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SOME CONVERGENCE RATES FOR EIGENVALUES OF INTERMEDIATE OPERATORS

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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, and bound state energy levels of atoms and molecules. In their analysis, we meet equations of the style $Au = \lambda u$ in Ω, 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. But the eigenvalues are not explicitly known in most cases, and thus sevral methods for their approximation have been presented and developed over many years. Since there is no method that provides a presise error estimation, the only reliables way is to use two ancillary methods that give upper and lower bounds, respectively, to the eigenvalues considered.

In the last quarter of the 19th century, Lord Rayleigh had initiated a development in the approximation of eigenvalues. With W. Ritz in 1909 this was developed to so–called *Rayleigh-Ritz method* which is the oldest method for obtaining numerical upper bounds. A. Weinstein developed a method for finding lower bounds for the eigenvalues of certain differential operators in 1937. This method was extended and simplified by N. Aronszajn in 1948 [1] by use of the properties of compact self-adjoint operators in Hilbert space, which is usually called the *intermediate problem method.* 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.

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Convergence rates for intermediate problem mehtods were first derived by Weinberger [16] for Weinstein type for a particular choice of approximating vectors. Somewhat later Fix [9], and Poznyak [13] obtained rate of convergence results for variants of Aronszajn's method with bounded or relatively bounded base operator perturbations. In case of totally unbounded base operator perturbation, Brown, Beattie and Greenlee, Greenlee showed the convergence [6,3,10], and Beattie and Greenlee also presented its rates [4,5]. In this paper we derive a convergence rate of the Aronszajn's method known as truncation including remainder [10], and also apply this result to a one dimensional Schrödinger operator. Section 2 deals with the main construction of a variant of the Aronszajn's method known as truncation including remainder. In section 3 we present a result of convergence rate for a sequence of semi–bounded operators. With the aid of this, we will derive a convergence rate of the method considered. Section 4 shows an example of one dimensional Schrödinger operator with a potential which arises in quantum mechanics.

2. On the Method of Intermediate Problems

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

$$\lambda_1(A) \leq \lambda_2(A) \leq \cdots \leq \lambda_\infty(A)$$

each having finite multiplicity. Here $\lambda_\infty(A)$ denotes the lowest limit point (if any) of the spectrum of A. For convenience we denote such a class of operators by $\mathcal{S}$. If A has compact resolvent, then we set $\lambda_\infty(A) = \infty$. We denote $a(u)$ by the closure of the quadratic form $\langle Au, u\rangle$.

The scheme of intermediate problems is following: Given an eigenvalue problem for an operator A of type $\mathcal{S}$, the first step is to find a base operator A_0 in $\mathcal{S}$, for which the eigenvalues of the base operator are all less than or equal to the corresponding eigenvalues of the given operator. The next step is to construct a sequence of eigenvalue problems in such a way as to yield computable eigenvalues which are between those of the base and given problem. It is thus necessary to have a knowledge of a related eigenvalue problem which is called a base problem,

$$A_0 u = \lambda u$$

where A_0 is in $\mathcal{S}$ and $A_0 \leq A$. We assume that the isolated eigenvalues of the base problem

$$\lambda_1(A_0) \leq \lambda_2(A_0) \leq \cdots \leq \lambda_\infty(A_0),$$

are known. Then $a_0(u) \leq a(u)$ for all $u \in Dom(a)$. The second monotonicity principle [17] implies that $\lambda_\infty(A_0) \leq \lambda_\infty(A)$, and that for each i such that $\lambda_i(A) < \lambda_\infty(A_0)$, $\lambda_i(A_0)$ exists and $\lambda_i(A_0) \leq \lambda_i(A)$. 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 $u \in Dom(b) = Dom(a) \subset Dom(a_0)$.

We now take a real number γ 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 γ 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 $A_0^{(\gamma)}$ has the same action as A_0 on the finite dimensional subspace, $\mathcal{U}_0^{(\gamma)} = Ran(E_{\gamma^-}[A_0])$, and acts as a scalar multiplication by γ on $(\mathcal{U}_0^{\gamma})^\perp$. The corresponding quadratic form $a_0^{(\gamma)}$ may be used to define a quadratic form

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

One may observe that $Dom(\tilde{a}) = Dom(a)$ where $\tilde{a}$ is a closed quadratic form and the corresponding self adjoint operator is given by

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

with $Dom(\tilde{A}) = Dom(A)$. 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.

