_h)\psi\| \leqslant c\|A_X\psi - I_h A_X\psi\|_X.$$

Lemma 2.3 yields our results. □

As a consequence one obtains

COROLLARY 2.2. *Consider the difference operator L_h used to compute the eigenvalues of the operator L defined by*

$$Ly = -y'' + q(x)y, \qquad 0 < x < \infty, \; y(0) = 0, \; y \text{ bounded}.$$

If L_h is chosen such that

$$\lim_{h \to 0} \sup_{\substack{\psi \in H_h \\ \|\psi\| = 1 \\ z = A_X\psi}} |r_h L_X z - L_h r_h z|_h = 0,$$

then L_h satisfies (A1) *and* (A2) *whenever the Galerkin approximation $G_h = A_h^{-1} - \gamma$ satisfies* (A1) *and* (A2).

This corollary enables us to use previous results obtained earlier for Galerkin approximations. In particular, by use of the Courant principle [2] and the notion of essential numerical range, Descloux [3] has clearly demonstrated that one obtains (A1) and (A2) for Galerkin approximations outside the essential numerical range ξ. In the particular case where q satisfies (Q)(1)–(Q)(3), ξ is exactly the interval $[0, 1/\gamma]$, which forms the continuous spectrum.

Outside such an interval, A has only isolated eigenvalues that can be approximated by the Galerkin method, and therefore by the difference operator L_h satisfying property (N).

2.4. *Verification of* (N) *for Numerov's Scheme.* Using the notations of Lemma 1.6, we write $\sigma_h = r_h L_X z - L_h r_h z$ for $z = A_X \psi$, $\psi \in U_h$.

We consider also the linear transformation in R^{N-1}, R_h, represented by the tridiagonal matrix

$$\frac{1}{12} \begin{pmatrix} 10 & 1 & & & & \\ & & & & & 0 \\ 1 & 10 & & \ddots & & \\ & & & & & \\ & & \ddots & \ddots & 1 & \\ & & & & & \\ 0 & & & 1 & 10 \end{pmatrix}.$$

Note that

$$(R_h \sigma_h)_i = -\left(z_{i-1}'' + 10 z_i'' + z_{i+1}''\right)/12$$

$$+ \left(z_{i-1} - 2z_i + z_{i+1}\right)/h^2, \qquad 1 \leqslant i \leqslant N - 1.$$

$(R_h \sigma_h)_i$ can be found to have the following expression:

$$(R_h \sigma_h)_i = \frac{1}{2h^2}\left[\int_{x_i}^{x_{i+1}} (x - x_i)^2 z'''(x)\, dx - \int_{x_{i-1}}^{x_i} (x - x_i)^2 z'''(x)\, dx\right]$$

$$+ \frac{1}{12}\left[\int_{x_i}^{x_{i+1}} z'''(x)\, dx - \int_{x_{i-1}}^{x_i} z'''(x)\, dx\right].$$

This leads to the following

LEMMA 2.5. *Assuming $z''' \in L^2(0, X)$, one has*

$$|R_h \sigma_h|_h \leqslant \alpha_0 h \left\{\int_0^X |z'''|^2\, dt\right\}^{1/2} \quad \text{with } \alpha_0 = \frac{1}{6} + \frac{4}{\sqrt{5}}.$$

Proof. Use standard arguments based on energy inequalities.   □

On the basis of Lemma 2.5 one obtains

LEMMA 2.6. *Under the assumptions* (Q)(1)–(Q)(3) *one has*

$$\lim_{h \to 0} \sup_{\substack{\psi \in H_h \\ z = A_X \psi \\ \|\psi\| = 1}} |r_h L_X z - L_h r_h z|_h = 0.$$

Proof. Since $-z'' + q(x)z = \psi$, $0 < x < X$, differentiation yields $z''' = q'z + qz' - \psi'$. Hence,

$$\left\{ \int_0^X |z'''|^2 \, dx \right\}^{1/2} \leqslant \left\{ \int_0^X (q'z)^2 \, dx \right\}^{1/2} + \left\{ \int_0^X (qz')^2 \, dx \right\}^{1/2}$$
$$+ \left\{ \int_0^X \psi'^2 \, dx \right\}^{1/2}.$$

