A STUDY OF THE COMPUTATION AND CONVERGENCE
BEHAVIOR OF EIGENVALUE BOUNDS
FOR SELF-ADJOINT OPERATORS

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Dissertation submitted to the Faculty of the
Virginia Polytechnic Institute and State University
in partial fulfillment of the requirements for the degree of
DOCTOR OF PHILOSOPHY
in
Mathematics

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May, 1991
Blacksburg, Virginia
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(ABSTRACT)

The convergence rates for the method of Weinstein and a variant method of
Aronszajn known as "truncation including the remainder" are derived in terms of
the containment gaps between exact and approximating subspaces, using analytical
techniques that arise in part in the convergence analysis of finite element methods
for differential eigenvalue problems. An example of a one dimensional Schrödinger
operator with a potential is presented which arises in quantum mechanics.

Examples using the recent eigenvector-free (EVF) method of Beattie and Goerisch
are considered. Since the EVF method uses finite element trial functions as approxi-
mating vectors, it produces sparse and well-structured coefficient matrices. For these
large-order sparse matrix eigenvalue problems, we adapt a spectral transformation
Lanczos algorithm for finding a few wanted eigenvalues. For a few particular examples
of vibration in beams and plates, convergence behavior is experimentally evaluated.
ACKNOWLEDGEMENTS

It is very pleasure for me to thank my advisor, Professor Christopher A. Beattie for his guidance and support. In the last three years I have been really indebted to him for having provided me a lot of knowledge on mathematics.

It is also my pleasure to thank my wife, Hyun-Sook, for her constant aid and patience.
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CHAPTER 1
PRELIMINARIES

1.1 Introduction.

It is important to compute accurately the eigenvalues and eigenvectors of differential operators in order to analyze successfully various natural phenomena. We easily find many examples including the frequencies of bars, beams and plates, critical values of the Reynolds number in hydrodynamics, and bound state energy levels of atoms and molecules. The importance of such problems has encouraged mathematicians to study methods for finding the eigenvalues of differential operators. However, the eigenvalues are not explicitly known in most cases, and thus several methods for their approximation have been presented and developed over many years. Since there is no method that provides precise error estimation in approximation, the only reliable way may be to use two ancillary methods that give upper and lower bounds, respectively, to the eigenvalues considered. In their analysis, we meet equations of the style \( Au = \lambda u \) in \( \Omega \), where \( A \) is considered as a semi-bounded self-adjoint operator on a Hilbert space, having eigenvalues of finite multiplicity below the lowest limit point (if any) of the spectrum.

Historically, in the last quarter of the 19th century, Lord Rayleigh had initiated a development in the approximation of eigenvalues, based on the so-called Rayleigh Principle which states that if one limits the freedom of vibration of a mechanical system, the frequencies of the obtained system can not be lower than those of the original system [55]. In 1909 W. Ritz illustrated that by choosing a constrained system with a finite but sufficiently large number of degrees of freedom, arbitrarily close approximations to the lower eigenvalues of the original continuous system could
be obtained. This observation leads to the oldest method for obtaining numerical upper bounds called the Rayleigh-Ritz method [44]. A much more difficult problem is that of finding accurate lower bounds, for which we will consider the method of intermediate eigenvalue problems, which gives a sequence of improvable lower bounds.

In 1937 A. Weinstein developed a method for finding lower bounds for the eigenvalues of certain differential operators [72]. This method was extended and simplified by N. Aronszajn in 1948 by use of the properties of compact self-adjoint operators in Hilbert space [2]. However, it initially proved to be very difficult to implement Aronszajn's method numerically. In 1959 N. Bazley achieved the first major innovation in the implementation of Aronszajn's method with the development of the method of special choice [7]. In the same year H. Weinberger published a method for improvable lower bounds and a method for simplifying the calculations involved in Weinstein's method [67]. Subsequently Bazley together with D. Fox developed a number of means for implementing Aronszajn's method for differential problems [8-14]. Very recently, Beattie and Goerisch have developed a method for finding lower bounds without having knowledge of eigenvectors of a base problem which otherwise are necessary in most intermediate eigenvalue problems [17]. Using both the Rayleigh-Ritz method and the intermediate problem method, one is able to find an interval, whose length can be made as small as desired, guaranteed to contain a selected eigenvalue.

This dissertation concentrates on both the usual method of intermediate problems as well as Beattie and Goerisch's eigenvector free (EVF) method, which may be found to be of use in classical and quantum mechanical eigenvalue problems that involve complex domain geometry or realistic potentials. Since we limit our attention to problems which can be formulated in terms of self-adjoint operators in Hilbert space, our approach will be operator theoretic in nature.

Section 2 presents some background for the variational approaches and Section 3
gives a brief explanation of the intermediate problem method. Section 4 contains some remarks. Chapter 2 introduces new results about convergence rates for a sequence of semi-bounded operators, which are applied to intermediate problems together with the method of *truncation including remainder* and also presents an example which comes from quantum mechanics. In Chapter 3 we deal with the Beattie and Goerisch EVF method with numerical examples that arise from the vibration of beams, and also analyze how to take advantage of the sparsity of a large-order matrix which comes from the EVF method as using finite element trial functions with an example of the vibration of a rectangular clamped plate.
1.2 Variational Principles of Eigenvalue Approximation.

In this section we outline the development of the variational principles for eigenvalues. Let $\mathcal{H}$ be a separable complex Hilbert space with norm $\|u\|$ and inner product $\langle u, v \rangle$. Let $A$ be a self adjoint operator with domain $\text{Dom}(A)$ dense in $\mathcal{H}$. We suppose that $A$ is bounded below and that the lower part of its spectrum consists of a finite or infinite number of isolated eigenvalues

$$\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_\infty$$

each having finite multiplicity. Here $\lambda_\infty$ denotes the lowest limit point (if any) of the spectrum of $A$. For convenience we denote such a class of operators by $S$. If $A$ has compact resolvent, then we set $\lambda_\infty = \infty$ (We say that $A$ has compact resolvent if $(A - z)^{-1}$ is compact for any $z \in \rho(A)$).

We note that many operators that arise in the eigenvalue problems of mathematical physics and engineering are in $S$ for some choice of Hilbert space $\mathcal{H}$. The lower eigenvalues of such operators have classical characterizations for which the oldest one is originally due to Lord Rayleigh [55] and Weber [63].

**Theorem 1.2.1.** (Rayleigh-Weber) The eigenvalues of $A \in S$ are given by the equations

$$\lambda_1 = \min_{u \in \text{Dom}(A)} \frac{\langle Au, u \rangle}{\langle u, u \rangle} \quad \text{and} \quad \lambda_n = \min_{\substack{u \in \text{Dom}(A) \setminus \{0\} \atop \langle u, u_i \rangle = 0 \atop i = 1, \ldots, n-1}} \frac{\langle Au, u \rangle}{\langle u, u \rangle},$$

where $u_1, u_2, \ldots, u_{n-1}$ denote eigenvectors corresponding to $\lambda_1, \lambda_2, \ldots, \lambda_{n-1}$.

We may find a modern proof of Theorem 1.2.1 in [73] and an extension of this result to semi-bounded, closed quadratic forms in [68] that is frequently more useful. It directly follows from Theorem 1.2.1 that for a unit vector $v_0 \in \text{Dom}(A)$, the value $\langle Av_0, v_0 \rangle$ provides an upper bound to the lowest eigenvalue $\lambda_1$. For more improved bounds to $\lambda_1$, we can take a sequence of orthonormal vectors $\{v_i\}_{i=1}^\infty \subset \text{Dom}(A)$
and compute the lowest eigenvalue of the matrices \([\langle Av_i, v_j \rangle]_{i,j=1}^n\) for \(n = 1, 2, \ldots\) successively.

While the classical characterization is very important as an analytical device, it has the disadvantage that it may not be used to determine higher eigenvalues without employing explicitly all preceding eigenvectors. Nearly a quarter of a century after the classical principle was given, the situation was considerably improved by Poincaré [50], who developed the Rayleigh-Weber result into a set of inequalities relating the eigenvalues of \(A\) to the eigenvalues of a finite-dimensional restriction of \(A\). For this purpose, we let \(\mathcal{P}_n\) be a \(n\)-dimensional subspace of \(\text{Dom}(A)\) with \(P_n\) representing the related orthogonal projection onto \(\mathcal{P}_n\). Then \(P_nAP_n\) is self-adjoint as a transformation from the finite-dimensional space \(\mathcal{P}_n\) into itself. If we consider \(P_nAP_n\) as an operator on \(\mathcal{H}\), its spectrum consists of the eigenvalues \(\Lambda_1, \Lambda_2, \ldots, \Lambda_n\) as well as the eigenvalue \(\Lambda = 0\) with infinite multiplicity.

**Theorem 1.2.2.** (Poincaré) For any \(n\)-dimensional space \(\mathcal{P}_n\), the eigenvalues \(\{\Lambda_i\}_{i=1}^n\) of \(P_nAP_n\) satisfy the inequalities

\[
\lambda_1 \leq \Lambda_1, \lambda_2 \leq \Lambda_2, \ldots, \lambda_n \leq \Lambda_n.
\]

Fischer [34] applied the Poincaré's inequalities for finite-dimensional spaces while Pólya [51] applied them to operators in infinite-dimensional spaces. The inequalities were formulated as a so-called minimum-maximum principle.

**Theorem 1.2.3.** (Fischer-Pólya : Minimum-Maximum Principle) The eigenvalues of \(A \in S\) may be characterized as

\[
\lambda_n = \min_{\mathcal{P}_n \subset \text{Dom}(A)} \max_{\dim \mathcal{P}_n = n} \frac{\langle Av_i, u \rangle}{\langle u, u \rangle}.
\]

As a related application of Theorem 1.2.2 or Theorem 1.2.3, we have an outstanding method for obtaining upper bounds for eigenvalues known as the Rayleigh-Ritz
method. This method provides an efficient means of computing nonincreasing upper bounds for an arbitrary but finite number of eigenvalues of any operator in class $S$. The main idea of this method is to restrict a given operator to a finite-dimensional subspace of its domain, yielding a matrix problem for which the eigenvalues are numerically computable. It follows then from Theorem 1.2.2 that the computed eigenvalues are all upper bounds to the corresponding eigenvalues of the given operator [73].

**Theorem 1.2.4. (Rayleigh-Ritz Method)** Let $\mathcal{P}_n = \text{span}\{p_1, p_2, \ldots, p_n\}$. Then the eigenvalues $\{\lambda_i\}_{i=1}^n$ of $\mathcal{P}_nA\mathcal{P}_n|_{\mathcal{P}_n}$ are the solutions to the general matrix eigenvalue problem in $\mathbb{C}^n$

$$[(Ap_i, p_j)]x = \lambda[(p_i, p_j)]x$$

for all $i, j = 1, \ldots, n$.

We have from this result an easy approach for finding upper bounds to the lower eigenvalues of $A$. With only these upper bounds it is difficult to realize how close they are to the eigenvalues of $A$. Thus we need rigorous lower bounds subsidiary to the upper bounds. For this we present an alternate characterization of the lower eigenvalues of $A$ that originally comes from an inequality of Weyl [74], which later was applied by Courant [31].

**Theorem 1.2.5. (Weyl's Inequality)** For any choice of vectors $p_1, p_2, \ldots, p_{n-1} \in \mathcal{H}$, we have the inequality

$$\min_{\substack{u \in \text{Dom}(A) \\ (u, p_i) = 0 \\ i=1,2,\ldots,n-1}} \frac{(Au, u)}{(u, u)} \leq \lambda_n.$$

Let us note in passing that the value in the left of Theorem 1.2.5 is the lowest eigenvalue of a problem $Au - PAu = \lambda u$ restricted to $Pu = 0$, where $P$ is the orthogonal projection onto the space spanned by $\{p_1, p_2, \ldots, p_{n-1}\}$, say $\mathcal{P}$ (cf. [73]).
THEOREM 1.2.6. (Courant-Weyl: Maximum-Minimum Principle) The eigenvalues of $A \in S$ are given by the equation

$$\lambda_n = \max_{P_1 \in \mathcal{H}} \min_{\substack{u \in \text{Dom}(A) \cap P_i = 0 \atop (u, p_i) = 0 \atop i = 1, \ldots, n-1}} \frac{\langle Au, u \rangle}{\langle u, u \rangle}.$$ 

for $n = 2, 3, \ldots$.

If $\mathcal{H}$ is a finite-dimensional space, the maximum-minimum principle and the minimum-maximum principle are in a sense equivalent, which is essentially due to the fact that in this case the orthogonal complement of a finite-dimensional space is itself finite-dimensional. But Theorem 1.2.6 (Max-min principle) is very different from Theorem 1.2.3 (Min-max principle) in spite of similarities in statement. The reason is mainly the usual infinite-dimensionality of the orthogonal complement to the space $\mathcal{P}$. The existence of the minimum in Theorem 1.2.5 has been proved recently for $A \in S$ [73]. The computational difficulties in obtaining rigorous lower bounds come from the infinite-dimensionality of $\mathcal{P}^\perp$. For example, let us take a finite-dimensional subspace $\mathcal{R}_m \subset \text{Dom}(A)$ with $\dim \mathcal{R}_m = m \leq n - 1$ (cf. [15]). Then

$$\lambda_n \leq \max_{\dim \mathcal{P} = n-1} \min_{u \in \mathcal{P}^\perp \cap \mathcal{R}_m} \frac{\langle Au, u \rangle}{\langle u, u \rangle} = \max_{\dim \mathcal{P} = n-m-1} \min_{u \in \mathcal{P}^\perp \cap \mathcal{R}_m^\perp} \frac{\langle Au, u \rangle}{\langle u, u \rangle}.$$ 

The right-hand side may be identified with the $(n-m)$-th eigenvalue of

$$Au - R_m Au = \lambda u \quad \text{with} \quad R_m u = 0$$ 

where $R_m : \mathcal{H} \rightarrow \mathcal{R}_m$ is the orthogonal projection. However $(A - R_m A)|_{R_m^\perp}$ is generally not a finite rank operator and does not usually have clear finite dimensional reducing spaces. Hence this approach does not seem to result in a computationally practical strategy. We now present an important application of the minimum-maximum principle.
**Definition.** Let \( \mathcal{P} \) be a closed subspace of \( \mathcal{H} \) and let \( P : \mathcal{H} \to \mathcal{P} \) be the orthogonal projection onto \( \mathcal{P} \). Let \( Q = I - P \). We say that \( A - PA \) on \( \mathcal{P}^\perp \) is the part of \( A \) in \( \mathcal{P}^\perp \), and that \( QAQ \) is the projection of \( A \) onto \( \mathcal{P}^\perp \).

**Theorem 1.2.7.** (Rayleigh's Theorem for r Constraints [44]) Let \( \mathcal{P} \) be an \( r \) dimensional subspace of \( \mathcal{H} \) and let \( P \) be the orthogonal projection onto \( \mathcal{P} \). Let \( \{\lambda'_i\} \) be the eigenvalues of the part of \( A \) in \( \mathcal{P}^\perp \) arranged in increasing order according to multiplicity. Then for all \( i = 1, 2, \ldots \),

\[
\lambda_i \leq \lambda'_i \leq \lambda_{i+r}.
\]

If \( A \) is self-adjoint, then the part of \( A \) is also self-adjoint [73]. The following theorems come from Theorems 1.2.3 or 1.2.7 and have important roles in the analysis of intermediate problems which follows in the next sections.

**Theorem 1.2.8.** (First Monotonicity Principle) Let \( A \) be an operator in \( S \) and \( A' \) be a part of \( A \) in the subspace \( Q \) of \( \mathcal{H} \). Then the eigenvalues \( \lambda'_i \) and \( \lambda_i \) of \( A' \) and \( A \), respectively, satisfy the inequalities

\[
\lambda_i \leq \lambda'_i
\]

for all \( i = 1, 2, \ldots \),

**Definition.** For symmetric operators \( S \) and \( T \) we define \( S \leq T \) if \( \text{Dom}(T) \subset \text{Dom}(S) \) and \( \langle Su, u \rangle \leq \langle Tu, u \rangle \), for all \( u \in \text{Dom}(T) \).

**Theorem 1.2.9.** (Second Monotonicity Principle) Let \( A' \) and \( A \) be operators of class \( S \) satisfying \( A \leq A' \). Then the eigenvalues \( \lambda'_i \) and \( \lambda_i \) of \( A' \) and \( A \), respectively, satisfy the inequalities

\[
\lambda_i \leq \lambda'_i
\]

for all \( i = 1, 2, \ldots \).
1.3 Construction of Intermediate Eigenvalue Problems.

In this section we review the methods presented by Weinstein in 1935 with his work on the estimation of buckling loads and vibration frequencies for plates [68–71] and by Aronszajn in 1951 [2] who proposed a similar estimation procedure for obtaining lower bounds that was applicable to a much wider class of eigenvalue problems than Weinstein’s procedure. As a variant of Aronszajn’s method, we present the method of truncation including the remainder which was first analyzed by Greenlee [43] and developed further by Greenlee and Beattie [19,20]. Finally we also present a variant of the Aronszajn method which was initiated by Bazley and Fox [10].

The scheme of intermediate problems is the following: Given an eigenvalue problem for an operator $A$ of type $S$, the first step is to find a base operator $A_0$ in $S$ whose eigenvalues are not greater than the corresponding eigenvalues of the given operator. The next step is to construct a sequence of eigenvalue problems, called intermediate eigenvalue problems, in such a way that they yield computable eigenvalues which are not smaller than those of the preceding problem in the sequence, not greater than those of the succeeding problem, and never greater than the eigenvalues of the original problem. The base problem

$$A_0u = \lambda u$$

is picked so that $A_0$ is in $S$ and $A_0 \leq A$. We assume that the isolated eigenvalues of the base problem

$$\lambda^0_1 \leq \lambda^0_2 \leq \cdots \leq \lambda^0_\infty$$

are computable to arbitrary precision. The closure of the quadratic form $(A_0u, u)$ is denoted by $a_0(u)$. Then $a_0(u) \leq a(u)$ for all $u \in Dom(a) \subset Dom(a_0)$. The second monotonicity principle implies that $\lambda^0_\infty \leq \lambda_\infty$, and that for each $i$ such that $\lambda_i < \lambda^0_\infty$, $\lambda_i^0$ exists and $\lambda_i^0 \leq \lambda_i$. Without loss of generality we may assume that the difference
between $a_0$ and $a$ is strictly positive, that is,

$$b(u) = a(u) - a_0(u) \geq \alpha \|u\|^2,$$

for some $\alpha > 0$ and all $u \in \text{Dom}(b) = \text{Dom}(a) \subset \text{Dom}(a_0)$.

We should note that most suitable base problems having computable eigenvalues and eigenvectors produce very poor and fixed bounds. The intermediate problem methods provide an approach for adding back incrementally what was lost in passing from $A$ to $A_0$ in a way that permits explicit resolution of the intermediate eigenvalue problems to improve lower bounds to the eigenvalues of $A$.

1.3.1 On the method of Weinstein. We suppose that the quadratic forms $a_0$ and $a$ are closed, densely defined and coercive in $\mathcal{H}$ such that $a_0(u) \leq a(u)$ for all $u \in \text{Dom}(a) \subset \text{Dom}(a_0)$. Then the corresponding self-adjoint operator $A_0$ is positive definite and the Hilbert space $\mathcal{H}_a$, which is the completion of $\text{Dom}(A_0)$ with respect to norm generated by $a_0(u,v)$, is continuously embedded in $\mathcal{H}$. The similarly defined Hilbert space $\mathcal{H}_a$ may be considered as a closed subspace of $\mathcal{H}_a$ (cf. [27]).

We assume that $P : \mathcal{H}_a \to \mathcal{H}_a \oplus \mathcal{H}_a$ is the $a_0$-orthogonal projection onto $\mathcal{H}_a \oplus \mathcal{H}_a$ and that $A = A_0 - PA_0$ on $\text{Dom}(A) \subset \text{Dom}(A_0)$. We note [45, 73] that the spectral resolution of the projection of $A_0$ to $\mathcal{H}_a$, $QA_0Q$, is obtained from the spectral theorem for the part of $A_0$ in $\mathcal{H}_a$ and adjoining the eigenvalue zero on $\mathcal{H}_a \oplus \mathcal{H}_a$. Here $Q = I - P : \mathcal{H}_a \to \mathcal{H}_a$ is a projection. Thus the positive eigenvalues of $QA_0Q$ are just those of $QA_0|\mathcal{H}_a$. Hence $A$ may be considered as $QA_0Q$, and the first monotonicity theorem implies that the base problem, $A_0u = \lambda u$, yields lower bounds to the eigenvalues of $A$. Let us take a sequence of finite dimensional subspaces, $\{\mathcal{P}_i\}$, in the orthogonal complement of $\mathcal{H}_a$ in $\mathcal{H}_a$,

$$\mathcal{P}_1 \subset \mathcal{P}_2 \subset \cdots \subset \mathcal{P}_k \subset \mathcal{P}_{k+1} \subset \cdots \subset \mathcal{H}_a \oplus \mathcal{H}_a$$
and let $P_k : \mathcal{H}_{a_0} \longrightarrow \mathcal{P}_k$ be the orthogonal projection. We now construct the intermediate operators as

$$A_k = Q_k A_0 Q_k$$

where $Q_k = I - P_k$. It follows [73] that if $A_0$ is compact, $Q_k A_0 Q_k$ is compact, and if $A \in S$, so is $Q_k A_0 Q_k$. The minimum-maximum principle provides that the eigenvalues of $A_k$ satisfy the inequality,

$$\lambda_i^0 \leq \cdots \leq \lambda_i^{(k)} \leq \lambda_i^{(k+1)} \leq \cdots \leq \lambda_i$$

for each $i$. That is, the intermediate operators provide improvable lower bounds to the eigenvalues of $A$ with increasing $k$.

The intermediate eigenvalue problem $A_k u = \lambda u$ on $\mathcal{P}_k^\perp$ yields the so-called Weyl-lstein matrix,

$$W_n(\lambda) = \langle R_\lambda^0 p_i, p_j \rangle,$$

where $R_\lambda^0 = (A_0 - \lambda)^{-1}$ and $\mathcal{P}_k = \text{span}\{p_1, p_2, \ldots, p_k\}$, because $P_k A_0 u \in \mathcal{P}_k$ and $Q_k$ is the identity on $\mathcal{P}_k^\perp$. The zeros and poles of the determinant of the matrix provide the eigenvalues of $A_k$. But a direct computation is obstructed by the difficulty in obtaining a functional expression for $R_\lambda^0 p_i$ in terms of $\lambda$. Using a truncation of $A_0$ as a base operator, we may overcome the difficulty [73].