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

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

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

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

By construction, we have

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

for all k and $u \in Dom(a)$ 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 $\lambda_i(A) < \gamma$.

3. Convergence Behavior

In this section we presente estimates which show how the eigenvalues of the operator A are approximated by those of A_k. Throughout this paper we denote that $\mathcal{U}$ is the eigenspace of A corresponding to the eigenvalue $\lambda_i(A) = \lambda_{i+1}(A) = \cdots = \lambda_{i+m-1}(A)$ with multiplicity m, and that $\mathcal{U}^{(k)}$ is the the eigenspace of A_k corresponding to the eigenvalues $\lambda_i(A_k), \lambda_{i+1}(A_k), \ldots, \lambda_{i+m-1}(A_k)$. We also denote E and E_k to be the orthogonal spectral projections of A and A_k onto $\mathcal{U}$ and $\mathcal{U}^{(k)}$, respectively. We introduce some convergence rates for the sequence of bounded operators whose proof may be found in [2].

THEOREM 3.1(BABUŠKA AND OSBORN). *Let (A_k) be a sequence of bounded operators which converges to A uniformly. Then for any i and $j = i, i+1, \ldots, i+m-1$, we have a sufficiently large k such that*

$$|\lambda_i - \lambda_j(A_k)| \le \max_{u \in \mathcal{U}, \|u\|=1} |\langle (A_k - A)u, u\rangle| + C \cdot \max_{u \in \mathcal{U}, \|u\|=1} \|(A_k - A)u\|^2$$

for a constant C independent of k.

We now assume that A_k and A are bounded below such that $A_k \le A_{k+1} \le A$, for all $k \ge 0$. With the aid of Weidmann [15] and the proof of Theorem 3.1 in [2], we have a main estimate result which plays a crucial role in our estimates. For detail, one may refer to [12].

THEOREM 3.2. *Let (A_k) be an increasing sequence of S which converges to A in the strong resolvent sense. Then for all i such that $\lambda_i < \lambda_\infty(A_0)$, $\lambda_i(A_k)$ converges to $\lambda_i(A)$ as k becomes large. Furthermore, if $\lambda_i(A)$ has multiplicity m with $\lambda_i(A) = \lambda_{i+1}(A) = \cdots = \lambda_{i+m-1}(A)$, we have the following estimates for any $j = i, i+1, \ldots, i+m-1$,*

(1)

$$|\lambda_i(A) - \lambda_j(A_k)| \le \max_{u \in \mathcal{U}, \|u\|=1} |\langle (A_k - A)u, u\rangle| + C_1 \cdot \max_{u \in \mathcal{U}, \|u\|=1} \|(A_k - A)u\|^2$$

(2)

$$\left|\frac{1}{\lambda_i(A)} - \frac{1}{\lambda_j(A_k)}\right| \le \max_{u \in \mathcal{U}, \|u\|=1} |\langle (A_k^{-1} - A^{-1})u, u\rangle| + C_2 \cdot \max_{u \in \mathcal{U}, \|u\|=1} \|(A_k^{-1} - A^{-1})u\|^2$$

for k sufficiently large and for some constants C_i's independent of k.

For any self adjoint operator A_k, the corresponding closed quadratic form is denoted by $a_k(u)$. It follows from [8] that we have the following theorem. One may also refer to Kato [11] and Simon [14].

THEOREM 3.3. *Let (A_k) be an increasing sequence of operators in $\mathcal{S}$ which is dominated by $A \in \mathcal{S}$ from above. We assume that for u in $\cap_{k\geq 0} Dom(a_k)$ such that $a_k(u)$ is uniformly bounded, the vector u is in $Dom(a)$ 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 $\lambda_i(A) < \lambda_\infty(A_0)$, $\lambda_i(A_k)$ converges to $\lambda_i(A)$ as k goes to ∞ .*

The set in the second hypothesis of Theorem 3.3 can be expressed as the domain of a_∞. That is,

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

and $a_\infty(u) = \lim_{k\to\infty} a_k(u)$, for all $u \in Dom(a_\infty)$. Both Theorem 3.2 and 3.3 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. We are now in a position to define the measure, the containment gap, [4], to show convergence rrate results.