From (Q)(1)–(Q)(3) one concludes

$$|z'''|_{L^2(0,X)} \leqslant l|z|_{L^2(0,X)} + M|z'|_{L^2(0,X)} + |\psi'|_{L^2(0,X)}.$$

Using standard energy inequalities, one may bound $|z|_{L^2(0,X)}$ and $|z'|_{L^2(0,X)}$ in terms of $|\psi|_{L^2(0,X)}$ which leads to

$$\left\{ \int_0^X |z'''|^2 \, dx \right\}^{1/2} \leqslant c\|\psi\|.$$

Lemma 2.5 completes the proof, as all the positive eigenvalues of R_h are bounded independently of h. $\square$

This proves

THEOREM 2.2. *Under the assumptions* (Q)(1)–(Q)(3), *the Numerov scheme satisfies condition* (A1) *for every isolated eigenvalue of finite multiplicity, and* (A2) *for every compact set of the resolvent set* $\zeta(L)$.

2.5. *Verification of* (N) *for the Central Difference Operator for the Regular Sturm-Liouville Operator.* For the purpose on hand, we apply Corollary 2.1 to the difference scheme (1.12)–(1.13) for the approximate solution of (1.11). To complete our notations, let

$$f \in L^2(a, b), \quad |f| = \left\{ \int_0^\infty |f(x)|^2 \, dx \right\}^{1/2},$$

$$f \in H^1(a, b), \quad \|f\| = \left\{ |f|^2 + |f'|^2 \right\}^{1/2},$$

$$f_h \in R^{N-1}, \quad |f_h|_h = \left\{ \sum_{i=1}^{N-1} h|f_{h_i}|^2 \right\}^{1/2}.$$

Moreover, the definitions of Subsection 2.1 with respect to H_h and R^{N-1} are maintained, and therefore relations (2.4) and (2.5) remain valid. To analyze the discretization error over the set of solutions $z(x)$ of

(2.9)
$$-(q(x)z')' + s(x)z = p(x)\psi(x), \quad a < x < b,$$
$$z(a) = z(b) = 0,$$

where $\psi \in H_h$, we use the following argument. Assuming $p, s \in H^1(a, b)$, $q \in H^2(a, b)$ and therefore $z \in H^3(a, b)$, $qz' \in H^2(a, b)$, one writes

$$\delta_{h/2}(q_i \delta_{h/2} z_i) = (q(x) z')_{x=x_i} + \frac{1}{h} \int_{x_{i-1/2}}^{x_{i+1/2}} (x - x_i)(q(x) z')'' dx$$

$$(2.10) \qquad\qquad + \frac{1}{2h^2} \left[q_{i+1/2} \int_{x_i}^{x_{i+1}} (x - x_{i+1/2})^2 z''' dx \right.$$

$$\left. - q_{i-1/2} \int_{x_{i-1}}^{x_i} (x - x_{i-1/2})^2 z''' dx \right].$$

If

$$\sigma_h = r_h L z - L_h r_h z,$$

then

$$\sigma_{h,i} = -(q(x) z')_{x=x_i} + \delta_{h/2}(q_i \delta_{h/2} z_i), \qquad 0 < i < N.$$

Using (2.10), one obtains by standard techniques the following lemma.

LEMMA 2.7. *Assuming $z \in H^3(a, b)$, $qz' \in H^2(a, b)$, the discretization error of the difference scheme (1.12)–(1.13) for (2.9) satisfies*

$$|r_h L z - L_h r_h z|_h \leqslant \frac{h}{2 \underline{p}} \max\{1, \bar{q}\} \left\{ 2|z'''|^2 + |(qz')''|^2 \right\}^{1/2}.$$

Again, using energy inequalities, one bounds the right-hand side of Lemma 2.7 in terms of $\|\psi\|$, which leads to

THEOREM 2.3. *Under the assumptions of Lemma 2.7, the central difference scheme for the regular Sturm-Liouville problem satisfies condition* (A1) *for each eigenvalue, and* (A2) *for every compact set of the resolvent set.*