1.3.2 On the method of Aronszajn. The method is designed for a different problem setting from the previous case. We recall that we have quadratic forms $a, a_0$ and $b$ such that

$$b(u) = a(u) - a_0(u) \geq \alpha \|u\|^2$$

for some $\alpha > 0$ and all $u \in \text{Dom}(b) = \text{Dom}(a) \subset \text{Dom}(a_0)$. Suppose that $b(u)$ is closable in $\mathcal{H}$ and denote its closure as $b$ again. There are densely defined self-adjoint operators, $A, A_0$ and $B$, associated with $a(u), a_0(u)$ and $b(u)$, respectively, such that
\( b(u, v) = \langle u, Bv \rangle \) for all \( u \in \text{Dom}(b) \) and \( v \in \text{Dom}(B) \). We assume that the operator \( A \) can be decomposed as the sum of two operators

\[
A = A_0 + B,
\]

where \( A_0 \) is a resolvable base operator. The theoretical basis for this scheme lies in the second monotonicity principle while that of the Weinstein lies in the first monotonicity principle. The main notion behind Aronszajn's method is to approximate \( B \) with finite rank perturbations of the resolvable operator \( A_0 \).

For this purpose we introduce a new Hilbert space \( \mathcal{H}_b \) which is the completion of \( \text{Dom}(B) \) in the norm generated by the new inner product \( \langle u, Bv \rangle \). Let a sequence of finite dimensional subspaces

\[
\mathcal{P}_1 \subset \mathcal{P}_2 \subset \cdots \subset \mathcal{P}_k \subset \mathcal{P}_{k+1} \subset \cdots \subset \text{Dom}(B)
\]

be given, and let \( P_k : \mathcal{H}_b \longrightarrow \mathcal{P}_k \) be the projection that is orthogonal with respect to the inner product \( \langle u, Bv \rangle \). That is, for any \( u \),

\[
P_ku = \sum_{i,j=1}^{k} \langle u, Bp_i \rangle b_{ij} p_j
\]

where the matrix \( (b_{ij}) \) is the inverse to the Gram matrix \( (\langle p_i, Bp_j \rangle) \) of order \( k \).

We now form the intermediate quadratic forms as

\[
a_k(u) = a_0(u) + b(P_ku)
\]

for all \( u \in \text{Dom}(a_k) = \text{Dom}(a_0) \) with the corresponding self-adjoint operators

\[
A_k = A_0 + BP_k,
\]

where \( k \) is called order of the intermediate operator. Since the operator \( BP_k \) is symmetric and bounded, it follows from [45, 64] that the operators \( A_k \) are self-adjoint.
and have the same domain as $A_0$. Moreover, since $BP_k$ is a compact operator, each of the operators $A_k$ has exactly the same limit points in its spectrum as does $A_0$ [58]. It follows from the boundedness of $BP_k$ that the operator $BP_k$ may be considered as an operator on the space $\mathcal{H}$ and thus we have

$$a_0(u) \leq \cdots \leq a_k(u) \leq a_{k+1}(u) \leq \cdots \leq a(u)$$

for all $u \in \text{Dom}(a) \subseteq \text{Dom}(a_k) = \text{Dom}(a_0)$. The second monotonicity theorem implies that the eigenvalues of $A_k$ satisfy the inequality,

$$\lambda_i^0 \leq \cdots \leq \lambda_i^{(k)} \leq \lambda_i^{(k+1)} \leq \cdots \leq \lambda_i$$

for all $i$ such that $\lambda_i \leq \lambda_0^0$. The eigenvalues of $A_k$ thus give lower bounds to the corresponding eigenvalues of $A$ that improve with increasing $k$.

We now turn to the problem of determining the eigenvalues and eigenvectors of the intermediate operators $A_k$. We will sketch the procedure; one may refer to [2,73] for details. First, let $\mathcal{P}_k = \text{span}_{1 \leq i \leq k}\{p_i\}$ and consider the eigenvalue problem,

$$A_k u = \lambda u.$$

Then for $\lambda$ that is not in the spectrum of $A_0$, we have

$$u = -\sum_{j=1}^{k} \alpha_j R^0_\lambda B p_j$$

where the coefficients $\alpha_j$'s satisfy the matrix equation

$$\sum_{j=1}^{k} \alpha_j \langle p_j + R^0_\lambda B p_j, B p_l \rangle = 0$$

for all $l = 1, 2, \ldots, k$. All of the $\alpha_j$'s cannot vanish if $u$ is to be nontrivial. Thus $\lambda$ must satisfy the determinantal equation

$$\det( \langle p_i + R^0_\lambda B p_i, B p_j \rangle ) = 0.$$
For the case that \( \lambda \) is in the spectrum of \( A_0 \), one may refer to [73]. We call the matrix \( (p_i + R^{0}_\lambda B p_i, B p_i)_{i,j=1}^k \) the \textit{Weinstein-Aronszajn (W-A)} matrix of order \( k \) and denote it again by \( W_k(\lambda) \). The matrix \( W_k(\lambda) \) has a meromorphic character with singularities at the isolated eigenvalues of \( A_0 \), but direct computation is obstructed by the problem of not having a functional expression for \( R^{0}_\lambda B p_i \) in terms of \( \lambda \) when the choice of vectors \( p_i \) is left general.

By a special choice of the vectors \( p_i \), Bazley first recognized [7] that the meromorphic function may be reduced to a rational function which can be written in an explicit form. In other words if we choose \( p_i \) so that \( B p_i \) is a unit eigenvector of \( A_0 \), say \( u^0_i \), the W-A matrix \( W_k(\lambda) \) can be represented by

\[
((\lambda^0_i - \lambda)\delta_{ij} + \langle B^{-1}u^0_i, u^0_j \rangle).
\]

Hence if the inverse of the operator \( B \) is explicitly known, the eigenvalue problem for \( A_k \) is easily resolvable. Bazley and Fox also extended this to the case where each \( p_i \) could be chosen so that \( B p_i \) was a known linear combination of eigenvectors of \( A_0 \) [8].

The method of special choice is not always possible. Thus it is important to consider a general choice of the \( p_i \). But in this case we may meet the difficulty described previously. That is, the resolvent operator \( R^0_\lambda \) for the base operator is rarely known in closed form. In many cases it can be expressed by infinite sums of integrals in general,

\[
R^0_\lambda u = \sum \frac{(u, u^0_i) u^0_i}{\lambda^0_i - \lambda} + \int_{\lambda^0_\infty}^{\infty} \frac{dE^0_{\mu} u}{ \mu - \lambda}
\]

where \( E^0_{\mu} \) is the spectral projection of \( A_0 \) for \( \mu \). To overcome this difficulty, Bazley and Fox proposed the use of the truncation of the base operator in [8] which Weinberger had initiated in [67] to his way, defined in terms of a spectral projection as

\[
A_0^{(n)} = A_0 E^0_{\lambda^n_0} + \lambda^0_{n+1}(I - E^0_{\lambda^n_0})
\]

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which is called a truncation of \( A_0 \) of order \( n \). Clearly, it satisfies

\[
A_0^{(n)} \leq A_0^{(n+1)} \leq A_0
\]

for \( n = 1, 2, \ldots \). The new intermediate operators \( A_{n,k} \) having \( A_0^{(n)} \) as a base operator are defined by

\[
A_{n,k} = A_0^{(n)} + BP_k
\]

for \( n, k = 1, 2, \ldots \). These are bounded, symmetric and monotonically increasing in \( n \) and \( k \). That is,

\[
A_{n,k} \leq \begin{bmatrix} A_{n+1,k} \\ A_{n,k+1} \end{bmatrix} \leq A
\]

for \( n, k = 1, 2, \ldots \). Thus they provide lower bounds to eigenvalues of \( A \) which improve with increasing \( n \) and \( k \).

The \( W \)-\( A \) matrix for this method may be represented by

\[
\left( \langle p_i + R_0^{(n)} B p_j, B p_j \rangle \right)_{i,j=1}^k
\]

in which the resolvent operator \( R_0^{(n)} \) of \( A_0^{(n)} \) is given by the closed expression,

\[
R_0^{(n)} v = \sum_{i=1}^n \frac{\langle v, u_i^0 \rangle u_i^0}{\lambda_i^0 - \lambda} + \frac{1}{\lambda_{n+1}^0 - \lambda} (v - \sum_{i=1}^n \langle v, u_i^0 \rangle u_i^0).
\]

Thus the \( W \)-\( A \) determinant, \( det W_k(\lambda) \), is a rational form instead of a (generally) transcendental function, which reduces the difficulty of determining roots. But we pay a price in that we are using a cruder base operator \( A_0^{(n)} \) than \( A_0 \).

As another method to overcome the difficulty of a special choice, Bazley and Fox used another projection, called the method of second projection. We will sketch this method (see [9] for further detail).

For any constant \( \delta \), the operator \( A_k \) may be rewritten by

\[
A_k = (A_0 - \delta^2) + (BP_k + \delta^2).
\]
Let \( B_k = B\delta^2 \), for each \( \delta \) and \( k \). The operator \( B_k \) produces a new inner product \( \langle u, B_k v \rangle \) on the Hilbert space \( \mathcal{H} \). Let a sequence of finite dimensional subspaces,
\[
\mathcal{P}_1 \subset \mathcal{P}_2 \subset \cdots \subset \mathcal{P}_n \subset \mathcal{P}_{n+1} \subset \cdots \subset \mathcal{H}.
\]
be given, and let \( \mathcal{P}_n : \mathcal{H} \rightarrow \mathcal{P}_n \) be the projection that is orthogonal with respect to this inner product \( \langle u, B_k v \rangle \). We form the intermediate operators as
\[
A_{k,n} = (A_0 - \delta^2) + B_k \mathcal{P}_n.
\]
The operators \( B_k \mathcal{P}_n \) are then bounded, symmetric and positive semidefinite such that
\[
B_k \mathcal{P}_n \leq B_k \mathcal{P}_{n+1} \leq B_k \mathcal{P}_n.
\]
It follows that the inequality holds
\[
A_0 - \delta^2 \leq A_{k,n} \leq \begin{bmatrix} A_{k,n+1} \\ A_{k+1,n} \end{bmatrix} \leq \begin{bmatrix} A_k \\ A_{k+1} \end{bmatrix} \leq A.
\]
Hence they provide lower bounds to eigenvalues of \( A \) which improve increasingly in \( n \) and \( k \).

The W-A matrix for this method may be expressed by
\[
\left( \langle \mathcal{P}_i + R_{\lambda+\delta^2} B_k \mathcal{P}_i, B_k \mathcal{P}_j \rangle \right)_{i,j=1}^n
\]
in which the operator \( B_k \) and the inverse have the explicit forms. In fact the inverse of \( B_k \) is expressed as
\[
B_k^{-1} u = \frac{1}{\delta^2} [I - B(\delta^2 + P_k B)^{-1} P_k] u
\]
\[
= \frac{1}{\delta^2} [u - \sum_{i,j=1}^k \langle u, B p_i \rangle c_{ij} B p_j]
\]
where \( (c_{ij}) \) is the matrix inverse to \( (\delta^2 \langle p_i, B p_j \rangle + \langle B p_i, B p_j \rangle) \). Therefore the operators \( A_{k,n} \) have been constructed so that a special choice of the \( \mathcal{P}_i \) is always possible. That is, \( \mathcal{P}_i = B_k^{-1} u_i^0 \). Thus we have the W-A matrix,
\[
W_{k,n}(\lambda) = ((\lambda_i^0 - \delta^2 - \lambda) \delta_{ij} + c_{ij})
\]
where \((c_{ij})\) is the inverse to \(\langle u_i^0, B_k u_j^0 \rangle\).

It follows from [9] that the operator \(A_{k,n}\) is monotonically increasing in \(\delta^2\) on the space spanned by \(\{u_1^0, \ldots, u_n^0\}\), but is decreasing on the orthogonal complement. The eigenvalues \(\lambda_i^{(k,n)}\) considered as functions of \(\delta\) converges to the eigenvalue \(\lambda_i^0\) as \(\delta\) goes to zero. For each \(k\) and \(n\), the best value of \(\delta^2\) for the estimation of \(\lambda_i\), \(i \leq n\), is that

\[\delta^2 = \lambda_{n+1}^0 - \lambda_i^{(k,n)}\]

Börsch-Supan first compared the methods of truncation and second projection. According to [25], if we take \(\delta^2 = \lambda_{n+1}^0 - \lambda\) and \(\hat{p}_i = B_k^{-1} u_i^0\), for \(i = 1, 2, \ldots, n\), then they have the same eigenvalues with slightly different eigenvectors. In the case of the second projection, the best value of \(\delta^2\) for \(\lambda_i\) is \(\delta^2 = \lambda_{n+1}^0 - \lambda_i^{(k,n)}\) and generally the method of truncation will produce better lower bounds.

1.3.3 On the method of truncation including the remainder. Bazley and Fox first introduced this method in [13], Greenlee analyzed it in [43] and later Beattie and Greenlee have developed further this method in [19,20]. For the following we adopt notations directly from [43,19,20]. Let us take a real number \(\gamma\) satisfying \(\lambda_1(A_0) < \gamma \leq \lambda_\infty(A_0)\), with the restriction that \(\gamma < \lambda_\infty(A_0)\) if \(A_0\) has an infinity of eigenvalues below \(\lambda_\infty(A_0)\).

Define the truncation of \(A_0\) at \(\gamma\) by

\[A_0^{(\gamma)} = A_0 E_{\gamma} - A_0 + \gamma (I - E_{\gamma} - A_0)\]

where \(E_\lambda[A_0]\) is the right continuous resolution of the identity for \(A_0\). We note that if \(\gamma = \lambda_{n+1}^0\), then the \(A_0^{(\gamma)}\) is the same as the previously defined \(A_0^{(n)}\). But we use the notation \(A_0^{(\gamma)}\) thereafter in order to follow their notations. We note that \(A_0^{(\gamma)}\) has the same action as \(A_0\) on the finite dimensional subspace, \(U_0^{(\gamma)} = \text{Ran}(E_{\gamma} - A_0)\), and acts as a scalar multiplication by \(\gamma\) on \((U_0^{(\gamma)})^\perp\). The corresponding quadratic form \(a_0^{(\gamma)}\) may be used to define a quadratic form

\[\tilde{a}(u) = a(u) - a_0^{(\gamma)}(u) \geq b(u) \geq a\|u\|^2.\]
One may observe that $\text{Dom}(\tilde{a}) = \text{Dom}(a)$ where $\tilde{a}$ is a closed quadratic form and the corresponding self adjoint operator is given by

$$\tilde{A} = A - A_0^{(\gamma)}$$

with $\text{Dom}(\tilde{A}) = \text{Dom}(A)$. The main notion behind this method is to approximate $\tilde{A}$ with a finite rank operator which consequently produces intermediate operators that are finite rank perturbations of the resolvable operator $A_0^{(\gamma)}$.

For this purpose, we introduce a new Hilbert space $\mathcal{H}_{\tilde{a}}$ which is the completion of $\text{Dom}(\tilde{A})$ in the norm generated by the new inner product $\langle u, \tilde{A}u \rangle$. Let a sequence of finite dimensional subspaces

$$\mathcal{P}_1 \subset \mathcal{P}_2 \subset \cdots \subset \mathcal{P}_k \subset \mathcal{P}_{k+1} \subset \cdots \subset \text{Dom}(\tilde{A})$$

be given, and let $P_k : \mathcal{H}_{\tilde{a}} \longrightarrow \mathcal{P}_k$ be the projection that is orthogonal with respect to the inner product $\langle u, \tilde{A}v \rangle$. For each $k$, we now define the intermediate form,

$$a_k(u) = a_0^{(\gamma)}(u) + \tilde{a}(P_k u)$$

for $u \in \text{Dom}(a_k) = \mathcal{H}$, with the corresponding self adjoint operator

$$A_k = A_0^{(\gamma)} + \tilde{A}P_k.$$ 

By construction, we have

$$a_0(u) = a_0^{(\gamma)}(u) \leq a_k(u) \leq a_{k+1}(u) \leq a(u)$$

for all $k$ and $u \in \text{Dom}(a)$ where the second monotonicity principle implies that

$$\lambda_i(A_0) = \lambda_i(A_0^{(\gamma)}) \leq \lambda_i(A_k) \leq \lambda_i(A_{k+1}) \leq \lambda_i(A),$$

for all $k$ and $i$ such that $\lambda_i(A) < \gamma$. 

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1.3.4 On the method of Basley-Fox. Let \( a(u) \) and \( a_0(u) \) be the quadratic forms which are the closures of \( \langle u, Au \rangle \) and \( \langle u, A_0u \rangle \), respectively, such that

\[
a_0(u) \leq a(u)
\]

for all \( u \in \text{Dom}(a) \subset \text{Dom}(a_0) \). We assume that the quadratic form \( a(u) \) is decomposed as

\[
a(u) = a_0(u) + \| Tu \|_*^2
\]

where \( T \) is a closed operator on \( \mathcal{H} \) to another Hilbert space \( \mathcal{H}_* \).

Let a sequence of finite dimensional spaces

\[
\mathcal{P}_1 \subset \mathcal{P}_2 \subset \cdots \subset \mathcal{P}_k \subset \mathcal{P}_{k+1} \subset \cdots \subset \text{Dom}(T^*) \subset \mathcal{H}_*
\]

be given, and let \( P_k : \mathcal{H}_* \longrightarrow \mathcal{P}_k \) be the projection that is orthogonal with respect to the inner product \( \langle u, v \rangle_* \). We construct the intermediate quadratic forms \( a_k(u) \) as

\[
a_k(u) = a_0(u) + \| P_k T u \|_*^2
\]

for all \( u \in \text{Dom}(a_k) = \text{Dom}(a_0) \cap \text{Dom}(T) \). Since \( \text{Ran}(P_k) \subset \text{Dom}(T^*) \), we may extend \( \| P_k T u \|_* \) to all of \( \mathcal{H} \) by continuity where \( a_k(u) \) may be associated with a self-adjoint operator given by

\[
A_k = A_0 + T^* P_k T
\]

with \( \text{Dom}(A_k) = \text{Dom}(A_0) \). By an argument similar to Section 1.3.2, the second monotonicity theorem with Bessel’s inequality yields that the eigenvalues of \( A_k \) provide lower bounds to the corresponding eigenvalues of \( A \) that improve increasingly in \( k \).

The W-A matrix, \( W_k(\lambda) \), whose zeros of determinant provide the eigenvalues of \( A_k \), may be represented as

\[
\left( \langle p_i, p_j \rangle_* + \langle P_k^2 T^* p_i, T^* p_j \rangle \right).
\]
By a special choice of the vectors $p_i$, i.e., $T^*p_i = u^0_i$, the matrix $W_k(\lambda)$ is compactly expressed as

$$\left(\frac{1}{\lambda^0 - \lambda}\delta_{ij} + \langle p_i, p_j \rangle_\ast\right).$$

For more information, one may refer to [19].

If we take a truncation of $A_0$ at $\lambda^0_n$, the intermediate operators are written by

$$A_{n,k} = A^0_0 + T^*P_kT$$

and the W-A matrix is obtained by

$$W_{n,k}(\lambda) = \left(\langle p_i, p_j \rangle_\ast + \left\langle R^{(n)}_\lambda T^*_\lambda p_i, T^*_\lambda p_j \right\rangle \right)$$

from the equation $A_{n,k}u = \lambda u$. Notice that $A_{n,k}$ has $\lambda^0_{n+1}$ as an eigenvalue of infinite multiplicity. Following [17], if we define for some fixed $\delta \neq 0$

$$B_k = T^*P_kT + \delta^2 I$$

then the operator $B_k$ is bounded, self-adjoint and positive definite. The intermediate operators for the second projection are defined to be the same form as in the previous section. The W-A matrix is also expressed as

$$\left(\langle \hat{p}_i + R^0_{\lambda + \delta^2}B_k\hat{p}_i, B_k\hat{p}_j \rangle \right)$$

in which $B_k$ has an explicit inverse given by

$$B_k^{-1}v = \frac{1}{\delta^2}(v - \sum_{i,j=1}^{k} \langle v, T^*_i p_i \rangle c_{ij} T^*_j p_j)$$

where $(c_{ij})$ is the matrix inverse to $(\delta^2 \langle p_i, p_j \rangle_\ast + \langle T^*_i p_i, T^*_j p_j \rangle)$. Therefore if we take a special choice of the $\hat{p}_i$, i.e., $\hat{p}_i = B_k^{-1}u^0_i$, the W-A matrix is explicitly computable as

$$\left[\left(\frac{1}{\delta^2} + \frac{1}{\lambda^0_i - \lambda - \delta^2}\right)\delta_{ij} - \frac{1}{\delta^2} \sum_{l,m=1}^{k} \langle u^0_i, T^*_i p_l \rangle c_{lm} \langle T^*_m p_m, u^0_j \rangle \right].$$

This expression (cf. [17]) is applied to build the EVF method.
1.4 Remarks.

We note that the Rayleigh–Ritz method does not always strictly improve previously obtained bounds at each successive stage [73]. For instance, if we take eigenvectors of the given operator as test functions, there is no improvement. But if trial functions are chosen from a set complete in a sufficiently strong topology, the bounds will converge to the eigenvalues. In the method of Weinstein, we can obtain the base problem by the removal of constraints. In the method of Aronszajn, the base problem is found by neglecting a positive term in the expression of the given operator. In applications we often have the advantage of the method of Bazley and Fox that the approximating functions, \( \{p_i\} \), may be chosen from \( \text{Dom}(T^*) \) rather than \( \text{Dom}(B) \) [44]. This usually means that the vectors \( \{p_i\} \) satisfy fewer boundary conditions.

In the method of Aronszajn, the essential spectrum of \( A_k \) is the same as that of \( A_0 \) since the operator \( BP_k \) is compact. Assume that \( \lambda_\infty^0 = \lambda_\infty \), and that \( A_0 \) and \( A \) have spectrum which begins with isolated eigenvalues of finite multiplicity, then so does \( A_k \). In order to succeed with Aronszajn’s method, the base problem must be selected in such a way that it has no essential spectrum below an eigenvalue to be approximated. There are important classes of problems for which rigorous lower bounds are of interest but for which Aronszajn’s method generally gives no more knowledge than was initially available from the base operator for the fixed essential spectrum. For such a problem, Fox presented [36] a method which can move the essential spectrum of the base operator. He used techniques on the tensor product structure of the underlying Hilbert space and on separation of variables so that the operator \( BP_k \) is noncompact. That is, the projecting space \( \mathcal{P}_k \) is of infinite dimension. Significantly, he showed how this could be done in such a way that it still allows \( A_k \) to be computationally resolvable.
CHAPTER 2
A STUDY OF CONVERGENCE RATES FOR SEMI-BOUNDED OPERATORS AND INTERMEDIATE PROBLEMS

2.1 Introduction.

In this chapter we present conditions sufficient to guarantee the convergence of eigenvalues of an increasing sequence of operators in $S$ and also derive convergence rates for the sequence of operators. These results will be applied to the methods of intermediate problems including a variant of a method of Aronszajn known as truncation including the remainder which was analyzed by Beattie and Greenlee [19,20,43]. We note that though the conditions for convergence we give may be the same as those of Brown [28] and Beattie and Greenlee [18], the convergence rates obtained are slightly improved over those obtained very recently by Beattie and Greenlee [20]. Moreover the convergence theorem for the method of truncation including the remainder follows as a special case. For the method of Weinstein, our result of convergence rate appears to be the first one for a general choice of approximating vectors $p_i$. For this purpose, we discuss the convergence rate of the eigenvalues and eigenvectors of the increasing sequence, $\{A_k\}_{k=0}^{\infty}$, of semi-bounded operators using techniques to analyze finite-element methods for the differential eigenvalue problem [6].