DEFINITION. Let $\mathcal{M}$ and $\mathcal{N}$ be two closed subspaces of $\mathcal{H}$ with $dim\,\mathcal{N} > 0$. The containment gap between $\mathcal{M}$ and $\mathcal{N}$ is defined as

$$\delta_{\mathcal{M}}(\mathcal{N}) = \max_{0\neq u\in\mathcal{N}} \frac{\|(I-Q)u\|}{\|u\|} = \|(I-Q)P\|,$$

where Q and P are the orthogonal projections onto $\mathcal{M}$ and $\mathcal{N}$, respectively.

Notice that the gap $\delta_{\mathcal{M}}(\mathcal{N})$ is not symmetric in $\mathcal{N}$ and $\mathcal{M}$ unlike that of Kato [11] and that $\delta_{\mathcal{M}}(\mathcal{N}) = 0$ if and only if $\mathcal{M} \supset \mathcal{N}$.

We recall that the intermediate forms are

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

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

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

Suppose that the set of vectors $\{p_i\}$ is taken to be dense in $Dom(\tilde{A})$ with respect to the graph norm $\|\tilde{A}u\|$. Then it follows from Lemmas 2.3.4 and 2.3.5 of [12] 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 3.3 implies that A_k converges to A in the strong resolvent sense. Since $\langle u, (A - A_k)u\rangle = \|(P_k - I)u\|_{\tilde{a}}^2$ and $\|(A - A_k)u\| = \|\tilde{A}(P_k - I)u\|$, we have the following estimate for this method.

LEMMA 3.4. *If the set of vectors $\{p_i\}$ is dense in $Dom(\tilde{A})$ with respect to the norm $\|\tilde{A}u\|$, then $\lambda_i(A_k)$ converges to $\lambda_i(A)$ for any i satisfying $\lambda_i(A) < \gamma$, and for all $j = i, i+1, \ldots, i+m-1$,*

$$|\lambda_i(A)-\lambda_j(A_k)| \leq \max_{u\in\mathcal{U},\|u\|=1} \|(I-P_k)u\|_{\tilde{a}}^2 + C\cdot \max_{u\in\mathcal{U},\|u\|=1} \|\tilde{A}(I-P_k)u\|^2$$

for a constant C independent of k.

For an interpretation of the expression $\max_{u\in\mathcal{U},\|u\|=1} \|\tilde{A}(I-P_k)u\|$, we adopt the following from [4]. We first assume that A is bounded, then

$$\|\tilde{A}(I-P_k)u\| = \|\tilde{A}^{\frac{1}{2}}\| \cdot \|(I-P_k)u\|_{\tilde{a}}.$$

Thus A_k converges strongly to A.

Define $Q_k : \mathcal{H} \longrightarrow span_{1\leq i\leq k}\{\tilde{A}p_i\}$ to be the orthogonal projection. Then

$$\begin{aligned}
\|(I-P_k)u\|_{\tilde{a}} &\leq \|\tilde{A}^{-\frac{1}{2}}\| \cdot \|(I-P_k^*)\tilde{A}u\| \\
&\leq \|\tilde{A}^{-\frac{1}{2}}\| \cdot \|(I-P_k^*)\| \cdot \|(I-Q_k)\tilde{A}u\| \\
&\leq \|\tilde{A}^{-\frac{1}{2}}\|(1+\|\tilde{A}P_k\tilde{A}^{-1}\|)\|(I-Q_k)\tilde{A}u\| \\
&\leq \|\tilde{A}^{-\frac{1}{2}}\|(1+\kappa)\|(I-Q_k)\tilde{A}u\|,
\end{aligned}$$

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

THEOREM 3.5. *Assume the hypotheses of Lemma 3.4. If A is bounded, then for $j = i, i+1, \ldots, i+m-1$,*

$$|\lambda_i(A) - \lambda_j(A_k)| \leq C \cdot \max_{u\in\mathcal{U},\|u\|=1} \|(I-Q_k)\tilde{A}u\|^2$$

for a constant C independent of k.