2.6. *Condition* (N) *for a 2-dimensional case.* Consider the problem of finding the eigenvalues of the differential operator L defined for a function $u(x, y)$ by

$$(2.11) \qquad L u = -\Delta u = -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2}, \qquad (x, y) \in D,$$

$$(2.12) \qquad u(x, y) = 0, \qquad (x, y) \in \partial D,$$

where

$$D = \{(x, y) \mid 0 < x < a, 0 < y < b\}.$$

Define the spaces $L^2(D)$ with norm $|\cdot|$ and inner product $[\cdot, \cdot]$, and $H^1(D)$ with norm $\|\cdot\|$ and inner product $(\cdot, \cdot)$. Let

$$H_0^1(D) = \{\phi \in H^1(D) \mid \phi = 0 \text{ on } \partial D\}.$$

With $h = (h_1, h_2) \in (0, 1) \times (0, 1)$, define the discrete domain

$$D_h = \{(x_i, y_j) \mid x_i = ih_1, \ y_j = jh_2, 0 < i < M, 0 < j < N, i, j \text{ integers}\}.$$

For $u_h \equiv \{u_{h,i,j}\}_{0 \leqslant i \leqslant M, 0 \leqslant j \leqslant N}$ define the five-point difference operator $-\Delta_h$ given for u_h: $D_h \to R$ by

$$(2.13) \qquad (-\Delta_h u_h)_{i,j} = (2u_{i,j} - u_{i-1,j} - u_{i+1,j})/h_1^2$$

$$+ (2u_{i,j} - u_{i,j-1} - u_{i,j+1})/h_2^2, \qquad i, j \in D_h,$$

$$(2.14) \qquad\qquad u_{h,i,j} = 0, \qquad i, j \in \partial D_h$$

(for simplicity we have written $u_{h,i,j} = u_{i,j}$). (2.13) and (2.14) can be reduced to finding the eigenvalues of the operator L_h: $R^{M-1} \times R^{N-1} \to R^{M-1} \times R^{N-1}$.

Let also

$$H_h = \left\{ \psi_h \in H^1(D) \cap C(D) \mid \psi_h = 0 \text{ on } \partial D, \right.$$

$$\left. \psi_h(x, y) = a + bx + cy + dxy, x, y \in D_{i,j}, 0 \leqslant i < M, 0 \leqslant j < N \right\},$$

with $D_{i,j} = \{(x, y) \in D \mid x_i \leqslant x \leqslant x_{i+1}, y_j \leqslant y \leqslant y_{j+1}\}$. H_h is the well-known piecewise bilinear space.

Note that $H_h \subset H_0^1(D)$; furthermore, $\psi \in H_h$, $\psi_{xy} \in L^2(D)$. On H_h consider the discrete norm $| \cdot |_h$ defined by

$$|\psi|_h = \left\{ \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} h_1 h_2 |\psi_{i,j}|^2 \right\}^{1/2},$$

induced by the discrete inner product

$$[\psi, \phi]_h = \sum_{i=1}^{M-1} \sum_{j=1}^{N-1} h_1 h_2 \psi_{i,j} \phi_{i,j},$$

where

$$\psi_{i,j} \equiv \psi_h(x_i, y_j), \qquad \phi_{i,j} \equiv \phi_h(x_i, y_j);$$

r_h: $H^1(D) \cap C(D) \to R^{M-1} \times R^{N-1}$ is defined by

$$(r_h f)_{i,j} = f(x_i, y_j), 0 < i < M, 0 < j < N.$$

Note that $| \cdot |_h$ can be considered as a norm on $R^{M-1} \times R^{N-1}$. Let σ_h be the discretization error, defined for $z \in C^2(D)$ by

$$\sigma_h(z) = r_h L z - L_h r_h z.$$

Our basic result is that L_h defined in (2.13), (2.14) satisfies condition (N). This will imply the stability results (A1)–(A2) for the 5-point difference scheme used to approximate the frequencies of vibration of the operator $-\Delta$. This is summarized in

THEOREM 2.4. *We have*

$$\lim_{h \to 0} \sup_{\substack{\psi \in H_h \\ \|\psi\| = 1 \\ z = A\psi}} |r_h L z - L_h r_h z|_h = 0.$$

Several preliminary results are needed, which we simply summarize to avoid technical details.