Throughout this chapter we denote by $U$ the eigenspace of $A$ corresponding to the eigenvalue $\lambda = \lambda_{i+1} = \cdots = \lambda_{i+m-1}$ with multiplicity $m$ which is less than $\lambda_0$, the lowest point of the essential spectrum of $A_0$. Similarly, $U^{(k)}$ denotes the eigenspace of $A_k$ corresponding to the eigenvalues $\lambda^{(k)}_i, \lambda^{(k)}_{i+1}, \ldots, \lambda^{(k)}_{i+m-1}$. We also represent the spectral projections of $A$ and $A_k$ onto $U$ and $U^{(k)}$ as $E$ and $E_k$ respectively.

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In Section 2 we review a result of Weidmann and the relevant theory for the finite element method usually used for differential eigenvalue problems. With the aid of these results, we will provide sufficient conditions for the convergence of eigenvalues and also derive the corresponding rate for a sequence of semi-bounded operators in $\mathcal{S}$. Section 3 deals with application of the derived results to the problem types of Aronszajn and Bazley–Fox as well as those of Weinstein. We derive a convergence rate for the method of truncation including the remainder in Section 4. Finally in Section 5 we present a numerical example of a one dimensional Schrödinger operator with a potential for the method of truncation including the remainder.
2.2 Convergence Rates for Semi-bounded Operators.

In this section we present some convergence results and estimates of convergence rates for the sequence, $\{A_k\}_{k=0}^{\infty}$, of operators and $A$ which are in $S$ as well as sufficient conditions for the convergence of their eigenvalues. We first assume that the $A_k$ and $A$ are bounded. It is then well known [58] that if $A_k$ converges to $A$ uniformly, then $\lambda_i^{(k)}$ converges to $\lambda_i$. For a sequence of compact operators we need only strong convergence to get convergence of their eigenvalues by an analog of Dini’s theorem [8].

**Theorem 2.2.1.** Let $A$ be a compact and self-adjoint operator and let $\{A_k\}$ be a sequence of compact and self-adjoint operators such that $A \leq A_{k+1} \leq A_k$. If $A_k$ converges to $A$ strongly, then $A_k$ converges uniformly to $A$.

**Proof:** We assume that $A_k$ does not converge to $A$ uniformly. Since $A_k - A$ is symmetric,

$$\|A_k - A\| = \sup_{\|u\|=1} \langle (A_k - A)u, u \rangle.$$ 

Thus there exists a positive number $\delta$ and a sequence $\{u_k\}$ with $\|u\| = 1$ such that $\langle (A_k - A)u_k, u_k \rangle \geq \delta$, for any $k$. Since the sequence $\{A_k\}$ is decreasing, we have for any fixed $N$,

$$\langle A_Nu_k, u_k \rangle \geq \langle A_ku_k, u_k \rangle \geq \langle Au_k, u_k \rangle + \delta$$

for any $k \geq N$. Since a Hilbert space is weakly compact, there is a subsequence of $\{u_k\}$, denoted again by $\{u_k\}$, and $u$ such that $u_k$ converges to $u$ weakly. Since $A$ and $A_N$ are compact, it follows that $A_Nu_k$ and $Au_k$ converge strongly to $A_Nu$ and $Au$, respectively. Consequently we have

$$\langle A_Nu, u \rangle \geq \langle Au, u \rangle + \delta$$

which is a contradiction to the assumption. $\blacksquare$

We introduce some convergence rates for the sequence of bounded operators whose proof may be found in [6].

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THEOREM 2.2.2 (Babuška and Osborn). Let \((A_k)\) be a sequence of bounded operators which converges to \(A\) uniformly. Then for any \(i\) and \(j = i, i + 1, \ldots, i + m - 1\) and \(u \in U\), we have a sufficiently large \(k\) such that

\[
(1) \quad |\lambda_i - \lambda_j^{(k)}| \leq \max_{u \in U, ||u|| = 1} |\langle (A_k - A)u, u \rangle| + C_1 \cdot \max_{u \in U, ||u|| = 1} \| (A_k - A)u \| ^2
\]

\[
(2) \quad \| u - E_k u \| \leq C_2 \cdot \max_{u \in U, ||u|| = 1} \| (A_k - A)u \|
\]

for some constants \(C_1\) and \(C_2\) independent of \(k\).

We now assume that \(A_k\) and \(A\) are bounded below such that \(A_k \leq A_{k+1} \leq A\), for all \(k \geq 0\). We recall the following definition. (e.g., [33, 45])

DEFINITION. Let \(A_k\) be a sequence of self-adjoint operators acting in a Hilbert space \(H\). We say that the \(A_k\) converges to \(A\) in the strong resolvent sense if

\[
(A_k - z)^{-1} \longrightarrow (A - z)^{-1}\quad \text{strongly}
\]

for some \(z\) which is bounded away from the spectra of the \(A_k\) and \(A\).

If the \(A_k\) and \(A\) are all coercive, convergence in the strong resolvent sense is equivalent to the strong convergence of \(A_k^{-1}\) to \(A^{-1}\). It has been well known \([44, 58]\) that if the self-adjoint operators \(A\) and \(B\) are compact (even bounded), then the differences of the corresponding eigenvalues of \(A\) and \(B\) are dominated by the norm of the difference of the operators. Thus the uniform convergence of a sequence of bounded operators implies the convergence of the corresponding eigenvalues. For a sequence of semi-bounded operators, we have

THEOREM 2.2.3. Let \(A\) be in \(S\) and let \(\{A_k\}\) be a sequence of operators in \(S\) such that \(A \leq A_{k+1} \leq A_k\) and \(\text{Dom}(A) = \text{Dom}(A_k)\) for all \(k\). If \(U\) is the eigenspace of \(A\) corresponding to the eigenvalues \(\lambda_1, \lambda_2, \ldots, \lambda_i\), then

\[
0 \leq \lambda_i^{(k)} - \lambda_i \leq \max_{u \in U, ||u|| = 1} \| (A_k - A)u \|.
\]
Proof: It easily follows from the minimum-maximum principle that
\[
\lambda_i^{(k)} = \min_{p \in \text{Dom}(A_k)} \max_{u \in \mathcal{U}, \|u\|=1} \langle A_k u, u \rangle \leq \max_{u \in \mathcal{U}, \|u\|=1} \langle A_k u, u \rangle \leq \lambda_i + \max_{u \in \mathcal{U}, \|u\|=1} \| (A_k - A) u \|.
\]

Hence we have the result.\[\square\]

The goal of this section is to get the same conclusion as in Theorem 2.2.2 for a sequence of semi-bounded operators in $S$. We modify a result of Weidmann for our problem setting. Notice that the result already had been applied to get sufficient conditions for the convergence of eigenvalues in [19–21, 27, 28].

Lemma 2.2.4 (Weidmann). Let $(A_k)$ be an increasing sequence of operators in $S$ which converges to $A$ in the strong resolvent sense. Let $\lambda_1^{(k)} \leq \lambda_2^{(k)} \leq \cdots \leq \lambda_\infty^{(k)}$ and $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_\infty$ be the isolated eigenvalues of $A_k$ and $A$, respectively. Then for all $i$ such that $\lambda_i < \lambda_\infty^0$, $\lambda_i^{(k)}$ converges to $\lambda_i$, where $\lambda_\infty^0$ denotes the lowest point of the essential spectrum of $A_k$.

With the aid of Lemma 2.2.4 and the proof of Theorem 2.2.2 in [6], we have the main estimate result which plays a crucial role in our estimates.

Theorem 2.2.5. Let $(A_k)$ be an increasing sequence of $S$ which converges to $A$ in the strong resolvent sense. Then for all $i$ such that $\lambda_i < \lambda_\infty^0$, $\lambda_i^{(k)}$ converges to $\lambda_i$ as $k$ becomes large. Furthermore, if $\lambda_i$ has multiplicity $m$ with $\lambda_i = \lambda_{i+1} = \cdots = \lambda_{i+m-1}$, we have the following estimates,

1. $|\lambda_i - \lambda_j^{(k)}| \leq \max_{u \in \mathcal{U}, \|u\|=1} \| (A_k - A) u, u \| + C_1 \cdot \max_{u \in \mathcal{U}, \|u\|=1} \| (A_k - A) u \|^2$
2. $|\frac{1}{\lambda_i} - \frac{1}{\lambda_j^{(k)}}| \leq \max_{u \in \mathcal{U}, \|u\|=1} \| (A_k^{-1} - A^{-1}) u, u \| + C_2 \cdot \max_{u \in \mathcal{U}, \|u\|=1} \| (A_k^{-1} - A^{-1}) u \|^2$
3. $\|u - E_k u\| \leq C_3 \cdot \max_{u \in \mathcal{U}, \|u\|=1} \| (A_k^{-1} - A^{-1}) u \|^2 \leq C_4 \cdot \max_{u \in \mathcal{U}, \|u\|=1} \| (A_k - A) u \|^2$

for $k$ sufficiently large and for some constants $C_i$'s independent of $k$. 26
Proof: We note that the spectral projection associated with \( \lambda_i \) is denoted by

\[
E = \frac{1}{2\pi i} \int_{\Gamma} R_z(A) \, dz,
\]

where \( \Gamma \) is a circle in the complex plane centered at \( \lambda_i \) which lies in the resolvent set, \( \rho(A) \), of \( A \) and which encloses no other points of the spectrum, \( \sigma(A) \), of \( A \) and \( R_z(A) \) is the resolvent operator of \( A \) at \( z \), i.e. \( R_z(A) = (z - A)^{-1} \). Since \( A_k \) converges monotonically to \( A \) in the strong resolvent sense, Lemma 2.2.4 implies that \( \lambda_j^{(k)} \) converges to \( \lambda_i \) as \( k \) goes to \( \infty \) for \( j = i, i+1, \ldots, i+m-1 \). There is thus a sufficiently large \( k \) such that \( \Gamma \) lies also in \( \rho(A_k) \) enclosing only \( \lambda_i \) and \( \{\lambda_j^{(k)}\}_{j=i}^{i+m-1} \). Thus the spectral projection \( E_k \) associated with \( A_k \) and \( \{\lambda_j^{(k)}\}_{j=i}^{i+m-1} \) may be expressed as

\[
E_k = \frac{1}{2\pi i} \int_{\Gamma} R_z(A_k) \, dz.
\]

Hence for any \( u \in \mathcal{U} \), we have

\[
\|(E - E_k)u\| = \left\| \frac{1}{2\pi i} \int_{\Gamma} (R_z(A_k) - R_z(A))u \, dz \right\|
\]

\[
\leq \frac{1}{2\pi} \left\| \int_{\Gamma} R_z(A_k)(A - A_k)R_z(A)u \, dz \right\|
\]

\[
\leq \frac{1}{2\pi} \cdot \ell(\Gamma) \cdot \max_{z \in \Gamma} \|R_z(A_k)\| \cdot \max_{u \in \mathcal{U}, \|u\|=1} \|(A_k - A)u\|
\]

\[
\cdot \max_{z \in \Gamma} \|R_z(A)\| \|u\|
\]

\[
\leq C \cdot \max_{u \in \mathcal{U}, \|u\|=1} \|(A_k - A)u\|, \quad \text{for some } C \text{ independent of } k
\]

because \( R_z(A_k) \) and \( R_z(A) \) are uniformly bounded on \( \Gamma \). Here \( \ell(\Gamma) \) is the arc length of \( \Gamma \). This gives (3). Since \( A_k \) converges to \( A \) in the strong resolvent sense with \( \mathcal{U} \) as a finite dimensional space, \( E_k \) converges to \( E \) on the space \( \mathcal{U} \).

Let \( \hat{E}_k : \mathcal{U} \rightarrow \mathcal{U}^{(k)} \) be the restriction of \( E_k \) to the space \( \mathcal{U} \). Suppose that \( \hat{E}_ku = 0 \) for some \( u \in \mathcal{U} \). Then

\[
\|u\| = \|(E - E_k)u\| \leq \max_{u \in \mathcal{U}, \|u\|=1} \|(E_k - E)u\||\|u\|.
\]
Since \( E_k \) converges to \( E \) on the space \( \mathcal{U} \), we have that \( u = 0 \) for \( k \) sufficiently large. Since \( \dim \mathcal{U} = \dim \mathcal{U}^{(k)} \), it follows that \( \hat{E}_k : \mathcal{U} \to \mathcal{U}^{(k)} \) is bijective for sufficiently large \( k \). Furthermore

\[
\| \hat{E}_k^{-1} \| \leq 2
\]

for \( k \) sufficiently large, since for any \( u \in \mathcal{U} \),

\[
\| u \| - \| \hat{E}_k u \| \leq \max_{u \in \mathcal{U}, \| u \| = 1} \| (E_k - E)u \| \cdot \| u \| \leq \frac{1}{2} \| u \|
\]

for \( k \) sufficiently large. For convenience, let \( T_k = \hat{E}_k^{-1} A_k \hat{E}_k \). Then \( T_k \) is an operator from \( \mathcal{U} \) onto \( \mathcal{U} \) having eigenvalues which are

\[
\sigma(T_k) = \{ \lambda_j^{(k)} \}_{j=i}^{i+m-1}.
\]

Let \( w_k \in \mathcal{U} \) be defined so that \( T_kw_k = \lambda_j^{(k)} w_k \) for some fixed \( i \geq j \geq i + m - 1 \) and \( \| w_k \| = 1 \). Then

\[
\lambda_i - \lambda_j^{(k)} = \langle (A - T_k)w_k, w_k \rangle.
\]

Since \( \hat{E}_k^{-1} E_k \) is the identity on \( \mathcal{U} \), we have for any \( v \in \mathcal{U} \) with \( \| v \| = 1 \),

\[
\langle (A - T_k)v, v \rangle = \langle \hat{E}_k^{-1} E_k A v, v \rangle - \langle \hat{E}_k^{-1} A_k \hat{E}_k v, v \rangle
\]

\[
= \langle \hat{E}_k^{-1} E_k (A - A_k)v, v \rangle
\]

\[
= \langle ((I - \hat{E}_k^{-1} E_k)(A_k - A)v, v \rangle - \langle (A_k - A)v, v \rangle.
\]

Since \( E_k \hat{E}_k^{-1} = I \) on \( \mathcal{U}^{(k)} \), we have that \( I - \hat{E}_k^{-1} E_k = (I - E_k)(I - \hat{E}_k^{-1} E_k) \) and \( (I - E_k)v = (E - E_k)v \) for any \( v \in \mathcal{U} \). Thus it follows from (3) that

\[
|\langle ((I - \hat{E}_k^{-1} E_k)(A_k - A)v, v \rangle| = |\langle ((I - \hat{E}_k^{-1} E_k)(A_k - A)v, (E - E_k)v \rangle|
\]

\[
\leq \| I - \hat{E}_k^{-1} E_k \| \| (A_k - A)v \| \| (E - E_k)v \|
\]

\[
\leq 3C \max_{u \in \mathcal{U}, \| u \| = 1} \| (A_k - A)u \|^2
\]

for sufficiently large \( k \). It leads to (1). By the same way (2) also follows. \( \blacksquare \)
Corollary 2.2.6. Let \((A_k)\) be an increasing sequence of operators in \(S\) and let \(A\) be in \(S\) such that \(A_k \leq A\) for all \(k\). If \(A_ku\) converges strongly to \(Au\) for any \(v \in \text{Dom}(A)\), then \(A_k\) converges to \(A\) in the strong resolvent sense. Thus we have the same results as in Theorem 2.2.5.

Proof: It easily follows from the fact that

\[
A_k^{-1} - A^{-1} = A_k^{-1}(A - A_k)A^{-1}.
\]

For any self adjoint operator \(A_k\), the corresponding closed quadratic form is denoted by \(a_k(u)\). It follows from [33] and Lemma 2.2.4 that we have the following theorem. One may also refer to Kato [45] and Simon [61].

Theorem 2.2.7. Let \((A_k)\) be an increasing sequence of operators in \(S\) which is dominated by \(A \in S\) from above. We assume that for \(u \in \cap_{k \geq 0} \text{Dom}(a_k)\) such that \(a_k(u)\) is uniformly bounded, the vector \(u\) is in \(\text{Dom}(a)\) and \(a_k(u)\) converges to \(a(u)\). Then \(A_k\) converges to \(A\) in the strong resolvent sense and thus for all \(i\) such that \(\lambda_i < \lambda^{(0)}\), \(\lambda_i^{(i)}\) converges to \(\lambda_i\) as \(k\) goes to \(\infty\).

The set in the second hypothesis of Theorem 2.2.7 can be expressed as the domain of \(a_{\infty}\). That is,

\[
\text{Dom}(a_{\infty}) = \{u \in \cap_{k \geq 1} \text{Dom}(a_k) : \sup a_k(u) < \infty\}
\]

and \(a_{\infty}(u) = \lim_{k \to \infty} a_k(u)\), for all \(u \in \text{Dom}(a_{\infty})\). Both Theorem 2.2.5 and 2.2.7 will be applied to get the sufficient conditions for the convergence of eigenvalues and also its rate for the intermediate problems with the method of truncation including remainder. If \(\text{Dom}(a) = \cap_{k \geq 1} \text{Dom}(a_k)\) is to be assumed, \(a_k(u)\) is uniformly bounded for \(u \in \text{Dom}(a)\) for \(a_k \leq a\). Thus we get the following useful corollaries.
Corollary 2.2.8. Let \((A_k)\) be an increasing sequence of operators in \(S\). Let \(A\) be in \(S\) such that \(A_k \leq A\) and assume that \(\text{Dom}(a) = \cap_{k \geq 1} \text{Dom}(a_k)\). If \(a_k(u) \rightarrow a(u)\) for all \(u \in \text{Dom}(a)\), then \(A_k\) converges to \(A\) in the strong resolvent sense and thus we have the same results as in Theorem 2.2.5.

Let \((A_k)\) be an increasing sequence of bounded and self-adjoint operators such that \(A_k\) converges weakly to a bounded and self-adjoint operator \(A\). It follows from Corollary 2.2.8 that \(A_k\) converges to \(A\) in the strong resolvent sense. Since \(A_k - A = A_k(A^{-1} - A_k^{-1})A\), we have the strong convergence of \(A_k\) to \(A\) but not the uniform convergence. However, we obtain the convergence of eigenvalues with its rate. One may compare this with Theorem 2.2.2.

Corollary 2.2.9. Let \((A_k)\) be an increasing sequence of bounded and self-adjoint operators. If \(A_k\) converges weakly to \(A\), then \(\lambda_i^{(k)}\) converges to \(\lambda_i\). Thus we have the same estimates as in Theorem 2.2.5.

We review the following basic results because they may be used in intermediate problems.

Theorem 2.2.10([30]). Let \(A\) and \(B\) be self-adjoint operators. Then

\[
\alpha < A \leq B \quad \text{if and only if} \quad (A - \alpha)^{-1} \geq (B - \alpha)^{-1} > 0.
\]

This allows us to transform a monotone increasing sequence of unbounded operators into an equivalent monotone decreasing sequence of bounded operators. That is,

\[
0 < \alpha \leq A_0 \leq \cdots \leq A_k \leq A_{n+1} \leq \cdots \leq A
\]

\[\iff \frac{1}{\alpha} \geq A_0^{-1} \geq \cdots \geq A_k^{-1} \geq A_{n+1}^{-1} \geq \cdots \geq A^{-1}.
\]

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THEOREM 2.2.11. Let $A$ and $B$ be self-adjoint such that $0 < B < A$. If $A$ is compact, then $B$ is compact.

Proof: We note that $A^\frac{1}{2}$ is compact because $A$ is positive and compact. Let $\{x_k\}$ be a sequence of vectors such that $x_k$ converges to 0 weakly. Since $A^\frac{1}{2}$ is compact, $A^\frac{1}{2}x_k$ converges to 0 strongly. Since

$$||B^\frac{1}{2}x_k||^2 = \langle B^\frac{1}{2}x_k, B^\frac{1}{2}x_k \rangle = \langle Bx, x \rangle$$

$$\leq \langle Ax, x \rangle = ||A^\frac{1}{2}x_k||,$$

$B^\frac{1}{2}$ is compact and thus $B$ is compact.\[\]

This implies that if the base operator $A_0$ has compact resolvent, then all intermediate operators with the given operator have compact resolvent.
2.3 Convergence Rate for Intermediate Problem Methods.

We introduce the following notation in order to lay out convergence rate results. For any densely defined closed positive coercive quadratic form \( c(u) \) on \( \mathcal{H} \), let \( \mathcal{M} \) and \( \mathcal{N} \) be subspaces of \( \text{Dom}(c) \) with \( \dim \mathcal{N} > 0 \). Beattie and Greenlee [19] define the containment gap relative to \( c(u) \) for the approximation of \( \mathcal{M} \) by \( \mathcal{N} \) as

\[
\delta_c(\mathcal{M}, \mathcal{N}) = \sup_{0 \neq u \in \mathcal{N}} \inf_{v \in \mathcal{M}} \frac{\|u - v\|_c}{\|u\|}.
\]

We note that \( \delta_c(\mathcal{M}, \mathcal{N}) \) is not symmetric in \( \mathcal{N} \) and \( \mathcal{M} \), and \( \delta_c(\mathcal{M}, \mathcal{N}) = 0 \) if and only if \( \mathcal{M} \supset \mathcal{N} \). Likewise we denote

\[
\delta_m(\mathcal{N}) = \sup_{0 \neq u \in \mathcal{N}} \inf_{v \in \mathcal{M}} \frac{\|u - v\|}{\|u\|}.
\]

We note that this is unlike the gap of Kato [45].