REMARK.

$$\begin{aligned}
\max_{u\in\mathcal{U}} \frac{\|(I-Q_k)\tilde{A}u\|}{\|u\|} &= \max_{u\in\mathcal{U}} \frac{\|\tilde{A}u - Q_k\tilde{A}u\|}{\|\tilde{A}u\|}\frac{\|\tilde{A}u\|}{\|u\|} \\
&\leq \max_{u\in\mathcal{U},\|u\|=1} \|\tilde{A}u\| \cdot \max_{v\in\tilde{A}\mathcal{U}} \min_{p\in\tilde{A}\mathcal{P}_k} \frac{\|v-p\|}{\|v\|} \\
&= O(\delta_{\tilde{A}\mathcal{U}}(\tilde{A}\mathcal{P}_k)).
\end{aligned}$$

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

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

where μ is chosen sufficiently large so that the corresponding quadratic form satisfies $\tilde{\tilde{a}}(u) \geq \frac{\alpha}{2}\|u\|^2$. See [10] for a proof that such a μ exists. We then have

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

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

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

LEMMA 3.6. *If $\{p_i\}$ is dense in $Dom(\tilde{A})$ with respect to the norm $\|\tilde{A}u\|$, then the set of $\{\hat{p}_i\}$ is dense in $Dom(\tilde{\tilde{A}})$ with respective to $\|\tilde{\tilde{A}}u\|$.*

Proof. We assume that $\left\langle \tilde{\tilde{A}}u, \tilde{\tilde{A}}\hat{p}_i \right\rangle = 0$ for some $u \in Dom(\tilde{\tilde{A}})$, then

$$0 = \left\langle \tilde{\tilde{A}}u, \tilde{A}p_i \right\rangle = \left\langle \tilde{A}\tilde{A}^{-1}\tilde{\tilde{A}}u, \tilde{A}p_i \right\rangle.$$

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

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

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

We define the intermediate operators as

$$A_k'' = A_0^{(\gamma)} + \tilde{\tilde{A}}\hat{P}_k.$$

Then we have for $u \in Dom(\tilde{a})$,

$$\begin{aligned} \tilde{\tilde{a}}(\hat{P}_k u) =& \tilde{\tilde{a}}(u - (I - \hat{P}_k)u) \leq \tilde{\tilde{a}}(u - (I - P_k)u) \\ &= \tilde{\tilde{a}}(P_k u) \leq \tilde{a}(P_k u) \leq \tilde{a}(u), \end{aligned}$$

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

$$\tilde{\tilde{a}}(u - (I - \hat{P}_k u)) \leq \tilde{\tilde{a}}(u - (I - P_k u)).$$

Therefore in this procedure the approximating vector $\{p_i\}$ should be considered as the graph norm $\|\tilde{A}u\|$.

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 3.7. *If the set of vectors $\{p_i\}$ is dense in $Dom(\tilde{A})$ with respect to the norm $\|\tilde{A}u\|$, then for $j = i, i+1, \ldots, i+m-1$,*

$$|\lambda_i(A) - \lambda_j(A_k)| \leq C \cdot \delta^2_{\tilde{A}\mathcal{U}}(\tilde{A}\mathcal{P}_k)$$

for a constant C independent of k.

Proof. Let $\hat{Q}_k : \mathcal{H} \longrightarrow span_{1 \leq i \leq k}\{\tilde{\tilde{A}}\hat{p}_i\}$ be the orthogonal projection. Since $\tilde{\tilde{A}}$ is bounded, it follows from Theorem 3.5 and Lemma 3.6 that we have

$$|\lambda_i(A) - \lambda_j(A_k)| \leq C \cdot \max_{u \in \mathcal{U}, \|u\|=1} \|(I - \hat{Q}_k)\tilde{\tilde{A}}u\|^2.$$

By the same argument as the remark of Theorem 3.5, we get

$$\max_{u \in \mathcal{U}} \frac{\|(I - \hat{Q}_k)\tilde{\tilde{A}}u\|}{\|u\|} = O(\delta_{\tilde{\tilde{A}}\mathcal{U}}(\tilde{\tilde{A}}\hat{\mathcal{P}}_k)).$$