LEMMA 2.8. *There exists a constant c independent of h such that*

$$|\sigma_h|_h^2 \leqslant c \left(h_1^2 |z_{xxx}|^2 + h_2^2 |z_{yyy}|^2 + h_1^2 h_2 |z_{xxxy}|^2 + h_2^2 h_1 |z_{yyyx}|^2 \right).$$

If z is the solution of $-\Delta z = \psi \in H_h$, $z = 0$ on ∂D, then using Fourier analysis one proves that

$$(2.15) \qquad \begin{aligned} |z_{xxx}|^2 &\leqslant |\psi_x|^2, & |z_{yyy}|^2 &\leqslant |\psi_y|^2, \\ |z_{xxxy}|^2 &\leqslant |\psi_{xy}|^2, & |z_{yyyx}|^2 &\leqslant |\psi_{xy}|^2, \end{aligned}$$

and by standard calculation on the subspace H_h one gets

(2.16) $\left| \psi_{xy} \right| \leqslant \dfrac{c}{h_1} \left| \psi_y \right|$, c independent of h.

Combining Lemma 2.8 with (2.15) and (2.16), one obtains

LEMMA 2.9. *There exists a constant c independent of h such that*

$$\left| r_h L z - L_h r_h z \right|_h^2 \leqslant c \left(h_1^2 + h_2^2 + h_1 + h_2 \right) \| \psi \|^2,$$

where

$$-\Delta z = \psi \in H_h, \qquad z = 0 \quad on \; \partial D.$$

Consequently, one obtains Theorem 2.4.

Department of Mathematics
American University of Beirut
Beirut, Lebanon

1. J. H. BRAMBLE & J. E. OSBORN, "Rate of convergence estimates for nonselfadjoint eigenvalue approximations," *Math. Comp.*, v. 27, 1973, pp. 525–549.

2. F. CHATELIN, *Théorie de l'Approximation des Opérateurs Linéaires, Application au Calcul des Valeurs Propres d'Opérateurs Différentiels et Intégraux*, Lecture Notes, Grenoble University, 1977.

3. J. DESCLOUX, "Essential numerical range of an operator with respect to a coercive form and the approximation of its spectrum by the Galerkin method," *SIAM J. Numer. Anal.*, v. 18, 1981, pp. 1128–1133.

4. J. DESCLOUX, N. R. NASSIF & J. RAPPAZ, "On spectral approximation, Part 1: The problem of convergence; Part 2: Error estimates for the Galerkin method," *RAIRO Anal. Numér.*, v. 12, 1978, pp. 97–112; pp. 113–119.

5. J. DESCLOUX, N. R. NASSIF & J. RAPPAZ, "On properties of spectral approximations," in *Equadiff IV*, Lecture Notes in Math., vol. 703, Springer-Verlag, Berlin and New York, 1977, pp. 81–85.

6. R. D. GRIGORIEFF, "Diskrete Approximation von Eigenwertproblemen, Part 1: Qualitative Konvergenz; Part 2: Konvergenzordnung; Part 3: Asymptotische Entwicklungen," *Numer. Math.*, v. 24, 1975, pp. 355–374; pp. 415–453; v. 25, 1975, pp. 79–97.

7. H. O. KREISS, "Difference approximations for boundary and eigenvalue problems for ordinary differential equations," *Math. Comp.*, v. 26, 1972, pp. 605–624.

8. B. V. NUMEROV, *Monthly Notices Roy. Astronom. Soc.*, v. 84, (180), 1924, p. 592.

9. E. C. TITCHMARSH, *Eigenfunction Expansions*, Oxford Univ. Press, London, 1962.

10. J. E. OSBORN, "Spectral approximations for compact operators," *Math. Comp.*, v. 29, 1975, pp. 712–725.

11. G. STRANG & G. J. FIX, *An Analysis of the Finite Element Method*, Prentice-Hall, Englewood Cliffs, N. J., 1973.

12. F. STUMMEL, "Elliptische Differenzenoperatoren unter Dirichlet Randbedingungen," *Math. Z.*, v. 97, 1967, pp. 169–211.

13. G. M. VAINIKKO, "A difference method for ordinary differential equations," *U.S.S.R. Comput. Math. and Math. Phys.*, v. 9, 1969, pp. 1–32.

14. J. H. WILKINSON, *The Algebraic Eigenvalue Problem*, Oxford Univ. Press, London, 1965.