For the speed of the convergence, Weinberger gave an error estimation for the convergence in 1952 [66] which is historically the first example of convergence rate for intermediate problems. For the basic convergence rate for the Rayleigh-Ritz method, one may refer to [6,20,35].

2.3.1 On the Weinstein type. We recall that the operator \( A \) and the intermediate operators \( A_k \) are written in terms of \( A_0 \) as

\[
A = Q A_0 Q \quad \text{and} \quad A_k = Q_k A_0 Q_k,
\]

where \( Q \) is the orthogonal projection of \( \mathcal{H}_{a_0} \) onto \( \mathcal{H}_a \) and \( Q_k : \mathcal{H}_{a_0} \rightarrow \mathcal{P}_k^\perp \) is the orthogonal projection onto \( \mathcal{P}_k^\perp \). We note that the sequence, \( \{ \mathcal{P}_k^\perp \} \), of subspaces with codimension \( k \) satisfies the inequality,

\[
\mathcal{H}_a \subset \cdots \subset \mathcal{P}_{k+1}^\perp \subset \mathcal{P}_k^\perp \subset \cdots \subset \mathcal{P}_0^\perp = \mathcal{H}_{a_0}.
\]

Thus the corresponding projections have the property

\[
I = Q_0 \supset Q_1 \supset \cdots \supset Q_k \supset Q_{k+1} \supset \cdots \supset Q.
\]
We suppose that the sequence of vectors, \( \{p_i\} \), in \( \mathcal{H}_{a_0} \) is selected such that it is complete in \( \mathcal{H}_{a_0} \oplus \mathcal{H}_a \). Each vector \( u \) in \( \mathcal{H}_{a_0} \) may be uniquely decomposed as \( u = v + w \), where \( v \in \mathcal{H}_a \) and \( w \in \mathcal{H}_{a_0} \oplus \mathcal{H}_a \). Thus

\[
\| (Q_k - Q)u \|_{a_0} = \| (P_k - P)u \|_{a_0} = \| (P_k - I)w \|_{a_0} \to 0 \quad \text{as} \quad n \to \infty,
\]

where \( P : \mathcal{H}_{a_0} \to \mathcal{H}_{a_0} \oplus \mathcal{H}_a \) is the orthogonal projection and \( Q_k = I - P_k \).

Aronszajn and Weinstein [4] showed in 1949 the convergence of the Weinstein method under the assumption that the base operator \( A_0 \) has a compact inverse and that \( \{p_i\} \) is complete in \( \mathcal{H}_{a_0} \oplus \mathcal{H}_a \). One may refer to [44,73] for the proof. In 1984 Brown [27] showed the convergence without any compactness assumption on \( A_0 \).

**Lemma 2.3.1.** Let the sequence, \( \{p_i\} \), of vectors be complete in \( \mathcal{H}_{a_0} \oplus \mathcal{H}_a \) and let \( A_0 \) be compact. Then \( Q_k A_0 Q_k \) converges uniformly to \( QA_0 Q \).

**Proof:** Since \( Q_k A_0 Q_k \) and \( QA_0 Q \) are compact, it suffices to show only the strong convergence. For any \( u \in \mathcal{H}_{a_0} \), we have

\[
\| (Q_k A_0 Q_k - QA_0 Q)u \|_{a_0} \leq \| (Q_k - Q) A_0 Q u \|_{a_0} + \| Q_k A_0 (Q_k - Q) u \|_{a_0} \\
\leq \| (Q_k - Q) A_0 Q u \|_{a_0} + \| A_0 \|_{a_0} \| (Q_k - Q) u \|_{a_0} \\
\to 0 \quad \text{as} \quad k \to \infty. \]

Let \( \mathcal{U} \) be the eigenspace of \( A \) corresponding to \( \lambda_i \) with multiplicity \( m_i \). Then

\[
\max_{u \in \mathcal{U}, \|u\|_{a_0} = 1} \| (Q_k A_0 Q_k - QA_0 Q)u \|_{a_0} = \max_{u \in \mathcal{U}, \|u\|_{a_0} = 1} \| (Q_k - Q) A_0 u \|_{a_0} \\
\leq \max_{u \in \mathcal{U}} \| A_0 u \|_{a_0} \cdot \| u \|_{a_0} \\
\leq \max_{u \in \mathcal{U}, \|u\|_{a_0} = 1} \| A_0 u \|_{a_0} \max_{v \in A_0 \mathcal{U}} \| (Q_k - Q) v \|_{a_0} \\
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and since $Q_k$ and $Q$ are identities on the space $\mathcal{U}$, it follows that for any $u \in \mathcal{U}$,
\[
\langle (Q_k A_0 Q_k - Q A_0 Q) u, u \rangle_{a_0} = \langle (Q_k - Q) A_0 u, u \rangle_{a_0}
\]
\[= \langle A_0 u, (Q_k - Q) u \rangle_{a_0}
\]
\[= 0.
\]

Therefore it follows directly from Theorem 2.2.2 that we have

**Theorem 2.3.2.** Let the sequence, $\{p_l\}$, of vectors be complete in $\mathcal{H}_a \oplus \mathcal{H}_b$ and let $A_0$ be compact. Then for $j = i, i + 1, \ldots, i + m - 1$, we have

\[
|\lambda_i - \lambda_j^{(k)}| \leq C_i \cdot \delta_{A_0 \mathcal{U}}(P_k)
\]

for some constant $C_i$ independent of $k$.

**Proof:** It is enough to show that

\[
\max_{v \in A_0 \mathcal{U}} \frac{\| (Q_k - Q) v \|_{a_0}}{\| v \|_{a_0}} = \max_{v \in A_0 \mathcal{U}} \frac{\| (P_k - I) v \|_{a_0}}{\| v \|_{a_0}}
\]

\[= \max \min_{v \in A_0 \mathcal{U}, p \in P_k} \frac{\| v - p \|_{a_0}}{\| v \|_{a_0}}
\]

\[= C_i \cdot \delta_{A_0 \mathcal{U}}(P_k). \quad \blacksquare
\]

### 2.3.2 On the Aronszajn type.
We recall that the intermediate operators of the Aronszajn method may be expressed as $A = A_0 + B$ and $A_k = A_0 + B P_k$ such that

\[0 < A_0 \leq A_k \leq A_{k+1} \leq A\]

with $\text{Dom}(A) \subset \text{Dom}(A_k) = \text{Dom}(A_0)$. Here $B$ is assumed to be coercive and $P_k : \mathcal{H}_b \rightarrow \mathcal{P}_k$ is a $b$-orthogonal projection. For any $v \in \text{Dom}(A)$, we have

\[
\|(A_k - A) v\| = \|B(P_k - I) v\| \quad \text{and} \quad \langle (A_k - A) v, v \rangle = \| (P_k - I) v \|^2_0.
\]

**Theorem 2.3.3.** If the set of vectors $\{p_l\}$ is chosen such that $\text{span}\{p_l\}$ is dense in $\text{Dom}(B)$ with respect to the norm $\|Bu\|$, then $\lambda_i^{(k)}$ converges to $\lambda_i$ for any $i$ satisfying $\lambda_i < \lambda_0^\circ$. Also for $j = i, i + 1, \ldots, i + m - 1$ and for any $u \in \mathcal{U}$,
\(1\) \( \lambda_i - \lambda_j^{(k)} \leq \max_{u \in U, \|u\| = 1} \| (I - P_k)u \|^2 + C_1 \cdot \max_{u \in U, \|u\| = 1} \| B(I - P_k)u \|^2 \)

\(2\) \( \| u - E_k u \| \leq C_2 \cdot \max_{u \in U, \|u\| = 1} \| B(I - P_k)u \| \)

for some \( C_i \)'s independent of \( k \).

For this we need the following lemmas.

**Lemma 2.3.4.** If the set of vectors \( \{p_i\} \) span a dense subspace in \( \text{Dom}(B) \) with respect to the graph norm \( \| Bu \| \), then \( \text{span}\{Bp_i\} \) is dense in \( H \) and thus \( \{p_i\} \) is a core of \( B \).

**Proof:** Suppose that there is a vector \( u \in H \) such that \( (u, Bp_i) = 0 \) for all \( i \). Since \( B \) is coercive and \( \text{Ran}(B) = H \), there is a bounded inverse \( B^{-1} \) such that \( u = BB^{-1}u \). Since \( \{p_i\} \) is dense in \( \text{Dom}(B) \) with respect to \( \| Bu \| \), it follows that \( B^{-1}u = 0 \). Thus \( u = 0 \).

**Lemma 2.3.5.** Let \( \{p_i\} \subset \text{Dom}(B) \) be chosen such that \( \text{span}\{Bp_i\} \) is dense in \( H \). Then the set of all vectors for which \( b(P_k u) \) is uniformly bounded with respect to \( k \) is the domain of \( b \). That is,

\[ \{ u \in H \mid b(P_k u) < \infty, \text{ for all } k \} = \text{Dom}(b). \]

**Proof:** Note that \( P_k u = \sum_{i,j=1}^{k} (u, Bp_i) b_{ij} p_j \) where \( [b_{ij}] \) is the inverse to the matrix \( [\langle p_i, Bp_j \rangle] \). Thus we have

\[
\langle P_k u, v \rangle = \sum_{i,j=1}^{k} (u, Bp_i) b_{ij} \langle p_j, v \rangle
\]

\[= \langle u, \sum_{i,j=1}^{k} Bp_i b_{ij} \langle p_j, v \rangle \rangle
\]

\[= \langle u, \sum_{i,j=1}^{k} \langle v, p_j \rangle b_{ij} Bp_i \rangle
\]

\[= \langle u, P_k^* v \rangle.
\]

That is,

\[
P_k^* v = \sum_{i,j=1}^{k} \langle v, p_i \rangle b_{ij} Bp_j.
\]
Hence
\[ P_k^* B v = \sum_{i,j=1}^{k} (B v, p_i) b_{ij} B p_j \]
\[ = \sum_{i,j=1}^{k} (v, B p_i) b_{ij} B p_j \]
\[ = B P_k v. \]

We note that for any \( n \) and \( m \), we have
\[ \lim_{n, m \to \infty} b(P_n u - P_m u) = \lim_{n, m \to \infty} |b(P_n u) - b(P_m u)| = 0 \]
since \( P_n P_n = P_m P_n = P_{\min(m,n)} \) and \( b(P_k u) < \infty \) for all \( k \). Thus there is a vector \( w \) in \( H_b \) such that \( P_k u \) converges to \( w \). For every \( i \), it follows that
\[ \langle w - u, B p_i \rangle = \lim_{n \to \infty} \langle P_n u, B p_i \rangle - \langle u, B p_i \rangle \]
\[ = \langle u, B p_i \rangle - \langle u, B p_i \rangle \]
\[ = 0 \quad \text{for sufficiently large } n. \]

Since \( \{B p_i\} \) is dense in \( H \), it follows that \( w = u \). The converse follows from the fact that \( P_k \) is a projection with respect to the norm induced by \( \langle u, B v \rangle \).

**Proof of Theorem 2.3.3**: By combining Lemmas 2.3.4 and 2.3.5 with Theorems 2.2.7 and 2.2.5, the result is obtained.

We note that it may not be easy to interpret the expression \( \|B(I - P_k)|u|\| \) since the projection \( P_k \) is orthogonal with respect to the inner product \( \langle u, B v \rangle \). However, if \( \|(P_k - I)|u|\|_3 = O(k^{-t}) \) and \( \|B(P_k - I)|u|\| = O(k^{-t}) \) as \( k \) becomes large for some constants \( s \) and \( t \), then we have
\[ |\lambda_i - \lambda_j^{(k)}| = O(k^{-2p}), \text{ where } p = \min(s, t) \]
for all \( j = i, i + 1, \ldots, i + m - 1 \). This is similar to the result Fix obtained in [24], although he assumed that \( B \) was bounded and used a special choice of the vectors \( p_i \)'s.
We assume that the operator $B$ is relatively bounded with respect to the base operator $A_0$ with bound $m$, i.e., $\|Bu\| \leq m\|A_0u\|$ and $\text{Dom}(A_0) \subseteq \text{Dom}(B)$. Thus $\text{Dom}(A) = \text{Dom}(A_k) = \text{Dom}(A_0)$. By the Heinz theorem [64], it follows that $\|B^{\frac{1}{2}}A_0^{-\frac{1}{2}}\| \leq m$. Now we consider the following:

\[
\|(A_k^{-1} - A^{-1})u\| = \|A_k^{-1}B(I - P_k)A^{-1}u\| \\
\leq \|A_k^{-1}B^\frac{1}{2}\|\|(I - P_k)A^{-1}u\|_b \\
\leq \|B^\frac{1}{2}A_0^{-\frac{1}{2}}\|\|A_0^\frac{1}{2}A_k^{-\frac{1}{2}}\|\|A_k^{-\frac{1}{2}}\|\|(I - P_k)A^{-1}u\|_b \\
\leq \frac{m\|A_0^{-\frac{1}{2}}\|}{\lambda_i}\|(I - P_k)u\|_b
\]

and

\[
\langle (A_k^{-1} - A^{-1})u, u \rangle = \langle (A_k^{-1}B(I - P_k)A^{-1}u, u \rangle \\
= \langle B(I - P_k)A^{-1}u, (I - P_k)A_k^{-1}u \rangle \\
\leq \|(I - P_k)A^{-1}u\|_b\|(I - P_k)A_k^{-1}u\|_b.
\]

Since

\[
\|(I - P_k)A_k^{-1}u\|_b \leq \|(I - P_k)(A_k^{-1} - A^{-1})u\|_b + \|(I - P_k)A^{-1}u\|_b \\
\leq \|A_k^{-1}B(I - P_k)A^{-1}u\|_b + \|(I - P_k)A^{-1}u\|_b \\
\leq \|B^\frac{1}{2}A_0^{-\frac{1}{2}}\|\|B^\frac{1}{2}(I - P_k)A^{-1}u\| + \|(I - P_k)A^{-1}u\|_b \\
\leq \|B^\frac{1}{2}A_0^{-\frac{1}{2}}\|\|(I - P_k)A^{-1}u\|_b + \|(I - P_k)A^{-1}u\|_b \\
= (\|B^\frac{1}{2}A_0^{-\frac{1}{2}}\|^2 + 1)\|(I - P_k)A^{-1}u\|_b,
\]

it follows that

\[
\langle (A_k^{-1} - A^{-1})u, u \rangle \leq \frac{m^2 + 1}{\lambda_i^2}\|(I - P_k)u\|_b^2.
\]

In 1961, Bazley and Fox showed that if the perturbation operator $B$ is relatively bounded with respect to $A_0$, $A_0$ has a compact inverse and the set of vectors $p_i$ is
complete in $\mathcal{H}_b$, then the inverses of the intermediate operators converge uniformly
to the inverse of the given operator, thus guaranteeing the convergence of the eigen-
values. In 1980, Weidmann introduced a weaker condition sufficient to guarantee the
convergence of eigenvalues of a sequence of operators in $\mathcal{S}$. He showed that the strong
resolvent convergence of a monotone operator sequence is enough for the convergence
of the eigenvalues. In 1982, Beattie proved that the completeness of $\{B_{p_1}\}$ in $\mathcal{H}$
implied strong resolvent convergence of $A_k$ to $A$ and so gave conditions for convergence
of intermediate problems.

**Theorem 2.3.6.** Let $B$ be relatively bounded with respect to $A_0$ and let $\{p_i\}$ be chosen
to be complete in $\text{Dom}(B)$ with respect to the quadratic form $b(u)$. Then for any $i$
satisfying $\lambda_i < \lambda^{(k)}_{\infty}$, $\lambda_i^{(k)}$ converges to $\lambda_i$, and for $j = i, i + 1, \ldots, i + m - 1$
and for any $u \in \mathcal{U}$,

1. $|\lambda_i - \lambda_j^{(k)}| \leq C_1 \cdot \max_{u \in \mathcal{U}, ||u|| = 1} \|(I - P_k)u\|_b$

2. $||u - E_k u|| \leq C_2 \cdot \max_{u \in \mathcal{U}, ||u|| = 1} \|(I - P_k)u\|_b$

for some constant $C_i$'s independent of $k$.

**Proof:** Since $P_k$ is the orthogonal projection with respect to $b(u)$, $P_k$ converges
strongly to $I$ with respect to $b(u)$. Since $\|A_k^{-1} - A^{-1}\| = O(\|(P_k - I)A^{-1}u\|_b)$ for
any $u \in \mathcal{H}$, it follows that $A_k^{-1}$ converges strongly to $A^{-1}$. The conclusion follows
from Theorem 2.2.5 and the fact that $\frac{1}{\lambda_j^{(k)}} - \frac{1}{\lambda_i} \geq \frac{\lambda_i - \lambda^{(k)}_j}{\lambda^2_i}$. ■

Theorem 2.3.6 may be considered as an extension of the results of Bazley and
Fox [8] and Poznyak [52] because we do not assume that $A$ and $A_0$ have compact
inverses. We note that the density condition in Theorem 2.3.6 is weaker than that in
Theorem 2.3.3 because the latter implies the former. If $B$ is not relatively bounded
with respect to $A_0$, we need the latter condition for the convergence of the eigenvalues.
For counter examples, one may refer to [28]. We note in passing that we need only the
relative form boundedness of $B$ to $A_0$ in the proof instead of the relative boundedness itself. Moreover, the latter is stronger than the former (Heinz Theorem). Beattie and Greenlee [21] showed that the relative boundedness may be replaced by the relative form boundedness under the assumption that $A_0 + B$ is essentially self-adjoint with unique self-adjoint extension $A$.

**Corollary 2.3.7.** Let $Q_k : \mathcal{H}_a \rightarrow \mathcal{P}_k$ be an $a$-orthogonal projection onto $\mathcal{P}_k$. Then the bound in Theorem 2.3.6 may be replaced by $\|(I - Q_k)u\|_a^2$.

**Proof:** The result follows from the fact that

$$\|(I - P_k)u\|_b = \|(I - P_k)(I - Q_k)u\|_b \leq \|(I - Q_k)u\|_b \leq \|B^\frac{1}{2}A_0^{-\frac{1}{2}}\|\|(I - Q_k)u\|_a \leq m\|(I - Q_k)u\|_a.$$

**Remark.**

$$\|(I - F_k)u\|_b = \max_{u \in \mathcal{U}, \|u\| = 1} \|u - P_ku\|_b = \max_{u \in \mathcal{U}, \|u\| = 1} \min_{p \in \mathcal{P}_k} \|u - p\|_b = \max_{u \in \mathcal{U}} \min_{p \in \mathcal{P}_k} \frac{\|B^\frac{1}{2}u - B^\frac{1}{2}p\| \|B^\frac{1}{2}u\|}{\|u\|} \leq \|B^\frac{1}{2}u\| \cdot \max_{v \in B^\frac{1}{2}\mathcal{U}} \min_{q \in B^\frac{1}{2}\mathcal{P}_k} \|v - q\| = O(\delta_B^\frac{1}{2}\mathcal{U} (B^\frac{1}{2}\mathcal{P}_k)),$$

since $\mathcal{U}$ is of finite dimension. Likewise it follows from $A_\frac{1}{2}\mathcal{U} \subseteq \mathcal{U}$ that

$$\|(I - Q_k)u\|_a = \max_{u \in \mathcal{U}, \|u\| = 1} \min_{p \in \mathcal{P}_k} \|u - p\|_a = O(\delta_\mathcal{U} (A_\frac{1}{2}\mathcal{P}_k)).$$

We note that if $p_i$ is selected to be a linear combination of $u_i$ which are the eigenvalues of $A$ corresponding to $\lambda_i$, then we have a bound $O(\delta_\mathcal{U}(\mathcal{P}_k))$. Also, if $B$ is bounded, then we have $O(\delta_\mathcal{U}(\mathcal{P}_k))$ as a bound.
Corollary 2.3.8. Let \( \{ p_i \} \) be selected to be complete in \( \mathcal{H} \). If \( B \) is bounded, then for \( j = i, i + 1, \ldots, i + m - 1 \) and for any \( u \in \mathcal{U} \),

1. \( |\lambda_i - \lambda_j^{(k)}| = O(\delta_u^2(\mathcal{P}_k)) \)
2. \( \|u - E_ku\| = O(\delta_u(\mathcal{P}_k)) \).

2.3.3 On the Bazley-Fox Type. We recall that the intermediate operators of the Bazley-Fox method are represented by \( A_k = A_0 + T^*P_kT \) such that

\[
0 < A_0 \leq A_k \leq A_{k+1} \leq A
\]

with \( \text{Dom}(A) \subset \text{Dom}(A_k) = \text{Dom}(A_0) \). Here \( P_k : \mathcal{H}_0 \to \mathcal{P}_k \) is the \( \mathcal{H}_0 \)-orthogonal projection onto \( \mathcal{P}_k \). For any \( v \in \text{Dom}(A) \), we have

\[
\|(A_k - A)v\| = \|T^*(P_k - I)Tv\| \text{ and } \langle (A_k - A)v, v \rangle = \|(P_k - I)Tv\|^2.
\]

Theorem 2.3.9. Let \( \{ P_k \} \) be an increasing sequence of orthogonal projections in \( \mathcal{H}_0 \) such that for each \( k \), \( \text{Ran}(P_kT) \subset \text{Dom}(T^*) \cap \text{Ran}(T) \). If \( \text{Ran}(P_kT) \) is a core of \( T^* \), then for any \( i \) satisfying \( \lambda_i < \lambda_0^0 \), \( \lambda_i^{(k)} \) converges to \( \lambda_i \), and for \( j = i, i + 1, \ldots, i + m - 1 \) and for any \( u \in \mathcal{U} \),

1. \( |\lambda_i - \lambda_j^{(k)}| \leq \max_{u \in \mathcal{U}, \|u\| = 1} \|(I - P_k)Tu\|^2 + C_1 \cdot \max_{u \in \mathcal{U}, \|u\| = 1} \|T^*(I - P_k)Tu\|^2 \)
2. \( \|u - E_ku\| \leq C_2 \cdot \max_{u \in \mathcal{U}, \|u\| = 1} \|T^*(I - P_k)Tu\| \)

for some constants \( \{ C_i \} \) independent of \( k \).

Proof: We note that \( \cup \text{Ran}(P_kT) \) is a core of \( T^* \) if and only if \( \cup \text{Ran}(P_kT) \) is dense in \( \text{Dom}(T^*) \) with respect to the graph norm of \( T^* \) (cf. [45]). It follows then from [28,18] that \( A_k \) converges to \( A \) in the strong resolvent sense. Thus Theorem 2.2.5 implies the result.