Since $\tilde{\tilde{A}}\mathcal{U} = \tilde{A}\mathcal{U}$ and $\tilde{\tilde{A}}\hat{\mathcal{P}}_k = \tilde{A}\mathcal{P}_k$, we have the results.■

REMARK. *With the same conditions as Theorem 3.7 has, Beattie and Greenlee obtained the following result to Theorem 3.7 [5]:*

$$|\lambda_i(A) - \lambda_j(A_k)| \le C \cdot \{\delta^2_{\mathcal{U}^\gamma}(\tilde{A}\mathcal{P}_k) + \delta^2_{\mathcal{U}+\mathcal{U}_0^\gamma}(\tilde{A}\mathcal{P}_k)\}.$$

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

4. 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 3.7 in terms of spectral projections of an auxiliary operator B. Let B be a positive definite and self adjoint operator in $\mathcal{H}$ such that $Dom(B) \subset Dom(\tilde{A})$ and $\|\tilde{A}u\| \le \beta\|Bu\|, \beta \ge 0$, for all $u \in Dom(B)$ with B^{-1} compact. Let

$$0 \le \mu_1 \le \mu_2 \le \cdots \nearrow \infty$$

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 in [4,5].

THEOREM 4.1. *If the eigenspace $\mathcal{U}$ is contained in $Dom(B^\tau)$ with $\tau > 1$, then*

$$\delta_{\tilde{A}\mathcal{U}}(\tilde{A}\mathcal{P}_k) = o(\mu_k^{1-\tau}), \text{ as } k \longrightarrow \infty,$$

where B^τ denotes the unique positive definite τ^{th} power of B.

This theorem implies that if we have such an operator B that the eigenspace of A corresponding to $\lambda_i(A)$ is contained in $Dom(B^\tau)$, then

$$|\lambda_i(A) - \lambda_i(A_k)| = o(\mu_k^{2-2\tau})$$

as $k \longrightarrow \infty$.

As an example, we estimate the rate of convergence of a differential problem with non-trivial continuous spectrum that was considered in [4,5]. The eigenvalue problem is for a Schrödinger operator with potential defined by

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

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 γ. The negative number γ will be our truncation point. We define the base operator A_0 by

$$A_0 u = -u'' + q_0 u,$$

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 $A_0 u = \lambda u$ 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 λ of

$$\tan(a\sqrt{ba^2 - \gamma + \lambda}) = \sqrt{\frac{\gamma - \lambda}{ba^2 - \gamma + \lambda}}$$

lying in the interval $(\gamma - ba^2, \gamma)$. The number of eigenvalues of A_0 smaller than γ is equal to the biggest integer, say N, smaller than

$\frac{a^2\sqrt{b}}{\pi}+1$. These eigenvalues below γ are labeled as $\lambda_1^0 \le \lambda_2^0 \le \cdots \le \lambda_N^0$. The corresponding eigenvectors, u_i^0, 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 $Dom(B) = H^2(\mathbb{R}) \cap Dom(x^2)$ Then B is self adjoint, and $\mu_k = \alpha(2k+1)$ for $k = 0, 1, 2, \ldots$ [7]. Moreover $\mathcal{U} \subset Dom(B^\tau)$, for all $\tau > 0$ [5]. 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 choose $\{p_k\}$ so that each p_k is an eigenvector of B with the corresponding eigenvalue μ_k. They are known as

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

where $H_k(\xi)$ is the Hermite polynomial. 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 $A_0^{(\gamma)}u = \sum_{l=1}^N \lambda_l^0 \langle u, u_l^0\rangle u_l^0 + \gamma(u - \sum_{l=1}^N \langle u, u_l^0\rangle u_l^0)$ and $\tilde{A} = A - A_0^{(\gamma)}$. Since the space $span\,\{u_1^0, \ldots, u_N^0\} \oplus span\,\{\tilde{A}p_1, \ldots, \tilde{A}p_k\}$ reduces the operator A_k, the intermediate problem $A_k u = \lambda u$ produces the matrix equation:

$$\begin{bmatrix} (\langle A_k u_i^0, u_j^0\rangle) & (\langle A_k u_i^0, \tilde{A}p_j\rangle) \\ (\langle \tilde{A}p_i, A_k u_j^0\rangle) & (\langle A_k \tilde{A}p_i, \tilde{A}p_j\rangle) \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

$$= \lambda \begin{bmatrix} ((u_i^0, u_j^0)) & ((u_i^0, \tilde{A}p_j)) \\ ((\tilde{A}p_i, u_j^0)) & ((\tilde{A}p_i, \tilde{A}p_j)) \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

whose rank is $k + N$. By a transformation, we get a simpler equation:

$$\begin{bmatrix} I & B \\ B^* & A \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = (\lambda - \gamma) \begin{bmatrix} (\Lambda - \gamma)^{-1} & 0 \\ 0 & C \end{bmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

where

$$A = ((\tilde{A}p_i, \tilde{A}p_j)), \qquad B = ((u_i^0, \tilde{A}p_j))$$
$$C = ((p_i, \tilde{A}p_j)) \quad \text{and } \Lambda = diag(\lambda_i^0).$$

and I is the identity matrix.

The inner products involved are expressed by the four basic ones $\langle u_i^0, p_j\rangle$, $\langle u_i^0, Ap_j\rangle$, $\langle Ap_i, Ap_j\rangle$ and $\langle Ap_i, p_j\rangle$. We express analytically the inner products $\langle Ap_i, p_j\rangle$ and $\langle Ap_i, Ap_j\rangle$. But the inner products $\langle u_i^0, p_j\rangle$ and $\langle u_i^0, Ap_j\rangle$ have to be approximated with numerical quadratures. 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 method to an estimated relative accuracy of 10^{-14}. The matrix eigenvalue problem was computed by the $\mathcal{QZ}$ method of Moler and Stewart. An order 30 Rayleigh-Ritz calculation using even-ordered Hermite trial functions were performed to provide complementary upper bounds.

For $a = 3, b = 2$ and $c = 0.01$ (thus $N = 5$), the computational results are given in Table 1 and the difference between upper and lower bounds are plotted against intermediate problem order k, on a log-log scale in Figure 1. The size of computational matrices is $k + 5$. We observe that no linear asymptote is appeared for any of the error curves, which is consistent with the predicted infinite order convergence.

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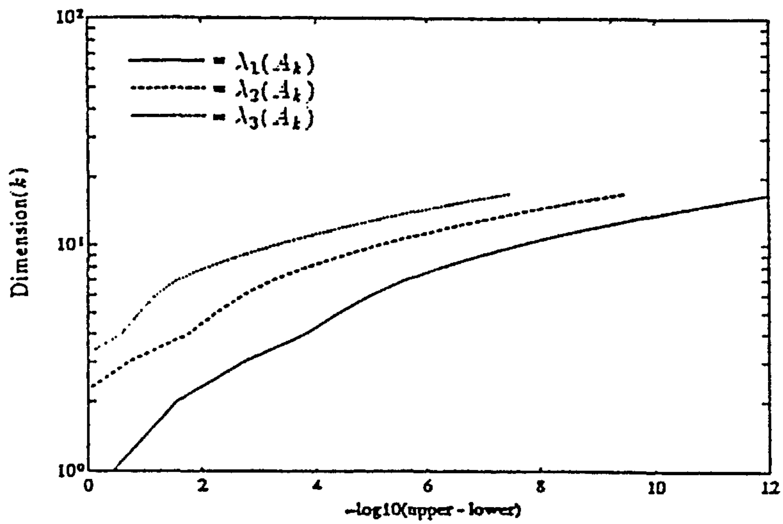
Table 1. Radial Schrödinger Equation: $\gamma = -0.1$

k	λ_1	λ_2	λ_3
Base	-17.864406220	-15.985358216	-12.262742720
5	-16.108571114	-9.0413075976	-3.1734022489
10	-16.108530500	-9.0354832125	-3.0515521939
15	-16.108530475	-9.0354751905	-3.0510018553
Ritz	-16.108530475	-9.0354751845	-3.0510013156

where Base means the base operator, i.e. $k = 0$, and Ritz means upper bounds come from Rayleigh–Ritz method.

Figure 1: Schrodinger equation: gamma=-0.1



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