We assume that the operator \( T^*T \) is relatively bounded with respect to the base operator \( A_0 \). Then \( \text{Dom}(a_0) \subset \text{Dom}(T) \) and thus \( \text{Dom}(a) = \text{Dom}(a_k) = \text{Dom}(a_0) \).
Now we consider that for any \( u \in \mathcal{U} \),
\[
\langle (A_k^{-1} - A^{-1})u, u \rangle = \langle (A_k^{-1} T^* (I - P_k) TA^{-1} u, u \rangle \\
= \|(I - P_k) TA^{-1} u, (I - P_k) TA_k^{-1} u \|_* \\
\leq \|(I - P_k) TA^{-1} u \|_* (\|T(A_k^{-1} - A^{-1})u \|_* + \|(I - P_k) TA^{-1} u \|_*) \\
\leq \|(I - P_k) TA^{-1} u \|_* (m^2 \|(I - P_k) TA^{-1} u \|_*) \\
+ \|(I - P_k) TA^{-1} u \|_* \\
\leq (m^2 + 1) \|(I - P_k) TA^{-1} u \|_*^2 \\
\leq \frac{m^2 + 1}{\lambda_i^2} \|(I - P_k) Tu \|_*^2
\]
with \( m = \| TA_0^{-\frac{1}{2}} \|_* \) and
\[
\|(A_k^{-1} - A^{-1})u \| = \| A_k^{-1} T^* (I - P_k) TA^{-1} u \| \\
\leq m \| A_0^\frac{1}{2} A_k^\frac{1}{2} \| \| A_k^{-\frac{1}{2}} \| \|(I - P_k) TA^{-1} u \|_* \\
\leq \frac{m \| A_0^\frac{1}{2} \|}{\lambda_i} \|(I - P_k) Tu \|_*.
\]

Hence we have the following estimation.

**Theorem 2.3.10.** Let \( T^*T \) be relatively bounded to \( A_0 \) and let \( P_k \) converge strongly to \( I \) in \( \mathcal{H}_* \). Then for any \( i \) satisfying \( \lambda_i < \lambda_0^0 \), \( \lambda_i^{(k)} \) converges to \( \lambda_i \), and for \( j = i, i+1, \ldots, i+m-1 \) and for any \( u \in \mathcal{U} \),
\[
(1) \quad |\lambda_i - \lambda_j^{(k)}| \leq C_1 \cdot \max_{u \in \mathcal{U}, \|u\| = 1} \|(I - P_k) Tu \|_*^2 \\
(2) \quad \|u - E_ku\| \leq C_2 \cdot \max_{u \in \mathcal{U}, \|u\| = 1} \|(I - P_k) Tu \|_*
\]
for some constants \( C_i \)'s independent of \( k \).

**Proof:** Since the assumption implies that \( A_k \) converges to \( A \) in the strong resolvent sense, the conclusion follows from Theorem 2.2.5 and the fact that \( \frac{1}{\lambda_j^{(k)}} - \frac{1}{\lambda_j} \geq \frac{\lambda_j - \lambda_j^{(k)}}{\lambda_j^2} \).

\[\Box\]
This may be considered as an extension of the result Pozryak [53] obtained because we do not assume that \( A \) and \( A_0 \) have compact inverses.

**Remark.**

\[
\max_{u \in U, \|u\|=1} \| (I - P_k)Tu \|_* = \max_{v \in U} \frac{\|Tu - P_kTu\|_* \|Tu\|_*}{\|Tu\|_*} \\
\leq \max_{u \in U, \|u\|=1} \|Tu\|_* \cdot \max_{v \in TU} \frac{\|v - P_kv\|_*}{\|v\|_*} \\
= \max_{u \in U, \|u\|=1} \|Tu\|_* \cdot \max_{v \in TU} \min_{p \in P_k} \|v - p\|_* \\
= O(\delta_{TU}(P_k))
\]

since \( U \) is of finite dimension.
2.4 Convergence Rates for the Method of Truncation including the Remainder.

We recall that the intermediate forms are

\[ a_\delta(u) = a_0^{(\gamma)}(u) + \tilde{a}(P_k u), \]

for \( u \in \text{Dom}(a_k) = \mathcal{H} \), with the corresponding self-adjoint operator

\[ A_k = A_0^{(\gamma)} + \tilde{A}P_k. \]

Here the quadratic form, \( \tilde{a} \), is

\[ \tilde{a}(u) = a(u) - a_0^{(\gamma)}(u) \geq b(u) \geq \alpha\|u\|^2 \]

and the corresponding self-adjoint operator

\[ \tilde{A} = A - A_0^{(\gamma)}, \]

where \( A_0^{(\gamma)} \) is the truncation of \( A_0 \) at \( \gamma \). Also, the operator \( P_k \) is the projection from \( \mathcal{H}_\delta \) onto \( P_k \) that is orthogonal with respect to the inner product \( \langle u, \tilde{A}v \rangle \). For clarity, we denote that \( \lambda(A) \) is an eigenvalue corresponding to the operator \( A \).

Suppose that the set of vectors \( \{p_i\} \) is taken to be dense in \( \text{Dom}(\tilde{A}) \) with respect to the graph norm \( \|\tilde{A}u\| \). Then it follows from Lemmas 2.3.4 and 2.3.5 that the set of all vectors with which \( \tilde{a}(P_k u) \) is uniformly bounded with respect to \( k \) is the domain of \( \tilde{a} \). Application of Theorem 2.2.7 implies that \( A_k \) converges to \( A \) in the strong resolvent sense. Since \( \langle u, (A - A_k)u \rangle = \|(P_k - I)u\|_\delta^2 \) and \( \|(A - A_k)u\| = \|\tilde{A}(P_k - I)u\| \), we have the following estimate for this method.

**Lemma 2.4.1.** If the set of vectors \( \{p_i\} \) is dense in \( \text{Dom}(\tilde{A}) \) with respect to the norm \( \|\tilde{A}u\| \), then \( \lambda_i^{(k)} \) converges to \( \lambda_i \) for any \( i \) satisfying \( \lambda_i < \gamma \), and for all \( j = i, i + 1, \ldots, i + m - 1 \) and \( u \in \mathcal{U} \),

\[ (1) \quad |\lambda_i(A) - \lambda_j(A_k)| \leq \max_{u \in \mathcal{U}, \|u\| = 1} \|(I - P_k)u\|_\delta^2 + C_1 \cdot \max_{u \in \mathcal{U}, \|u\| = 1} \|\tilde{A}(I - P_k)u\|^2 \]
\[(2) \|u - E_k u\| \leq C_2 \cdot \max_{u \in \mathcal{U}, \|u\| = 1} \|\tilde{A}(I - P_k)u\|,\]

for some \(C_i\)'s independent of \(k\).

It may not be easy to interpret the expression \(\max_{u \in \mathcal{U}, \|u\| = 1} \|\tilde{A}(I - P_k)u\|\). In order to get an interpretation for the expression, we adopt the following from [19]. We first assume that \(A\) is bounded, then

\[\|\tilde{A}(I - P_k)u\| = \|\tilde{A}^\frac{1}{2}\|(I - P_k)u\|_a.\]

Thus \(A_k\) converges strongly to \(A\).

Define \(Q_k : \mathcal{H} \rightarrow \text{span}_{1 \leq i \leq k}\{\tilde{A}P_i\}\) to be the orthogonal projection. Then

\[\|(I - P_k)u\|_a \leq \|\tilde{A}^{-\frac{1}{2}}\|(I - P_k^*)\tilde{A}u\|\]
\[\leq \|\tilde{A}^{-\frac{1}{2}}\|(I - P_k)\|\|(I - Q_k)\tilde{A}u\|\]
\[\leq \|\tilde{A}^{-\frac{1}{2}}\|(1 + \|\tilde{A}P_k\tilde{A}^{-1}\|)\|(I - Q_k)\tilde{A}u\|\]
\[\leq \|\tilde{A}^{-\frac{1}{2}}\|(1 + \kappa)\|(I - Q_k)\tilde{A}u\|,\]

where \(\kappa = \|\tilde{A}^{\frac{1}{2}}\|\|\tilde{A}^{-\frac{1}{2}}\|\). It follows that we have

**Theorem 2.4.2.** Assume the hypotheses of Lemma 2.4.1. If \(A\) is bounded, then for \(j = i, i + 1, \ldots, i + m - 1\) and \(u \in \mathcal{U}\),

\[\begin{enumerate}
  \item \(|\lambda_i(A) - \lambda_j(A_k)| \leq C_1 \cdot \max_{u \in \mathcal{U}, \|u\| = 1} \|(I - Q_k)\tilde{A}u\|^2\)
  \item \(\|u - E_k u\| \leq C_2 \cdot \max_{u \in \mathcal{U}, \|u\| = 1} \|(I - Q_k)\tilde{A}u\|\)
\end{enumerate}\]

for some constants \(C_i\)'s independent of \(k\).

**Remark.**

\[\max_{u \in \mathcal{U}} \frac{\|(I - Q_k)\tilde{A}u\|}{\|u\|} = \max_{u \in \mathcal{U}} \frac{\|\tilde{A}u - Q_k\tilde{A}u\|}{\|\tilde{A}u\|} \frac{\|\tilde{A}u\|}{\|u\|}\]
\[\leq \max_{u \in \mathcal{U}, \|u\| = 1} \|\tilde{A}u\| \cdot \min_{v \in \tilde{A}u} \frac{\|v - p\|}{\|v\|}\]
\[= O(\delta_{\tilde{A}u}(\tilde{A}P_k)).\]
For the following argument we are indebted to Greenlee [43] and Beattie and Greenlee [19,20]. We assume that $A$ is unbounded. It could happen that $P_k$ fails to converge strongly to $I$ so that $\{P_k\}$ may not be uniformly bounded. In order to bypass this difficulty, Greenlee introduced the auxiliary operator

$$\tilde{A} = A^{(\mu)} - A_0^{(\gamma)}$$

where $\mu$ is chosen sufficiently large so that the corresponding quadratic form satisfies $\tilde{a}(u) \geq \frac{\alpha}{2}\|u\|^2$. See [43] for a proof that such a $\mu$ exists. We then have

$$a^{(\mu)}(u) = a_0^{(\gamma)}(u) + \tilde{a}(u),$$

applying the Aronszajn method to this decomposition of $a^{(\mu)}$.

Given the approximating vectors $\{p_i\}$, we define $\{\hat{p}_i\}$ by $\hat{p}_i = \tilde{A}^{-1}\tilde{A}p_i$, for each $i = 1, 2, \ldots$. Then the following lemma easily follows.

**Lemma 2.4.3.** If $\{p_i\}$ is dense in $\text{Dom}(\tilde{A})$ with respect to the norm $\|\tilde{A}u\|$, then the set of $\{\hat{p}_i\}$ is dense in $\text{Dom}(\tilde{A})$ with respect to $\|\tilde{A}u\|$.

**Proof:** We assume that $\left< \tilde{A}u, \tilde{A}\hat{p}_i \right> = 0$ for some $u \in \text{Dom}(\tilde{A})$, then

$$0 = \left< \tilde{A}u, \tilde{A}\hat{p}_i \right> = \left< \tilde{A}\tilde{A}^{-1}\tilde{A}u, \tilde{A}\hat{p}_i \right>.$$

Since $\{p_i\}$ is complete in $\text{Dom}(\tilde{A})$ with respect to the graph norm $\|\tilde{A}u\|$, it follows that $\tilde{A}^{-1}\tilde{A}u = 0$. Hence $u = 0$.  $lacksquare$

Now we define $\hat{P}_k : \mathcal{H}_{\tilde{A}} \rightarrow \hat{P}_k$ to be the orthogonal projection, where $\hat{P}_k = \text{span}_{1 \leq i \leq k}\{\hat{p}_i\}$. Since $\tilde{A}$ is bounded, the projections $\hat{P}_k$ and $\hat{P}_k^*$ converges to $I$ strongly. Furthermore

$$\text{Ran}(I - \hat{P}_k) = \text{Ker}\hat{P}_k = (\tilde{A}\hat{P}_k)^\perp = (\tilde{A}\mathcal{P}_k)^\perp = \text{Ker}P_k = \text{Ran}(I - P_k).$$

We define the intermediate operators as

$$A''_k = A_0^{(\gamma)} + \tilde{A}\hat{P}_k.$$
Then we have for $u \in \text{Dom}(\tilde{a})$,
\[
\tilde{a}(\tilde{P}_k u) = \tilde{a}(u - (I - \tilde{P}_k)u) \leq \tilde{a}(u - (I - P_k)u) = \tilde{a}(P_k u) \leq \tilde{a}(P_k u) \leq \tilde{a}(u),
\]
since $\text{Ran}(I - \tilde{P}_k) = \text{Ran}(I - P_k)$ and $I - \tilde{P}_k$ is orthogonal with respective to $\tilde{a}$, but $I - P_k$ is not.

**Remark.** We note that if $\{p_i\}$ is chosen to be dense with respect to $\tilde{a}(u)$ and $\hat{p}_i$ is defined by $\tilde{A}^{-\frac{1}{2}} A^{-\frac{1}{2}} p_i$, then the set $\{\hat{p}_i\}$ is complete in $\text{Dom}(\hat{A})$ with respect to $\tilde{a}(u)$. But the set of $\{\hat{p}_i\}$ does not produce $\text{Ran}(I - \hat{P}_k) = \text{Ran}(I - P_k)$. The reason is that since $(\hat{A}\hat{P}_k)^\perp \neq (\tilde{A}P_k)^\perp$, we may not have
\[
\tilde{a}(u - (I - \hat{P}_k u)) \leq \tilde{a}(u - (I - P_k u)).
\]

The above inequality yields that for any $i$ with $\lambda_i(A) < \gamma$,
\[
\lambda_i(A''_k) \leq \lambda_i(A_k) \leq \lambda_i(A)
\]
so that
\[
|\lambda_i(A) - \lambda_j(A_k)| \leq |\lambda_i(A) - \lambda_j(A'')_k|.
\]

**Theorem 2.4.4.** If the set of vectors $\{p_i\}$ is dense in $\text{Dom}(\tilde{A})$ with respect to the norm $\|\tilde{A}u\|$, then for $j = i, i + 1, \ldots, i + m - 1$,
\[
|\lambda_i(A) - \lambda_j(A_k)| \leq C \cdot \delta_{\tilde{A}U} (\tilde{A}\hat{P}_k)
\]
for some constants $C$ independent of $k$.

**Proof:** Let $\hat{Q}_k : \mathcal{H} \longrightarrow \text{span}_{1 \leq i \leq k}\{\tilde{A}\hat{p}_i\}$ be the orthogonal projection. Since $\tilde{A}$ is bounded, it follows from Theorem 2.4.2 and Lemma 2.4.3 that we have
\[
|\lambda_i(A) - \lambda_j(A_k)| \leq C \cdot \max_{u \in U, \|u\|=1} \| (I - \hat{Q}_k) \tilde{A}u \|^2.
\]
By the same argument as the remark of Theorem 2.4.2, we get
\[
\max_{u \in U} \frac{\| (I - \hat{Q}_k) \tilde{A}u \|}{\|u\|} = O(\delta_{\tilde{A}U} (\tilde{A}\hat{P}_k)).
\]
Since $\tilde{A}U = \tilde{A}U$ and $\tilde{A}\hat{P}_k = \tilde{A}P_k$, we have the results. $\blacksquare$
Remark. With the same conditions as Theorem 2.4.4 has, Beattie and Greenlee obtained a similar result to Theorem 2.4.4 [20]:

$$|\lambda_i(A) - \lambda_i(A_k)| \leq C \cdot \{\delta_{\gamma^2}(\bar{A}P_k) + \delta_{\gamma^2}(\bar{A}P_k)\}.$$ 

where $\mathcal{U}^\gamma$ and $\mathcal{U}_0^\gamma$ are the eigenspaces of $A$ and $A_0$, respectively, corresponding to the eigenvalues less than $\gamma$. 
2.5 Application to a Schrödinger Operator.

In order to apply the preceding estimates to differential eigenvalue problems, it is convenient to dominate the containment gap of Theorems 2.4.4 in terms of spectral projections of an auxiliary operator $B$. For this we cite Beattie and Greenlee's papers [19,20]. Let $B$ be a positive definite and self-adjoint operator in $\mathcal{H}$ such that $\text{Dom}(B) \subset \text{Dom}(\tilde{A})$ and $\|\tilde{A}u\| \leq \beta \|Bu\|, \beta \geq 0$, for all $u \in \text{Dom}(B)$ with $B^{-1}$ compact. Let

$$0 \leq \mu_1 \leq \mu_2 \leq \cdots \to \infty$$

be the eigenvalues of $B$ with corresponding eigenvectors $\{p_i\}$ orthonormal in $\mathcal{H}$. If these vectors $\{p_i\}$ are employed as the trial vectors to construct the projection operators $\{P_k\}$, then the following estimation is obtained.

**Theorem 2.5.1 (Beattie and Greenlee [19]).** If the eigenspace $\mathcal{U}$ is contained in $\text{Dom}(B^\tau)$ with $\tau > 1$, then

$$\delta_{\mathcal{AU}}(\tilde{A}P_k) = o(\mu_{k+1}^{1-\tau}), \quad \text{as } k \to \infty,$$

where $o$ is the usual Landau symbol and $B^\tau$ denotes the unique positive definite $\tau^{th}$ power of $B$.

Theorem 2.5.1 implies that if $\mathcal{U} \subset \text{Dom}(B^\tau)$, then

$$|\lambda_i(A) - \lambda_i(A_k)| = o(\mu_{k+1}^{2-2\tau})$$

$$\|u - E_ku\| = o(\mu_{k+1}^{1-\tau}),$$

as $k \to \infty$.

As an example, we experimentally verify the rate of convergence of a differential problem with non-trivial continuous spectrum that was considered in [19,20].

The eigenvalue problem is for a one-dimensional Schrödinger operator with potential defined by

$$q(x) = b(x^2 - a^2)\exp(-cx^2),$$

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where \( b \) and \( c \) are positive constants. That is, the operator \( A \) is given by

\[
Au = -u'' + qu
\]

for \( u \in H^2(\mathbb{R}) \) with the corresponding form,

\[
a(u) = \int_{-\infty}^{\infty} (|u'|^2 + q|u|^2)dx,
\]

for \( u \in H^1(\mathbb{R}) \). Let the square well potential \( q_0 \) be

\[
q_0(x) = \begin{cases} 
q(0) + \gamma, & -a < x < a \\
\gamma, & \text{otherwise,}
\end{cases}
\]

where \( \gamma < 0 \) is so big that all negative eigenvalues of \( A \) are less than \( \gamma \). The negative number \( \gamma \) will be our truncation point. We define the base operator \( A_0 \) by

\[
A_0u = -u'' + q_0u,
\]

for \( u \in H^2(\mathbb{R}) \) with the corresponding form

\[
a_0(u) = \int_{-\infty}^{\infty} (|u'|^2 + q_0|u|^2)dx,
\]

for \( u \in H^1(\mathbb{R}) \). The base problem \( A_0u = \lambda u \) is explicitly solvable. In fact, if we consider only the even symmetry class of functions for convenience, the lower spectrum of \( A_0 \) consists of simple eigenvalues which are the solutions in \( \lambda \) of

\[
\tan(\alpha \sqrt{ba^2} - \gamma + \lambda) = \sqrt{\frac{\gamma - \lambda}{ba^2 - \gamma + \lambda}}
\]

lying in the interval \((\gamma - ba^2, \gamma)\). The lowest point of the essential spectrum of \( A_0 \) is given by \( \gamma \) and the number of eigenvalues of \( A_0 \) smaller than \( \gamma \) is equal to the biggest integer, say \( N \), smaller than \( \frac{\alpha \sqrt{\lambda}}{\pi} + 1 \). These eigenvalues below \( \gamma \) are labeled as \( \lambda_1^0 \leq \lambda_2^0 \leq \cdots \leq \lambda_N^0 \). The corresponding (unnormalized) eigenvectors of \( A_0 \) are given by

\[
\begin{cases} 
\exp(-a\sqrt{\gamma - \lambda_i^0}) \cos(\sqrt{ba^2 + \lambda_i^0} - \gamma x), & -a < x < a \\
\cos(a\sqrt{ba^2 + \lambda_i^0} - \gamma) \exp(-\sqrt{\gamma - \lambda_i^0} |x|), & \text{otherwise.}
\end{cases}
\]
For the auxiliary operator $B$, we take the harmonic oscillator, that is,

$$B = -\frac{d^2}{dx^2} + \alpha^2 x^2,$$

with $\text{Dom}(B) = H^2(\mathbb{R}) \cap \text{Dom}(x^2)$. Then $B$ is self adjoint, and $\mu_k = \alpha(2k - 1)$ for $k = 1, 2, \ldots [32]$. Moreover $\mathcal{U} \subset \text{Dom}(B^*)$, for all $\tau > 0 [20]$. It follows that we have an estimation

$$|\lambda_i(A) - \lambda_i(A_k)| = o(k^{-\delta}) \text{ as } k \to \infty, \text{ for all } \delta > 0,$$

which is called infinite order convergence.

For the intermediate problem, we must choose $\{p_i\}$ so that the set becomes dense in $H^2(\mathbb{R})$. A useful choice appears to be the solutions to $Bp = \mu p$. The eigenvalues and eigenvectors are known as

$$p_k(x) = \left(\frac{1}{2^k k! \sqrt{\alpha \pi}}\right)^{\frac{1}{2}} H_k(\sqrt{\alpha} x) \exp(-\frac{1}{2} \alpha x^2)$$

and $\mu_k = \alpha(2k + 1)$ for $k = 0, 1, 2, \ldots$, where $H_k(\xi)$ is the Hermite polynomials satisfying the following recursion:

$$H_k(\xi) = 2\xi H_{k-1}(\xi)$$

$$H_{k+1}(\xi) = 2\xi H_k(\xi) - 2k H_{k-1}(\xi).$$

Since we restrict ourselves to the even symmetry subspace of $L^2(\mathbb{R})$, we need to consider only the even functions $\{p_{2k}\}$.

Now we consider the intermediate operators

$$A_k = A_0^{(\gamma)} + \tilde{A}P_k$$

where $A_0^{(\gamma)} u = \sum_{i=1}^{N} \lambda_i^{(0)} (u, u_i^0) u_i^0 + \gamma (u - \sum_{i=1}^{N} (u, u_i^0) u_i^0)$ and $\tilde{A} = A - A_0^{(\gamma)}$. Since the space $\text{span} \{u_1^0, \ldots, u_N^0\} \oplus \text{span} \{\tilde{A}p_1, \ldots, \tilde{A}p_k\}$ reduces the operator $A_k$, the intermediate problem $A_k u = \lambda u$ produces the matrix equation:
\[
\begin{bmatrix}
\langle A_k u_i^0, u_j^0 \rangle & \langle A_k u_i^0, \tilde{A} p_j \rangle \\
\langle \tilde{A} p_i, A_k u_j^0 \rangle & \langle A_k \tilde{A} p_i, \tilde{A} p_j \rangle
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix}
= \lambda
\begin{bmatrix}
\langle u_i^0, u_j^0 \rangle & \langle u_i^0, \tilde{A} p_j \rangle \\
\langle \tilde{A} p_i, u_j^0 \rangle & \langle \tilde{A} p_i, \tilde{A} p_j \rangle
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix}
\]
whose rank is \( k + N \). We recall that \( P_k u = \sum_{i,j=1,k}^k \langle u, \tilde{A} p_i \rangle b_{ij} p_j \) where the matrix \((b_{ij})\) is the inverse to the Gram matrix \((\langle p_i, \tilde{A} p_j \rangle)\). Notice then that if we assume the eigenvectors, \( u_i^0 \), of \( A_0 \) are normalized, the inner products in the above equation are expressed as the following:

\[
\langle A_k u_i^0, u_j^0 \rangle = \Lambda + B C^{-1} B^*
\]

\[
\langle A_k u_i^0, \tilde{A} p_j \rangle = \Lambda B + B C^{-1} A
\]

\[
\langle A_k \tilde{A} p_i, \tilde{A} p_j \rangle = B^* (\Lambda - \gamma) B + \gamma A + A C^{-1} A
\]
where

\[
A = (\langle \tilde{A} p_i, \tilde{A} p_j \rangle), \quad B = (\langle u_i^0, \tilde{A} p_j \rangle)
\]

\[
C = (\langle p_i, \tilde{A} p_j \rangle) \quad \text{and} \quad \Lambda = \text{diag}(\lambda_i^0).
\]
It follows from [16] that the above equation can be represented as a compact equation:

\[
\begin{bmatrix}
I & B \\
B^* & A
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2
\end{bmatrix}
= (\lambda - \gamma)
\begin{bmatrix}
(\Lambda - \gamma)^{-1} & 0 \\
0 & C
\end{bmatrix}
\begin{bmatrix}
y_1 \\
y_2
\end{bmatrix}
\]
where \( I \) is the identity matrix.

The matrices \( A, B \) and \( C \) may be expressed as

\[
A = (Ap_i, Ap_j) - \sum_{i=1}^N (\lambda_i^0 - \gamma) \langle p_i, u_i^0 \rangle \langle u_i^0, Ap_j \rangle + \langle p_j, u_i^0 \rangle \langle u_i^0, Ap_i \rangle
\]

\[
+ \sum_{i=1}^N (\lambda_i^0 - \lambda_i^2) \langle p_i, u_i^0 \rangle \langle p_j, u_i^0 \rangle - 2\gamma \langle Ap_i, p_j \rangle + \gamma^2 \langle p_i, p_j \rangle
\]

\[
B = \langle u_i^0, Ap_j \rangle - \lambda_i^0 \langle u_i^0, p_j \rangle
\]

\[
C = (Ap_i, p_j) - \sum_{i=1}^N (\lambda_i^0 - \gamma) \langle p_i, u_i^0 \rangle \langle u_i^0, p_j \rangle - \gamma \langle p_i, p_j \rangle.
\]
Thus the inner products involved may be expressed in terms of the four basic ones

\[ \langle u_i^0, p_j \rangle, \langle u_i^0, Ap_j \rangle, \langle Ap_i, A p_j \rangle \text{ and } \langle Ap_i, p_j \rangle. \]

Analytical expressions may be obtained for \( \langle Ap_i, p_j \rangle \) and \( \langle Ap_i, Ap_j \rangle \). But the inner products \( \langle u_i^0, p_j \rangle \) and \( \langle u_i^0, Ap_j \rangle \) must be approximated with numerical quadratures. For reasons of economy and precision they are determined from recurrence relations that are derived from the basic three-term recurrence for Hermite polynomials. In the appendix we will express how to compute the basic four inner products in detail using the recurrence relations of Hermite polynomials. The transcendental integral evaluations are reduced to the evaluation of the complementary error function and the quadrature of

\[ \int_0^a \cos(\sqrt{b}a^2 - \gamma + \lambda_i^0 x) \exp(-\frac{x^2}{2}) \, dx \]

for \( i = 1, 2, \ldots, N. \)

Calculations were performed on a Vax 8800 in double precision carrying a unit roundoff \( \approx 1.4 \times 10^{-17} \). Numerical quadratures were carried out using Gauss-Kronrod scheme to an estimated relative accuracy of \( 10^{-14} \). The matrix eigenvalue problem was solved using the QZ method of Moler and Stewart with eigenvalues participating in bounds to a relative accuracy of better than \( 10^{-11} \). An order 30 Rayleigh-Ritz calculation using even-ordered Hermite trial functions were performed to provide complementary upper bounds. The computational results are given in Table 1 and Table 2 and the difference between upper and lower bounds are plotted against intermediate problem order \( k \), on a log-log scale in Figures 1 and 2. We observe that no linear asymptote is apparent for any of the error curves, which is consistent with the predicted infinite order convergence.
Table 1. Radial Schrödinger Equation: $\gamma = 0$

<table>
<thead>
<tr>
<th>N</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>-17.764406220</td>
<td>-15.885358216</td>
<td>-12.162742720</td>
</tr>
<tr>
<td>5</td>
<td>-16.108567768</td>
<td>-9.0407459021</td>
<td>-3.1574282306</td>
</tr>
<tr>
<td>10</td>
<td>-16.108530509</td>
<td>-9.0354830733</td>
<td>-3.0515306038</td>
</tr>
<tr>
<td>Ritz</td>
<td>-16.108530475</td>
<td>-9.0354751845</td>
<td>-3.0510013156</td>
</tr>
</tbody>
</table>

Table 2. Radial Schrödinger Equation: $\gamma = -0.1$

<table>
<thead>
<tr>
<th>N</th>
<th>$\lambda_1$</th>
<th>$\lambda_2$</th>
<th>$\lambda_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>-17.864406220</td>
<td>-15.985358216</td>
<td>-12.262742720</td>
</tr>
<tr>
<td>5</td>
<td>-16.108571114</td>
<td>-9.0413075976</td>
<td>-3.1734022489</td>
</tr>
<tr>
<td>10</td>
<td>-16.108530500</td>
<td>-9.0354832125</td>
<td>-3.0515521939</td>
</tr>
<tr>
<td>Ritz</td>
<td>-16.108530475</td>
<td>-9.0354751845</td>
<td>-3.0510013156</td>
</tr>
</tbody>
</table>
Figure 1: Schrödinger equation; \( \gamma = 0 \)
Figure 2: Schrödinger equation; gamma=0.1
2.6 Appendix.

In this section we express how to compute the four basic inner products

\[ \langle A_{p_i}, p_j \rangle, \langle A_{p_i}, A_{p_j} \rangle, \langle u_{i}^{0}, p_j \rangle \text{ and } \langle u_{i}^{0}, A_{p_j} \rangle \]

and how to relate with the matrix pencil.

For the computations of \( \langle A_{p_i}, p_j \rangle \text{ and } \langle A_{p_i}, A_{p_j} \rangle \), we denote that

\[
P_{ij} = \langle p_i', p_j' \rangle \quad A_{1ij} = \langle p_i'', p_j'' \rangle \quad A_{4ij} = \langle x^2 e^{-cx^2} p_i, e^{-cx^2} p_j \rangle
\]

\[
S_{ij} = \langle e^{-cx^2} p_i, p_j \rangle \quad A_{2ij} = \langle p_i', x^2 e^{-cx^2} p_j \rangle \quad A_{5ij} = \langle e^{-cx^2} p_i, e^{-cx^2} p_j \rangle
\]

\[
T_{ij} = \langle x^2 e^{-cx^2} p_i, p_j \rangle \quad A_{3ij} = \langle p_i'', e^{-cx^2} p_j \rangle \quad A_{6ij} = \langle x^2 e^{-cx^2} p_i, x^2 e^{-cx^2} p_j \rangle
\]

for \( i, j = 0, 1, \ldots, 2(k - 1) \). Then the inner products \( \langle A_{p_i}, p_j \rangle \text{ and } \langle A_{p_i}, A_{p_j} \rangle \) can be expressed as

\[
\langle A_{p_i}, p_j \rangle = P_{ij} + bT_{ij} - ba^2 S_{ij}
\]

\[
\langle A_{p_i}, A_{p_j} \rangle = A_{1ij} - b(A_{2ij} + A_{2ji}) + ba^2(A_{3ij} + A_{3ji}) - b^2a^2(A_{4ij} + A_{4ji})
\]

\[
+ b^2a^4 A_{5ij} + b^2 A_{6ij}.
\]

Thus we need to compute the matrices \( P, S, T, A_1, A_2, A_3, A_4 \) and \( A_5 \). For \( i \) and \( j \geq 0 \) we have

\[
P_{ij} = \frac{\alpha}{2} \left[ (\sqrt{i+j} + \sqrt{(i+1)(j+1)})\delta_{ij} - \sqrt{i(j+1)}\delta_{i-1,j+1} - \sqrt{j(i+1)}\delta_{i+1,j-1} \right]
\]

\[
S_{ij} = \frac{\alpha}{\alpha + c} \sqrt{\frac{j}{i}} S_{i-1,j-1} - \frac{c}{\alpha + c} \sqrt{\frac{i-1}{i}} S_{i-2,j}
\]

\[
T_{ij} = \frac{1}{2\alpha} \left[ \sqrt{(i+1)(j+1)}S_{i+1,j+1} + \sqrt{i(j+1)}S_{i-1,j+1} + \sqrt{j(i+1)}S_{i+1,j-1}
\right.
\]

\[
\left. + \sqrt{ij}S_{i-1,j-1} \right]
\]

\[
A_{1ij} = \frac{\alpha^2}{4} \left[ \sqrt{(i+1)(i+2)(j+1)(j+2)} + (2i+1)(2j+1) + \sqrt{i(i-1)}j(j-1)\delta_{ij}
\right.
\]

\[
- (2j+1)\sqrt{(i+1)(i+2)} + (2i+1)\sqrt{j(j-1)}\delta_{i+2,j} + \sqrt{(i+1)(i+2)}j(j-1)\delta_{i+2,j-2} \right]
\]

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\[ A_{2ij} = \frac{\alpha}{2} \left[ (i+1)(i+2)T_{i+2,j} - (2i+1)T_{ij} + \sqrt{i(i-1)}T_{i-2,j} \right] \]
\[ A_{3ij} = \frac{\alpha}{2} \left[ (i+1)(i+2)S_{i+2,j} - (2i+1)S_{ij} + \sqrt{i(i-1)}S_{i-2,j} \right] \]
\[ A_{4ij} = \hat{T}_{ij} \quad \text{and} \quad A_{5ij} = \hat{S}_{ij} \]
\[ A_{6ij} = \frac{1}{2\alpha} \left[ (i+1)(i+2)A_{4i+2,j} + (2i+1)A_{4ij} + \sqrt{i(i-1)}A_{4i-2,j} \right] \]

with \( S_{00} = \sqrt{\frac{\alpha}{\alpha + c}} \). Here \( \hat{T}_{ij} \) and \( \hat{S}_{ij} \) are the same as \( S_{ij} \) and \( T_{ij} \) except that \( c \) is replaced by \( 2c \) and we use the symmetry of \( S_{ij} \), i.e. \( S_{ij} = S_{ji} \), to get the value \( S_{0j} \).

For the computation of \( \langle u_i^0, p_j \rangle \) and \( \langle u_i^0, A p_j \rangle \), we define by

\[ \lambda_i = \lambda_i^0 - \gamma, \quad \beta_i = e^{-\sqrt{-\lambda_i^0}}, \quad \alpha_i = \cos(\sqrt{ba^2 + \lambda_i^0}) \quad \text{and} \quad d_i = \sqrt{ba^2 + \lambda_i^0}, \]

for \( i = 1, 2, \ldots, N \). We denote again by

\[ A_{ij} = \int_0^a \cos(d_i x) \cdot H_j(\sqrt{\alpha x}) \cdot e^{-\frac{1}{2}\alpha x^2} \, dx \]
\[ B_{ij} = \int_a^{\infty} \, e^{-\sqrt{-\lambda_i^0} x} \cdot H_j(\sqrt{\alpha x}) \cdot e^{-\frac{1}{2}\alpha x^2} \, dx, \]
\[ A'_{ij} = \int_0^a \cos(d_i x) \cdot H_j(\sqrt{\alpha x}) \cdot e^{-\frac{1}{2}(\alpha + c)x^2} \, dx \]
\[ B'_{ij} = \int_a^{\infty} \, e^{-\sqrt{-\lambda_i^0} x} \cdot H_j(\sqrt{\alpha x}) \cdot e^{-\frac{1}{2}(\alpha + c)x^2} \, dx, \]
\[ A''_{ij} = \int_0^a \cos(d_i x) \cdot H_j(\sqrt{\alpha x}) \cdot x^2 \cdot e^{-\frac{1}{2}(\alpha + c)x^2} \, dx \]
\[ B''_{ij} = \int_a^{\infty} \, e^{-\sqrt{-\lambda_i^0} x} \cdot H_j(\sqrt{\alpha x}) \cdot x^2 \cdot e^{-\frac{1}{2}(\alpha + c)x^2} \, dx, \]

for \( i = 1, 2, \ldots, N \) and \( j = 0, 1, \ldots, 2(k - 1) \). Then we have

\[ \langle u_i^0, p_j \rangle = 2C_j(\beta_i A_{ij} + \alpha_i B_{ij}) \]
\[ \langle u_i^0, A p_j \rangle = 2C_j(d_i^2 \beta_i A_{ij} + \lambda_i \alpha_i B_{ij}) - 2ba^2C_j(\beta_i A'_{ij} + \alpha_i B'_{ij}) + 2b.C.(\beta_i A''_{ij} + \alpha_i B''_{ij}), \]

where \( C_j = \left( \frac{1}{(2j)!} \sqrt{\pi} \right)^{\frac{3}{2}} \). The recurrence formula for \( A_{ij}, A'_{ij}, A''_{ij}, B_{ij}, B'_{ij} \) and \( B''_{ij} \) are
for $i \geq 1$ and $j \geq 0$,

$$A_{i,j+2} = (4j + 2 - \frac{4}{\alpha}d^2)A_{ij} - 4j(j - 1)A_{ij-2} + \frac{4}{\alpha}d_iH_j(\sqrt{\alpha}a)e^{-\frac{1}{2}\alpha a^2} \sin(d_ia)$$

$$- \frac{1}{\sqrt{\alpha}}[-8jH_{j-1}(0) + 2H_{j+1}(\sqrt{\alpha}a) - 2jH_{j-1}(\sqrt{\alpha}a)e^{-\frac{1}{2}\alpha a^2} \cos(d_ia)]$$

$$A'_{i,j+2} = \frac{1}{\alpha}(\frac{2\alpha}{\alpha + 2c})^2[d_iH_j(\sqrt{\alpha}a) \sin(d_ia)e^{-\frac{1}{2}\alpha a^2} + \sqrt{\alpha}H_{j+1}(0)]$$

$$+ 2j\sqrt{\alpha}(\frac{1}{2} - \frac{c}{\alpha})H_{j-1}(\sqrt{\alpha}a) - \sqrt{\alpha}(\frac{1}{2} + \frac{c}{\alpha})H_{j+1}(\sqrt{\alpha}a)e^{-\frac{1}{2}\alpha a^2} \cos(d_ia)$$

$$- 4j(j - 1)\alpha(\frac{1}{2} - \frac{c}{\alpha})^2A_{ij-2} + 2(2j + 1)\alpha(\frac{1}{2} - \frac{c}{\alpha})(\frac{1}{2} + \frac{c}{\alpha}) - d^2A_{ij}]$$

$$A''_{ij} = \frac{1}{\alpha}(A'_{i,j+2} + (j + \frac{1}{2})A'_{ij} + j(j - 1)A'_{i,j-2}),$$

and for $i \geq 1$ and $j \geq 1$,

$$B_{ij} = \frac{2}{\sqrt{\alpha}}[H_{j-1}(\sqrt{\alpha}a)e^{-\frac{1}{2}\alpha a^2} - \sqrt{-\lambda_i}B_{ij-2} - \sqrt{-\lambda_i}B_{ij-1}]$$

$$B'_{i,j} = \frac{2\sqrt{\alpha}}{\alpha + 2c}[H_{j-1}(\sqrt{\alpha}a)e^{-\frac{1}{2}\alpha a^2} - \sqrt{-\lambda_i}B_{ij-2} - \sqrt{-\lambda_i}B_{ij-1}]$$

$$B''_{ij} = \frac{1}{(\alpha + 2c)^2}[(a(\alpha + 2c) - \sqrt{-\lambda_i})H_j(\sqrt{\alpha}a) + 2j\sqrt{\alpha}H_{j-1}(\sqrt{\alpha}a)$$

$$e^{-\frac{1}{2}\alpha a^2} - \sqrt{-\lambda_i} + (a + 2c - \lambda_i)B'_{ij} - 4j\sqrt{-\lambda_i}eB''_{ij-1}$$

$$+ 4j(j - 1)\alpha B'_{ij-2}]$$

with

$$A_{i0} = \int_0^a \cos(d_ia)e^{-\frac{1}{2}\alpha a^2} \, dx$$

$$A'_{i0} = \int_0^a \cos(d_ia)e^{-\frac{1}{2}\alpha a^2} \, dx$$

$$B_{i0} = \sqrt{\frac{2}{\alpha}}e^{-\frac{1}{2\alpha}}(\frac{\sqrt{\pi}}{2}) - \frac{\sqrt{\pi}}{2}\sqrt{\frac{\alpha}{2} + \frac{\alpha}{2c}}$$

$$B_{i0}' = \sqrt{\frac{2}{\alpha}}e^{-\frac{1}{2\alpha}}(\frac{\sqrt{\pi}}{2}) - \frac{\sqrt{\pi}}{2}\sqrt{\frac{\alpha}{2} + \frac{\alpha}{2c}}$$

We note here that it may not be necessary to compute if $j$ is odd because of even symmetry.
CHAPTER 3

A STUDY OF THE EIGENVECTOR FREE METHOD
WITH CONVERGENCE BEHAVIOR

3.1 Introduction.

With the method of intermediate eigenvalue problems we may consider the original operator eigenvalue problem as a perturbation of a simpler, resolvable, self-adjoint eigenvalue problem, called a base problem, that gives rough lower bounds. The full perturbation is approximated systematically by related finite-rank perturbations. The associated intermediate eigenvalue estimates are obtained by computing the spectrum of the base operator summed with a positive semi-definite finite rank operator approximating the full perturbation. Intermediate problem methods have some limitations. In practice, they require not only explicit knowledge of reducing spaces and spectrum of the base operator but also special choices for the range space of the approximating finite rank operators. This makes the resulting problem involve dense matrices so that heavy burdens may be imposed on available computational resources. These practical obstructions primarily come from the explicit involvement of the base problem eigenfunctions which are typically supported throughout the problem domain and consequently may be difficult to handle practically. In the case of the Lehmann-Maehly method, even if one uses finite-element trial functions which make the computational matrix banded and well-structured, the method still depends on the knowledge of numbers that are known to separate adjacent eigenvalues of the given operator.

The so-called eigenvector free method (EVF) which has been developed by Beattie and Goerisch [17] may overcome such problems since it does not need information of eigenvectors of the base problem and permits the effective use of finite-element trial
functions so that it yields final computational matrices which are sparse and well-structured. Moreover it needs only information about separation of the spectrum of the base operator instead of the given operator itself, so it encompasses both the Weinstein–Aronszajn theory and the Lehmman–Maehley’s theory in a certain sense.

Bounds are derived ultimately from eigenvalues of generalized symmetric matrix eigenvalue problems. Highly accurate bounds require large matrix order which may make impractical the use of the QZ method [46] which, in spite of great stability, is unable to exploit any existing sparsity in the original coefficient matrices. For large-order problems, the necessity of retaining the sense of these derived bounds in the face of finite-precision arithmetic and finite computing resources leads to the consideration of iterative algorithms having a variational component. Such a component provides, at every step, intermediate results that may be used to deduce rigorous bounds, even if the method terminates prematurely.

In Section 2 we review the eigenvector free method (EVF) of Beattie and Geverisch. With EVF we explore experimentally in Section 3 convergence behavior of two one-dimensional examples which arise from the vibrations of beams. Section 4 deals with how to take advantage of the sparsity of large-order matrix eigenvalue problems as well as how to choose shifts to make the number of iterations small. With these shifts we explore experimentally in Section 5 convergence behavior of a two-dimensional example of vibrational frequencies of a clamped plate on rectangular domains. Section 6 presents convergence behavior of bounds for each problem and contains some remarks on this topic.
3.2 The Eigenvector Free Method of Beattie and Goerisch.

In this section we present a brief description of the EVF method. For more detail, one should refer to [17]. We recall from Chapter 1 that the associated $n \times n$ W-A matrix of the operator $A_{k,n} = A_0 - \delta^2 + B_k \hat{p}_n$ is given by

$$W_{k,n}(\lambda) = [(\hat{p}_i + R_{\lambda + \delta^2}B_k \hat{p}_i, B_k \hat{p}_j)]$$

(2.1)

for $i, j = 1, \ldots, n$. If we let $\mu = \lambda + \delta^2$ and introduce the change of variable $q_i = R_{\mu}B_k \hat{p}_i$ into the W-A matrix (2.1), we get

$$W_{k,n}(\lambda) = [(B_k^{-1}(A_0 - \mu)q_i, (A_0 - \mu)q_j) + \langle q_i, (A_0 - \mu)q_j \rangle]$$

which may be further simplified with the aid of the formula for $B_k^{-1}$ to get

$$W_{k,n}(\lambda) = [(q_i, (A_0 - \mu)q_j) + \frac{1}{\mu - \lambda} \{(q_i, (A_0 - \mu)q_i, (A_0 - \mu)q_j)

- \sum_{i,m=1}^{k} \langle (A_0 - \mu)q_i, T^* p_i \rangle c_{im} \langle T^* p_m, (A_0 - \mu)q_j \rangle]$$

If we define the matrices as

$$F_1 = [(q_i, (A_0 - \mu)q_j)] \in \mathbb{C}^{n \times n}, \quad F_2 = [(p_i, p_j)_*] \in \mathbb{C}^{k \times k},$$

$$G_1 = [(q_i, (A_0 - \mu)q_j)] \in \mathbb{C}^{n \times n}, \quad G_2 = [(T^* p_i, T^* p_j)] \in \mathbb{C}^{k \times k},$$

and

$$H = [(T^* p_i, T^* p_j)] \in \mathbb{C}^{n \times k},$$

then the W-A matrix , $W_{k,n}(\lambda)$, may be compactly expressed as

$$W_{k,n}(\lambda) = F_1 + \frac{1}{\mu - \lambda} \{G_1 - H[(\mu - \lambda) F_2 + G_2]^{-1} H^*\}.$$

(2.2)

Based on this W-A matrix, Beattie and Goerisch introduced the following method which is called the eigenvector free method.
Theorem 3.2.1 (Beattie and Goersch). Let $\mu$ and $r$ be chosen so that $\lambda^0_{r-1} < \mu \leq \lambda^0_r$. Suppose that $\{p_i\}_{i=1}^k \subset \text{Dom}(T^*)$ and $\{q_i\}_{i=1}^n \subset \text{Dom}(A_0)$. If the generalized matrix eigenvalue problem

$$
\begin{bmatrix}
F_1 & 0 \\
0 & F_2
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix} = \zeta
\begin{bmatrix}
G_1 & H \\
H^* & G_2
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix}
$$

has discrete finite eigenvalues ordered as

$$
\zeta_1 \leq \zeta_2 \leq \ldots \leq \zeta_i < 0 \leq \zeta_{i+1} \leq \ldots
$$

($l = 0$ if all discrete eigenvalues are either nonnegative or infinite), then for each eigenvalue $\zeta_p$ with $p \leq l$ we have a corresponding lower bound for an eigenvalue of $A$,

$$
\mu + \frac{1}{\zeta_p} \leq \lambda_{r-d-m(p)} \leq \lambda_{r-d-p} \leq \lambda_{r-p}
$$

where $m(p) = \max \{m|\zeta_m = \zeta_p\}$ and $d$ is the number of negative eigenvalues of $[\nu_1^* F_1 \nu_1 + \nu_2^* F_2 \nu_2]$ for $\nu = \begin{pmatrix} \nu_1 \\ \nu_2 \end{pmatrix}$ having columns that form a basis for $\ker \begin{bmatrix} G_1 & H \\ H^* & G_2 \end{bmatrix}$.

Notice that the number of negative eigenvalues of (2.3) is less than $r$ because the Gram matrix and $F_2$ are positive semi-definite and because the number of eigenvalues of $A_0$ less than $\mu$ is at most $r - 1$. We then arrive at the following useful result.

Corollary 3.2.2. In addition to the assumptions of Theorem 3.2.1, if $\{p_i\}$ and $\{q_i\}$ are chosen such that $\{(A_0 - \mu)q_i\}_{i=1}^n$ and $\{T^* p_i\}_{i=1}^k$ are jointly linearly independent, then

$$
\mu + \frac{1}{\zeta_p} \leq \lambda_{r-m(p)} \leq \lambda_{r-p}.
$$

Eigenvector-Free Method ([17]).

(i) Select trial vectors $\{q_i\}_{i=1}^n \subset \text{Dom}(A_0)$ and $\{p_j\}_{j=1}^k \subset \text{Dom}(T^*)$.

(ii) Pick a value $\mu \in (\lambda^0_{r-1}, \lambda^0_r)$ for a selected $r > 1$.

(iii) Form and solve the matrix eigenvalue problem defined by (2.3).
(iv) The finite negative discrete eigenvalues computed from (2.3) may each be associated with eigenvalue bounds as given in (2.4).

We note that if \( \{q_i\}_{i=1}^n \) and \( \{p_j\}_{j=1}^k \) are chosen to have local support as with finite-element trial functions, then the resulting matrices will be sparse and the matrix eigenvalue problem may be efficiently handled using sparse techniques, even for quite large values of \( n \) and \( k \). Furthermore, the only need for \( a \ priori \) spectral information comes through the selection of \( \mu \) as a sufficiently good lower bound to \( \lambda_0 \) to separate it from \( \lambda_{v-1} \). No eigenvector data for \( A_0 \) are necessary nor are exact values for the eigenvalues of \( A_0 \) needed for appropriate selection of \( \mu \).

We next consider a relation between eigenpairs of the matrix pencil (2.3) and those of intermediate operators \( A_{k,n} \). Let \( u \) be an eigenvector of \( A_{k,n} \) corresponding to an eigenvalue \( \lambda \). Then \( \lambda \) satisfies the determinant equation of \( W-A \) matrix (2.1) and \( u = -\sum_{j=1}^n \alpha_j R_{\lambda+i \epsilon}^0 B_k \hat{p}_j \) with \( \alpha \in \ker W_{k,n}(\lambda) \). Since \( q_i = R_\mu^0 B_k \hat{p}_i \), we have

\[
F_1 \alpha = \zeta \left\{ G_1 - H \left[ -\frac{1}{\zeta} F_2 + G_2 \right]^{-1} H^* \right\} \alpha
\]

with \( \zeta = \frac{1}{\lambda - \mu} \) and \( v = -\sum_{j=1}^n \alpha_j q_j \). If we define

\[
\beta = \zeta (F_2 - \zeta G_2)^{-1} H^* \alpha,
\]

the vector \( \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \) is an eigenvector of (2.3) corresponding to an eigenvalue \( \zeta \). Conversely, let \( \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \) be an eigenvector of (2.3) corresponding to an eigenvalue \( \zeta \). Then

\[
F_1 \alpha = \zeta \left\{ G_1 - H \left[ -\frac{1}{\zeta} F_2 + G_2 \right]^{-1} H^* \right\} \alpha.
\]

Therefore, \( u = -\sum_{j=1}^n \alpha_j q_j \) is an eigenvector of \( A_{k,n} \) corresponding to an eigenvalue \( \lambda = \mu + \frac{1}{\zeta} \), which leads to the following.

**Theorem 3.2.3.** If \( \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \) is an eigenvector of the matrix pencil (2.3) with a corresponding eigenvalue \( \zeta \), then \( -\sum_{j=1}^n \alpha_j q_j \) is an eigenvector of intermediate operator \( A_{k,n} \) with a corresponding eigenvalue \( \mu + \frac{1}{\zeta} \). The converse holds for \( \beta \) in (2.5).
3.3 Application to Beam Problems.

We consider the free vibration of a uniform rotating beam clamped at one end and free at the other. This may be modeled by the differential equation

\[ EI \frac{d^4 u}{dz^4} - \frac{mC\Omega^2}{2} \frac{d}{dz} (l^2 - z^2) \frac{du}{dz} - 4\pi^2 f^2 mCu = 0, \quad 0 < z < l \]

with boundary conditions

\[ u(0) = \frac{du}{dz}(0) = \frac{d^2 u}{dz^2}(l) = \frac{d^3 u}{dz^3}(l) = 0, \]

where \( u \) is the transverse displacement of the beam, \( I \) is the moment of inertia of the cross section about the principal axis in the plane of rotation, \( E \) is the modulus of elasticity, \( m \) is the mass per unit volume, \( l \) is the length of the beam, \( C \) is the cross-section area, \( \Omega \) is the angular velocity of rotation, and \( f \) is the natural frequency. This problem has been treated previously with other methods in [12,59].

For convenience, we introduce the nondimensional variable \( x = \frac{z}{l} \) and write the above differential equation as an eigenvalue problem,

\[ \frac{d^4 u}{dz^4} - \frac{a^2}{2} \frac{d}{dx} (1 - x^2) \frac{du}{dx} = \lambda u, \quad 0 < x < 1 \]

(3.1)

with boundary conditions

\[ u(0) = \frac{du}{dz}(0) = \frac{d^2 u}{dz^2}(1) = \frac{d^3 u}{dz^3}(1) = 0 \]

Here the parameter \( a^2 \) is proportional to the angular velocity of rotation, \( a^2 = \frac{mC\Omega^2}{EI} \), and the eigenvalue \( \lambda \) is related to the natural frequency \( f \) by \( 4\pi^2 \frac{mC\Omega^2 l^2}{EI} \). We denote by \( A \) the differential operator of the equation (3.1) and by \( \text{Dom}(A) \) its domain, i.e.,

\[ Au = \frac{d^4 u}{dz^4} - \frac{a^2}{2} \frac{d}{dx} (1 - x^2) \frac{du}{dx} \]

and

64
\[ \text{Dom}(A) = \{ u \in H^4(0,1) \mid u(0) = \frac{du}{dx}(0) = \frac{d^2u}{dx^2}(0) = \frac{d^3u}{dx^3}(1) = 0 \}. \]

The quadratic form associated with the operator \( A \) is given by

\[ a(u) = \int_0^1 \left( \left| \frac{d^2u}{dx^2} \right|^2 + \frac{a^2}{2} (1 - x^2) \left| \frac{du}{dx} \right|^2 \right) dx \]

with the domain

\[ \text{Dom}(a) = \{ u \in H^2(0,1) \mid u(0) = \frac{du}{dx}(0) = 0 \}. \]

If we take the base operator \( A_0 \) as

\[ A_0u = -\frac{a^2}{2} \frac{d}{dx} (1 - x^2) \frac{du}{dx} \]

with

\[ \text{Dom}(A_0) = \{ u \in H^3(0,1) \mid u(0) = \lim_{x \to 1^-} (1 - x) \frac{du}{dx} = 0 \}, \]

and the perturbation operator \( T \) as

\[ Tu = -\frac{d^2u}{dx^2} \]

with

\[ \text{Dom}(T) = \{ u \in H^2(0,1) \mid u(0) = \frac{du}{dx}(0) = 0 \}, \]

then the quadratic forms associated with the operators \( A \) and \( A_0 \) are

\[ a(u) = a_0(u) + \| Tu \|^2, \quad a_0(u) = \frac{a^2}{2} \int_0^1 (1 - x^2) \left| \frac{du}{dx} \right|^2 dx \]

with \( \text{Dom}(a_0) = \{ u \in H^1(0,1) \mid u(0) = 0 \} \), and the adjoint operator of \( T \) is obtained as

\[ T^*u = -\frac{d^2u}{dx^2} \]

with

\[ \text{Dom}(T^*) = \{ u \in H^2(0,1) \mid u(1) = \frac{du}{dx}(1) = 0 \}. \]
The eigenvalues of $A_0$ are easily found by

$$\lambda_i^0 = a^2 l(2l - 1), \quad \text{for } l = 1, 2, 3, \ldots.$$  

It follows that for a given function $u \in \text{Dom}(a)$, the quadratic forms $a$ and $a_0$ satisfy the inequality

$$a_0(u) \leq a(u).$$

The eigenvalues associated with these quadratic forms thus satisfy the inequality

$$\lambda_\nu^0 \leq \lambda_\nu, \quad \text{for } \nu = 1, 2, 3, \ldots.$$

Define a uniform mesh on $[0, 1]$ with a mesh size $h = \frac{1}{N}$. Furthermore, define cubic spline functions on this mesh, $B_i(x)$, centered at $x_i = ih$ for $i = -1, 0, 1, \ldots, N + 1$ so that

$$B_i(x_i) = 1, \quad B_i(x_{i+1}) = \frac{1}{4} \quad \text{and} \quad B_i(x_{i+2}) = 0.$$

In order to take the projecting vectors $\{q_i\}$ and $\{p_j\}$ within $\text{Dom}(A_0)$ and $\text{Dom}(T^*)$ respectively, we define them by

$$q_1 = B_0 - 4B_{-1}, \quad q_2 = B_0 - 4B_1, \quad q_i = B_{i-1}, \quad \text{for } i = 3, \ldots, N + 2$$

and

$$p_j = B_{j-2}, \quad \text{for } j = 1, \ldots, N, \quad p_{N+1} = B_{N-1} - \frac{1}{2} B_N + B_{N+1}.$$  

This provides an $(N+2, N+1)$-order problem. Since the order is dependent only on the mesh size, the eigenvalue estimates will be denoted by $\lambda_\nu^{(N)}$. The elements of
matrices $F_1, F_2, G_1, G_2$ and $H$ of (2.3) are given by the inner products:

\[ F_{1}^{ij} = \frac{a^2}{2} \left( \int_{0}^{1} q_i' \cdot q_j' \, dx - \int_{0}^{1} q_i' \cdot x^2 q_j' \, dx \right) - \mu \int_{0}^{1} q_i \cdot q_j \, dx, \]

\[ F_{2}^{ij} = \int_{0}^{1} p_i \cdot p_j \, dx, \]

\[ G_{1}^{ij} = \frac{a^4}{4} \left( \int_{0}^{1} q_i'' \cdot q_j'' \, dx - 2 \int_{0}^{1} q_i'' \cdot x q_j' \, dx + \int_{0}^{1} q_i'' \cdot x^2 q_j' \, dx - 2 \int_{0}^{1} q_i' \cdot x q_j' \, dx + \int_{0}^{1} q_i' \cdot x^2 q_j' \, dx + 2 \int_{0}^{1} q_i' \cdot x^2 q_j' \, dx + 4 \int_{0}^{1} q_i' \cdot x^2 q_j' \, dx + 2 \int_{0}^{1} q_i' \cdot x^2 q_j' \, dx \right), \]

\[ - a^2 \mu \left( \int_{0}^{1} q_i' \cdot q_j' \, dx - \int_{0}^{1} q_i' \cdot x q_j' \, dx \right) + \mu^2 \int_{0}^{1} q_i \cdot q_j \, dx, \]

\[ G_{2}^{ij} = \int_{0}^{1} p_i'' \cdot p_j'' \, dx, \]

\[ H^{ij} = \frac{a^2}{2} \left( \int_{0}^{1} q_i'' \cdot p_j'' \, dx - 2 \int_{0}^{1} a q_i' \cdot p_j'' \, dx - \int_{0}^{1} x^2 q_i'' \cdot p_j'' \, dx \right) - \mu \int_{0}^{1} q_i' \cdot p_j' \, dx. \]

For the upper bounds the basis functions are chosen as

\[ \phi_1 = B_{-1} - \frac{1}{2} B_0 + B_1 \quad \text{and} \quad \phi_i = B_i, \quad \text{for} \quad i = 2, \ldots, N + 1 \]

to satisfy the boundary conditions. Upper bounds to the eigenvalues of the rotating beam are obtained as the eigenvalues $\lambda$ of $(N + 1)$-st order symmetric generalized algebraic eigenvalue problem,

\[ \begin{pmatrix} \langle A_0 \phi_i, \phi_j \rangle + \langle T \phi_i, T \phi_j \rangle \end{pmatrix} x = \lambda (\langle \phi_i, \phi_j \rangle) x \]

for $i, j = 1, \ldots, N + 1$. Here

\[ \langle A_0 \phi_i, \phi_j \rangle = \frac{a^2}{2} \left( \int_{0}^{1} \phi_i' \cdot \phi_j' \, dx - \int_{0}^{1} \phi_i' \cdot x^2 \phi_j' \, dx \right), \]

\[ \langle T \phi_i, T \phi_j \rangle = \int_{0}^{1} \phi_i'' \cdot \phi_j'' \, dx \quad \text{and} \quad \langle \phi_i, \phi_j \rangle = \int_{0}^{1} \phi_i \cdot \phi_j \, dx. \]

The result is contained in Table 3. Here the upper bounds come from Rayleigh–Ritz problem of $N = 200$. 67
Table 3. Clamped Beam Problem (CBP)

\[ a^2 = 200 \quad \mu = 65000 \quad r = 13 \]

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\[ a^2 = 10000 \quad \mu = 910000 \quad r = 7 \]

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Next we consider the free vibration of a uniform rotating beam simply supported at one end and free at the other. The differential equation governing this problem is the same as the clamped case but with a different boundary condition

\[
u(0) = \frac{d^2 u}{dx^2}(0) = \frac{d^2 u}{dx^2}(1) = \frac{d^3 u}{dx^3}(1) = 0.
\]

Then the base operator \( A_0 \) and its domain are the same as in the clamped case, but the domain of \( a \) is \( \text{Dom}(a) = \{ u \in H^1(0,1) | u(0) = 0 \} \) and the domain of \( T^* \) is

\[
\text{Dom}(T^*) = \{ u \in H^2(0,1) | u(0) = u(1) = \frac{du}{dx}(1) = 0 \}.
\]
The projecting vectors \( \{ q_i \} \) are the same as those of the previous case, but the vectors \( p_j \) are defined as

\[
p_1 = B_0 - 4B_{-1}, \quad p_2 = B_1 - 4B_{-1}
\]

and

\[
p_i = B_{i-1}, \quad \text{for } i = 3, \ldots, N - 1, \quad p_N = B_{N-1} - \frac{1}{2}B_N + B_{N+1}.
\]

This yields \((2N + 2)\)-order eigenvalue problem.

For the upper bounds the trial functions are chosen to be

\[
\phi_1 = B_0 - 4B_{-1}, \quad \phi_2 = B_0 - 4B_1, \phi_i = B_{i-1}, \quad \text{for } i = 3, \ldots, N + 2
\]

in order to satisfy boundary conditions. Table 4 contains the result. Here the upper bounds come from Rayleigh–Ritz problem of \( N = 200 \).

**Table 4. Simply Supported Beam Problem (SBP)**

\[
a^2 = 5 \quad \mu = 2805 \quad r = 17
\]

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\[
a^2 = 500 \quad \mu = 138000 \quad r = 12
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3.4 Numerical Realisation of Eigenvalue Bounds.

In this section we deal with large order matrix eigenvalue problem which comes from the EVF method. For this purpose, we consider the generalized matrix eigenvalue problem

\[ Ax = \Lambda Bx \tag{4.1} \]

where \( A \) is a symmetric positive-definite matrix and \( B \) is a symmetric positive semi-definite matrix. A variety of approaches exist for computing selected eigenpairs of (4.1) when \( A \) and \( B \) are very large and very sparse. The simplest of these is subspace iteration (cf. [48]). Starting with full rank \( S^{(0)} \in \mathbb{R}^{n \times m} (m \ll n) \) and \( \theta_i^{(0)} = 1 \), iterate

Form \( \tilde{S}^{(k)} = (A - \sigma B)^{-1} B S^{(k-1)} \text{diag}(\theta_i^{(k-1)}) \)

For \( A^{(k)} = \tilde{S}^{(k)^*} A \tilde{S}^{(k)} \) and \( B^{(k)} = \tilde{S}^{(k)^*} B \tilde{S}^{(k)} \)

Solve \( A^{(k)} G^{(k)} = B^{(k)} G^{(k)} \text{diag}(\theta_i^{(k)}) \)

Form \( S^{(k)} = \tilde{S}^{(k)} G^{(k)} \)

for \( k = 1, 2, \ldots \). Since for each \( k \geq 1 \), \( \{\theta_i^{(k)}\}_{i=1}^m \) are the result of Ritz approximations to (4.1) out of \( \text{span}(S^{(k)}) \), it is clear that \( \lambda_i \leq \Lambda_i \leq \theta_i^{(k)} \), independent of \( \sigma \). While the convergence rate is linear, it will be more rapid to those eigenvalues of (4.1) closest to the shift \( \sigma \) since it depends on the ratio \( \max \frac{|\theta_j^{(k-1)}|}{|\lambda - \sigma|} \).

The slow linear rate of convergence and the necessity for solving \( m \) linear systems, where \( m \) should be selected larger than the number of eigenvalues actually wanted, at each step ultimately make subspace iteration less appealing than the Lanczos method. Since we are interested in a few eigenvalues, the spectral transformation Lanczos method (STLM) may be useful. Thus if one is willing to live with the expense of an occasional factorization of \( A - \sigma B \), STLM is often substantially more effective than subspace iteration. Moreover, if \( B \) is singular, STLM does not suffer the same
degradation of the accuracy [47]. Eqn. (4.1) is transformed to

\[(A - \sigma B)^{-1}Bx = \frac{1}{\Lambda - \sigma}x.\]  \hspace{1cm} (4.2)

For convenience, let \(\mathcal{M} = (A - \sigma B)^{-1}B\). All eigenvectors of (4.1) corresponding to finite eigenvalues are also eigenvectors of \(\mathcal{M}\), and they lie in the range of \(\mathcal{M}\). The semi-inner product induced by \(\mathcal{B}\) is a true inner product on the range of \(\mathcal{M}\), and also the eigenvalue problem (4.2) is self-adjoint with respect to this inner product even though the problem is not symmetric [47]. STLM requires calculating the action of \(\mathcal{M}\) on a vector of the range of \(\mathcal{M}\) at each iteration step. It constructs a symmetric tridiagonal matrix, \(T_j \in \mathbb{R}^{j \times j}\), in the course of \(j\) iteration steps, whose eigenvalues approximate those of (4.2). A set of Lanczos vectors \(\{q_i\}_{i=1}^j\) that form a \(\mathcal{B}\)-orthogonal basis for the order \(j\) Krylov subspace is generated by \(\mathcal{M}\) and \(q_1\). In floating point arithmetic, \(\mathcal{B}\)-orthogonality is volatile and expensive to maintain, but so long as the \(\{q_i\}_{i=1}^j\) are kept robustly independent (\(\mathcal{B}\)-"semiorthogonal"), one can guarantee up to terms on the order of the machine precision that \(T_j\) is the Rayleigh-Ritz restriction of (4.2) to \(\text{span}(\{q_i\}_{i=1}^j)\) with respect to the \(\mathcal{B}\)-inner product [49]. The eigenvalues of \(T_j\) will be associated with upper bounds to corresponding eigenvalues of (4.2) and thus it will be associated with lower bounds to corresponding eigenvalues of (4.1).

We recall from the EVF method that eigenvalues of the given operator may be associated with lower bounds according to

\[\mu + \frac{1}{\zeta_p} \leq \lambda_{r-p}\]

for each \(p = 1, 2, \ldots, r-1\). If \(\hat{\zeta}_p \geq \zeta_p\) is an estimate of \(\zeta_p\), then \(\mu + (1/\hat{\zeta}_p) \leq \mu + (1/\zeta_p) \leq \lambda_{r-p}\). Hence we seek upper bounds to the negative eigenvalues of (2.3) or (4.1) so as to maintain consistent lower bounds to \(\{\lambda_i\}_{i=1}^{r-1}\). Practically, if \(m\) is such that \(\Lambda_m < \mu < \Lambda_{m+1}\), then it makes sense to find lower bounds only to \(\{\lambda_i\}_{1}^{m}\). In
other words we need only the \( m \) biggest negative eigenvalues of \( \{\zeta_i\} \) instead of the entire set of negative eigenvalues.

Let \( A = \begin{bmatrix} F_1 & 0 \\ 0 & F_2 \end{bmatrix} \) and \( B = \begin{bmatrix} G_1 & H \\ H^* & G_2 \end{bmatrix} \). Now we consider how to select the shift \( \sigma \) for the equation (4.1). It is desirable to choose a zero shift in order to preserve the sparsity of \( A \). However, small magnitude eigenvalues may need many iterations to get a reasonable accuracy. In our model of the clamped plate problem the negative eigenvalues of \((A, B)\) have very small magnitudes compared to the extreme positive eigenvalues. Moreover, the number of Lanczos steps required exceeds half of the size of its computational matrix to get a reasonable accuracy. In order to overcome such trouble, it may be possible to take the shift so that the wanted eigenvalue of \( M \) has the biggest magnitude. For this purpose, let \( m \) be such that \( \Lambda_m < \mu \) and let \( p = r - m \). If we take \( \sigma = (\Lambda_m - \mu)^{-1} \), then \( \zeta_{r-m-1} < \sigma < \zeta_{r-m} \). Without loss of generality we may assume \( \sigma \) is closer to \( \zeta_{r-m} \) than to \( \zeta_{r-m-1} \) since \( \Lambda_m \) can be taken to be closer to \( \lambda_m \) than to \( \lambda_{m+1} \). For clarity we may refer to Figure 3.

If \( \nu_i' \)'s are the ordered eigenvalues of \((A - \sigma B)^{-1}B\), then we have

\[
\zeta_{r-m} = \frac{1}{\nu_S} + \sigma, \ldots, \zeta_{r-1} = \frac{1}{\nu_{S-m+1}} + \sigma,
\]

where \( S \) is the rank of \( B \). We note that the eigenvalue \( \nu_S \) has the biggest magnitude. Since we only need few extreme eigenvalues, \( \nu_S, \ldots, \nu_{S-m+1} \), of \((A - \sigma B)^{-1}B\), the Lanczos method is expected to be quite efficient. Moreover, if \( A \) and \( B \) are large and sparse, we can efficiently reduce the storage for \( A \) and \( B \) as storing only their nonzero entries because the STLM requires calculating the action of \((A - \sigma B)^{-1}B\) on a vector at each iteration step, even if it needs additional storage for factorization of \((A - B)\).

Since we seek upper bounds to the negative eigenvalues of (2.3) or (4.1), we have to find lower bounds to the corresponding eigenvalues of \((A - \sigma B)^{-1}B\). It is appropriate to comment here that the modifications to Rutishauser's subspace iteration \textit{ritzit
(cf. [48]) that extend its applicability to (4.1) are straight-forward, but the resulting eigenvalue estimates are lower bounds to $\Lambda_i$ of (4.1). Hence it is impossible to directly deduce upper bounds to $\lambda_i$. Remarkably, it can be recovered with a rank-one modification of $T_j$ and so regain the sense of derived bounds for $\lambda_i$. We give a brief description. For more detail, one may refer to [47]. Let $T_j = Q_j^*B(A - \sigma B)^{-1}BQ_j$ be the tridiagonal matrix in STLM and define $W_j = Q_j^*(A - \sigma B)Q_j$, where $Q_j$ is a matrix whose columns are Lanczos vectors. Then the eigenvalues of $W_j$ are the Ritz value approximations to $\zeta_i - \sigma$ and thus the eigenvalues of $W_j^{-1}$ are lower bounds to $\nu_i$ which we want. Moreover, the matrix $W_j^{-1}$ differs from $T_j$ only in the last diagonal entry. Hence we easily modify the Lanczos algorithm for our goal. The following is a modified algorithm with full reorthogonalization.

Set $q_0 = 0$ and take $r_1 \in ran(M)$ and let $\beta_1 = ||r_1||$.

For $j = 1, \ldots, \text{maxit}$, do

\begin{align*}
q_j & \leftarrow \frac{r_j}{\beta_j} \quad \text{(normalization)} \\
\alpha_j & \leftarrow q_j^tBMq_j \\
\text{if } j = 1; & \quad \omega_1 \leftarrow q_1^t(A - \sigma B)q_1 \text{ and } \mu_1 \leftarrow \frac{1}{\omega_1} - \alpha_1 \\
\text{else; } & \quad \mu_j \leftarrow -\alpha_j - \frac{\beta_j^2}{\mu_{j-1}} \\
r & \leftarrow (M - \alpha_j)q_j - \beta_jq_{j-1} \\
r_{j+1} & \leftarrow r - \sum_{i=1}^{j} q_i(q_i^tBr) \quad \text{(orthogonalization)} \\
\beta_{j+1} & \leftarrow (r_{j+1}^tBr_{j+1})^{\frac{1}{2}} \quad \text{(norm of } r_{j+1} \text{ with respect to } B) \\
\text{end for}
\end{align*}

We next consider that the mapping from the eigenvalues of (2.3) to the final lower bounds to $\lambda_i$ introduces potential error magnification. The relative error in a bound
to $\lambda_{r-p}$ caused by approximating $\zeta_p$ with $\hat{\zeta}_p > \zeta_p$ may be expressed as

$$\left(\text{relative error in the estimate to } \lambda_{r-p}\right) = \left(\frac{1}{\mu |\zeta_p| - 1}\right) \frac{|\hat{\zeta}_p - \zeta_p|}{|\hat{\zeta}_p|}.$$  

The coefficient $1/(\mu |\zeta_p| - 1)$ may be assumed to be positive without loss of generality since all eigenvalues $-1/\mu \leq \zeta_p < 0$ produce nonpositive lower bounds to $\lambda_{r-p}$ (which are already known to be positive). The error in $\zeta_p$ will be either magnified or diminished depending on whether $\zeta_p > -2/\mu$ or $\zeta_p < -2/\mu$.

Figure 3: Relation Between Spectra
3.5 Application to a Clamped Plate Problem.

In this section we give rigorous upper and lower bounds to vibrations of uniform clamped plates on a rectangular domain. The estimation of these vibrations has been treated previously in [14,73]. The lower bounds are obtained by EVF using bicubic spline functions as trial functions, while the upper bounds are obtained by the finite element method using the same trial functions.

Let Ω denote the open rectangle \((\frac{-1}{2}, \frac{1}{2}) \times (-\frac{1}{2}, \frac{1}{2})\) in \(\mathbb{R}^2\). Consider the following simple model of vibration of a clamped plate:

\[
\Delta^2 u = \lambda u \text{ on } \Omega \quad \text{with} \quad u = \frac{\partial u}{\partial n} = 0 \text{ on } \partial \Omega.
\]

That is, the operator \(A\) is defined on a core of \(C^\infty_0(\Omega) \subset L^2(\Omega) = \mathcal{H}\) by

\[
A u = \frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial y^4} + 2 \frac{\partial^4 u}{\partial x^2 \partial y^4} \quad \text{with} \quad u = \frac{\partial u}{\partial n} = 0 \text{ on } \partial \Omega.
\]

We now define a base operator \(A_0\) on a core of \(C^\infty_0(\Omega) \subset L^2(\Omega)\) by

\[
A_0 u = 2 \frac{\partial^4 u}{\partial x^2 \partial y^4} \quad \text{with} \quad u = 0 \text{ on } \partial \Omega
\]

and \(T\) on a core of \(C^\infty_0(\Omega) \subset L^2(\Omega)\) into \(L^2(\Omega) \times L^2(\Omega) = \mathcal{H}_u\) by

\[
T u = \begin{bmatrix}
\frac{\partial^2 u}{\partial x^2} & \frac{\partial^2 u}{\partial y^4}
\end{bmatrix} \quad \text{with} \quad u = \frac{\partial u}{\partial n} = 0 \text{ on } \partial \Omega.
\]

The adjoint operator \(T^*\) of \(T\) is then defined on sufficiently smooth functions of \(L^2(\Omega) \times L^2(\Omega)\) by

\[
T^* (v, w) = -\left( \frac{\partial^2 v}{\partial x^4} + \frac{\partial^2 w}{\partial y^4} \right)
\]

with free boundary conditions.

Notice that the region, the differential equation and the boundary conditions, share common properties of symmetry. Thus we can take advantage of this so that
we restrict the problem on the space of functions even with respect to both $x$-axes and $y$-axes. Then we need extra boundary conditions of

$$\frac{\partial u}{\partial n} = 0 \text{ on } \{(0, y), (x, 0) \mid 0 < x < \frac{a}{2} \text{ and } 0 < y < \frac{b}{2}\}.$$  

We define $\Omega = (0, \frac{a}{2}) \times (0, \frac{b}{2})$, $\Gamma_1 = \{(\frac{a}{2}, y), (x, \frac{b}{2}) \mid 0 < x < \frac{a}{2} \text{ and } 0 < y < \frac{b}{2}\}$ and $\Gamma_2 = \{(0, y), (x, 0) \mid 0 < x < \frac{a}{2} \text{ and } 0 < y < \frac{b}{2}\}$.

The boundary conditions for $A, A_0$ and $T^*$ restricted to even–even symmetry class are as follows:

1. For $A, u = \frac{\partial u}{\partial n} = 0$ on $\Gamma_1$ and $\frac{\partial u}{\partial n} = 0$ on $\Gamma_2$
2. For $A_0, u = 0$ on $\Gamma_1$ and $\frac{\partial u}{\partial n} = 0$ on $\Gamma_2$
3. For $T^*, \frac{\partial u}{\partial n} = 0$ on $\Gamma_2$.

The eigenvalues of $A_0$ with these boundary conditions are easily found to be

$$\frac{2\pi^4}{a^2b^2}(2i - 1)^2(2j - 1)^2 \text{ for } i, j \geq 1.$$  

Now we are in a position to construct approximating vectors for both the EVF and the Rayleigh–Ritz methods. Let $N \times N$ finite-element mesh be overlaid on $\Omega$. Trial functions will be constructed from the associated set of bicubic splines so as to satisfy necessary boundary conditions. Let $B_i$ be cubic spline functions on $[0, 1]$ for $i = -1, \ldots, N + 1$. For approximating vectors within $Dom(A_0)$, we define

$$\tilde{B}_0 = B_0, \quad \tilde{B}_1 = B_1 + B_{-1},$$
$$\tilde{B}_j = B_j, \quad \text{for } j = 2, \ldots, N - 2,$$
$$\tilde{B}_{N-1} = 4B_{N-1} - B_N, \quad \tilde{B}_N = 4B_{N+1} - B_N.$$
Then the approximating vectors are defined as $q_{ij}(x, y) = \tilde{B}_i(x)\tilde{B}_j(y)$ for $0 \leq i, j \leq N$ so that the dimension of the finite element space for $\text{Dom}(A_0)$ is $(N + 1)^2$. For approximating vectors within $\text{Dom}(T^*)$, define

$$\tilde{B}_0 = B_0, \quad \tilde{B}_1 = B_1 + B_{-1}$$
$$\tilde{B}_j = B_j, \quad \text{for } j = 2, \ldots, N + 1.$$

Then the approximating vectors are defined as $\{\tilde{B}_i(x)B_j(y), 0\}$ and $\{0, B_k(x)\tilde{B}_l(y)\}$ for $0 \leq i, l \leq N + 1$ and $-1 \leq j, k \leq n + 1$ so that the dimension is $2(N + 2)(N + 3)$. Thus we have $n = (N + 1)^2$ and $k = 2(N + 2)(N + 3)$ for the EVF method.

For upper bounds, we define

$$\tilde{B}_0 = B_0, \quad \tilde{B}_1 = B_1 + B_{-1}$$
$$\tilde{B}_j = B_j, \quad \text{for } j = 2, \ldots, N - 2$$
$$\tilde{B}_{N-1} = B_{N-1} - \frac{1}{2}B_N + B_{N+1}.$$

The approximating vectors for $\text{Dom}(a)$ are defined by $\phi_{ij}(x, y) = \tilde{B}_i(x)\tilde{B}_j(y)$ for $0 \leq i, j \leq N - 1$ so that we have $n = N^2$ for the Rayleigh–Ritz problem.

For the computation of each entry of the matrices of EVF and Rayleigh–Ritz problem, we need not compute all the integrations that come from the inner products of approximating vectors directly. Instead, we need only find 4 local overlap matrices of dimension $4 \times 4$ and later compute matrix entries by assembly. For this purpose we denote by $S_{-1}, S_0, S_1$ and $S_2$ the cubic spline functions on $[0, 1]$ with mesh size of 1. Let $S'_1$ and $S''_1$ be the first and second derivatives of $S_1$. Then we have the following local $4 \times 4$ matrices:

<table>
<thead>
<tr>
<th></th>
<th>$S_1$</th>
<th>$S_0$</th>
<th>$S_1$</th>
<th>$S_1$</th>
</tr>
</thead>
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<tr>
<td>$1/7$</td>
<td>129/140</td>
<td>3/7</td>
<td>1/140</td>
<td></td>
</tr>
<tr>
<td>$129/140$</td>
<td>297/35</td>
<td>933/140</td>
<td>3/7</td>
<td></td>
</tr>
<tr>
<td>$3/7$</td>
<td>933/140</td>
<td>297/35</td>
<td>129/140</td>
<td></td>
</tr>
<tr>
<td>$1/140$</td>
<td>3/7</td>
<td>129/140</td>
<td>1/7</td>
<td></td>
</tr>
</tbody>
</table>
Let $B_i$’s be the cubic spline functions on $[0, \ell]$ with $N$ uniform meshes and let $h = \frac{\ell}{N}$. Then the global $N + 3$ by $N + 3$ matrices $[\langle B_i, B_j \rangle, [\langle B_i', B_j' \rangle], \langle B_i', B_j'' \rangle]$ and $[\langle B_i', B_j' \rangle]$ are obtained by assembling the corresponding local matrices and multiplying by $h$, $\frac{1}{h^3}$, $\frac{1}{h}$ and $\frac{1}{h}$, respectively. Moreover each entry of the matrices $[\langle B_i, B_j \rangle, [\langle B_i, B_j' \rangle], [\langle B_i', B_j \rangle]$ with matrices of their derivatives are formed to be a linear combination of each entries of $[\langle B_i', B_j \rangle]$ with matrices of its derivatives. From these, the final matrices $F_1, F_2, G_1, G_2,$ and $H$ are built. The matrix $A - \sigma B$ and $B$ have at most $441N^2 + 196N + 103$ nonzero entries since $\langle B_i, B_j \rangle = 0$ if $|i - j| \geq 4$. If we store only the nonzero entries of the matrix, then the size of storage may be reduced from $O(N^4)$ to $O(N^2)$ even though additional storage for factorization of $(A - \sigma B)$ is needed. In Tables 5 and 6 we show upper and lower bounds for rectangular clamped plate problem and square clamped plate problem, respectively. Here the upper bounds come from Rayleigh–Ritz problem of $N = 30$.

Table 5: Vibration of a clamped rectangular plate; $a = 2$ and $b = 3$

<table>
<thead>
<tr>
<th>shift($\sigma$)</th>
<th>45.6</th>
<th>276.6</th>
<th>981.2</th>
<th>1299.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$</td>
<td>$\lambda_1$</td>
<td>$\lambda_2$</td>
<td>$\lambda_3$</td>
<td>$\lambda_4$</td>
</tr>
<tr>
<td>Base</td>
<td>5.41161632</td>
<td>48.7045469</td>
<td>48.7045469</td>
<td>135.290408</td>
</tr>
<tr>
<td>8</td>
<td>45.57898297</td>
<td>276.5527261</td>
<td>980.6751978</td>
<td>1287.381572</td>
</tr>
<tr>
<td>12</td>
<td>45.57909607</td>
<td>276.5678153</td>
<td>981.0796336</td>
<td>1297.112053</td>
</tr>
<tr>
<td>16</td>
<td>45.57912595</td>
<td>276.5708077</td>
<td>981.1509026</td>
<td>1298.862718</td>
</tr>
<tr>
<td>20</td>
<td>45.57913693</td>
<td>276.5717255</td>
<td>981.1703925</td>
<td>1299.314289</td>
</tr>
<tr>
<td>Ritz</td>
<td>45.57915548</td>
<td>276.5728822</td>
<td>981.1859568</td>
<td>1299.639980</td>
</tr>
</tbody>
</table>
Table 6: Vibration of a clamped square plate; $a = b = \pi$

(even-even symmetry class)

<table>
<thead>
<tr>
<th>shift((\sigma))</th>
<th>13.3</th>
<th>177.8</th>
<th>179.5</th>
<th>497.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>N</td>
<td>(\lambda_1)</td>
<td>(\lambda_2)</td>
<td>(\lambda_3)</td>
<td>(\lambda_4)</td>
</tr>
<tr>
<td>Base</td>
<td>2.00000000</td>
<td>18.00000000</td>
<td>18.00000000</td>
<td>50.00000000</td>
</tr>
<tr>
<td>8</td>
<td>13.29371618</td>
<td>177.7164393</td>
<td>179.4028827</td>
<td>496.1218673</td>
</tr>
<tr>
<td>12</td>
<td>13.29375278</td>
<td>177.7352417</td>
<td>179.4238800</td>
<td>496.8199162</td>
</tr>
<tr>
<td>16</td>
<td>13.29376216</td>
<td>177.7385483</td>
<td>179.4278173</td>
<td>496.9514904</td>
</tr>
<tr>
<td>20</td>
<td>13.29376564</td>
<td>177.7394530</td>
<td>179.4289743</td>
<td>496.9901598</td>
</tr>
<tr>
<td>Ritz</td>
<td>13.29377089</td>
<td>177.7403470</td>
<td>179.4302061</td>
<td>497.0222355</td>
</tr>
</tbody>
</table>

STLM was used with a random starting vector and shifts derived from the corresponding Ritz values estimating \(\lambda_1, \lambda_2, \lambda_3,\) and \(\lambda_4\). For simplicity, full reorthogonalization was used. The sparse \(LU\) factorization needed by STLM was performed with the Harwell subroutine MA28. Calculations were performed on a Vax 3800 in double precision. The single biggest eigenvalue of \((A - \sigma B)^{-1}B\) stabilized to full machine accuracy within 2 Lanczos steps, independent of \(N\). It should be noted again that if we use zero shift, the number of Lanczos steps required exceeds half of the size of its computational matrix, i.e. \((N + 1)^2 + 2(N + 2)(N + 3)\), to get the same accuracy as nonzero shift has.
3.6 Concluding Remarks.

We note that the inner products of cubic spline functions $B_i$ and $B_j$ vanish if the difference between $i$ and $j$ is greater than or equal to 4 (i.e., $|i - j| \geq 4$). The inner product matrices $F_1, F_2, G_1, G_2$ and $H$ have a full-band width of 7. The $(i,j)$ entry of each matrix is expressible as the sum of $4 - |i - j|$ integrals of polynomials of degree 6 or less over some, up to 4, consecutive subintervals $[x_k, x_{k+1}]$ with $x_k = \frac{k}{n}$ and $0 \leq k \leq n - 1$. These integrals may be computed analytically in principle but this may be highly tedious. Since each integrand is a polynomial of degree no greater than 6, a Gauss quadrature rule with 4-points is adequate to compute exactly each subinterval integration.

In the case of the simply supported beam problem, each Gram matrix we have encountered is always positive definite while the clamped beam problem is singular. Both problems have the parameter $d = 0$ and $m(p) = p$ which implies the negative eigenvalue of the computational eigenvalue problem is simple.

In the case of simply supported beam problem, the smallest eigenvalue of $A$ is the same as that of $A_0$ so that we don't actually need to compute it because the lower bound is between those of $A_0$ and of $A$. Thus convergence is moot in this case.

In the case of clamped plate problem, we need a couple of Lanczos steps (exactly two steps) to get better than 10 digit accuracy so that it does not make sense to use reorthogonalization. In our model problem we have used Rayleigh–Ritz values when taking shifts. But if we have a priori knowledge of separation of eigenvalues of the given operator, we don't need to find upper bounds before computing lower bounds. On the other hand, if we have some information on eigenvectors of the matrix pencil (2.3) corresponding to the wanted eigenvalues, it might be desirable to try to use zero shift in STLM. As seen in Section 4, we know the relationship between eigenvectors of the matrix pencil and those of the intermediate operators $A_{k,n}$, and we may think
that the eigenvectors of intermediate eigenvalue problems and those of Rayleigh–Ritz problem are close in a sense.

Since the EVF has been developed very recently, it still has open questions. First, we don’t know analytically how fast (or slowly) the bounds converge as the $N$ increases. From Figures 4, 5, 6 and 7, we may predict its behavior is like $O(N^{-\alpha})$ for some positive $\alpha$. The rate suggested from CBP, SBP and CPP is always $O(N^{-4})$, which is the same as the rate obtained from the Rayleigh–Ritz method using the same trial functions. Second, we don’t know how sensitive the bounds are depending on the choice of $\mu$. As seen in Table 7, the bounds seem to converge to some value less than the corresponding upper bounds for fixed $N$ as increasing $\mu$, which makes us have a conjecture that there is a close relationship between $\mu$ and the convergence of bounds. In Table 7 we have used $\sigma = 45.6$ as a shift fixed (i.e. $m = 1$ in Section 4 is used).

Table 7: Bounds depending on $\mu$

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\mu$</th>
<th>48.7</th>
<th>438.3</th>
<th>1217.6</th>
<th>1563.9</th>
</tr>
</thead>
<tbody>
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<td>6</td>
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<td>45.57873757</td>
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<td></td>
</tr>
<tr>
<td>10</td>
<td>45.57510808</td>
<td>45.57894476</td>
<td>45.57904766</td>
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<td></td>
</tr>
<tr>
<td>14</td>
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<td>45.57906744</td>
<td>45.57910952</td>
<td>45.57911501</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>45.57845109</td>
<td>45.57910860</td>
<td>45.57912984</td>
<td>45.57913276</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>45.57845649</td>
<td>45.57911893</td>
<td>45.57913488</td>
<td>45.57913686</td>
<td></td>
</tr>
</tbody>
</table>

Table 7 suggests us to take $\mu$ as big as possible to get high accuracy for the fixed $N$.

Rayleigh-Ritz calculations of order 200 and 30 were performed to provide complementary upper-bounds for the beam problem and plate problems, respectively. We note that as the parameter $a$ in beam problems gets larger and larger, we need smaller $N$ for the mesh to get the same accuracy. The reason is that if $a$ gets bigger and bigger, the eigenvalues of the base operator $A_0$ get closer to those of the given operator $A$ so that small value of $\tau$ is enough to get some lower bounds, directly making the dimension of coefficient matrices smaller. The relative differences between upper
bounds and lower bounds (i.e., $\frac{\text{upper-lower}}{\text{upper}}$ for a fixed upper bound and $\frac{\text{upper-lower}}{\text{lower}}$ for a fixed lower bound) are plotted against the number, $N$, of mesh element on a log-log scale in Figures 4, 5, 6, and 7. Linear asymptotes are evident in each case. For a few large values of $N$, a slight deterioration in convergence rate occurs which apparently is an artifact of insufficiently accurate Ritz calculation. The graphs are all drawn using MATLAB on a VAXstation 3800.
Figure 4: Error Behavior for CBP
Figure 5: Error Behavior for SBP
Figure 6: Error Behavior for Rectangular CPP
Figure 7: Error Behavior for Square CPP
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