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# Numerical verification method for spectral problems 

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#### Abstract

In this paper we will show how guaranteed bounds for eigenvalues（together with eigenvectors）are obtained and how non－existence of eigenvalues in a concrete region could be assured．Especially we focus on an application to the eigenvalue excluing of 1－D Schrödinger operators in the spectral gaps．


## 1 Introduction

Up to now we have developed a method to enclose and exclude eigenvalues for differential operators［8，10］．This method is based on Nakao＇s theory known as a numerical verification method for partial differential equations［ $15,16,17,18$ ］，and it has a merit that it could be applied even in case the operator is not symmetric．A remarkable point of this eigenvalue enclosing／excluding is to assure an existence and non－existence range of eigenvalues in mathe－ matically rigorous sense．This means not only a reliability of computed eigenpairs（e．g．［12］） but also that such evaluation of eigenvalues（and eigenvectors）can be applied to related another problems，e．g．another numerical verification method for nonlinear problems［9，11］or stability analysis of bifurcation phenomenon in hydrodynamics［13］．

This paper aims to show how eigenvalues（and eigenvectors）are enclosed or excluded in mathematically rigorous sense．At first in Section 2，we introduce some eigenvalue enclosure methods，especially for symmetric operators．Our original method is described in Section 3， and an application to a spectral problem for one dimensional Schrödinger operator is presented in Section 4.

## 2 Enclosure methods for symmetric operators

Let $H$ be an infinite dimensional Hilbert space with an inner product $\langle\cdot, \cdot\rangle$. For a linear symmetric operator $L: \mathcal{D}(L) \rightarrow H$, we consider the eigenvalue problem

$$
\begin{equation*}
L u=\lambda u, \quad u \in \mathcal{D}(L) \backslash\{0\} . \tag{2.1}
\end{equation*}
$$

An eigenvalue of an operator takes an important role to understand a nonlinear phenomenon in science and engineering. Especially, it often becomes a key value when we consider a behavior of dynamical systems.

Several methods to enclose eigenvalues for symmetric operators have been proposed, and now we introduce some of those methods below. Here we assume that all eigenvalues of $L$ are bounded below and ordered as $\lambda_{1} \leq \lambda_{2} \leq \cdots$.

## Krylov-Weinstein's bounds [4]

As one of the simplest way of eigenvalue enclosure, Krylov-Weinstein's bounds is well known.
Let $(\widetilde{u}, \tilde{\lambda}) \in \mathcal{D}(L) \times \mathbf{R}$ be an approximate eigenpair and compute

$$
\delta \equiv \frac{\|L \tilde{u}-\tilde{\lambda} \tilde{u}\|}{\|\widetilde{u}\|}
$$

Then the interval $[\tilde{\lambda}-\delta, \tilde{\lambda}+\delta]$ contains at least one eigenvalue of $L$.
This bound is easy to compute, but the width of the enclosed interval is not so narrow. And it also has another defect that no information is obtained concerning the index of eigenvalue.

## Kato-Temple's bounds [6]

As an improved version of Krylov-Weinstein's bounds, there is a Kato-Temple's bounds which was proposed in 1949 [6].

Let $(\bar{u}, \tilde{\lambda})$ be an approximate eigenpair satisfying

$$
\tilde{\lambda}=<L \tilde{u}, \tilde{u}\rangle /\langle\tilde{u}, \tilde{u}\rangle
$$

and compute

$$
\delta \equiv \frac{\|L \tilde{u}-\tilde{\lambda} \widetilde{u}\|}{\|\tilde{u}\|}
$$

For the nth eigenvalue $\lambda_{n}$ with finite multiplicity, suppose that an open interval ( $\alpha, \beta$ ) does not contain any spectrum except for $\lambda_{n}$. Then for $\rho \in \mathbf{R}$ satisfying $\alpha<\rho<\beta$, we have

$$
\begin{equation*}
\lambda_{n} \in\left[\rho-\frac{\delta^{2}}{\beta-\rho}, \rho+\frac{\delta^{2}}{\rho-\alpha}\right] . \tag{2.2}
\end{equation*}
$$

The quality of this bounds is better than Krylov-Weinstein's bounds. Indeed it has an $O\left(\delta^{2}\right)$ quality compared with an $O(\delta)$ quality of Krylov-Weinstein's bounds. But it also has a difficulty that it needs a precise information on eigenvalue distribution in advance, i.e. a (rough) upper bound for $\lambda_{n-1}$ and (rough) lower bound for $\lambda_{n+1}$ are needed to obtain the result.

## Rayleigh-Ritz bounds [4]

The Rayleigh-Ritz method is well known as a method to obtain very accurate upper bounds for the first $N$ eigenvalues of $L$.

Let $\widetilde{u}_{1}, \ldots, \widetilde{u}_{N} \in \mathcal{D}(L)$ be linearly independent functions and define two $N \times N$ - matrices

$$
\begin{aligned}
& A_{1} \equiv\left(<L \widetilde{u}_{i}, \widetilde{u}_{j}>\right)_{i, j=1, \ldots, N}, \\
& A_{2} \equiv\left(\left\langle\widetilde{u}_{i}, \widetilde{u}_{j}>\right)_{i, j=1, \ldots, N}\right.
\end{aligned}
$$

Then, for $N$ eigenvalues $\Lambda_{i}(i=1, \ldots, N)$ of the matrix eigenvalue problem

$$
\begin{equation*}
A_{1} x=\Lambda A_{2} x, x \in \mathbf{R}^{N} \backslash\{0\}, \tag{2.3}
\end{equation*}
$$

we have

$$
\begin{equation*}
\lambda_{i} \leq \Lambda_{i}(i=1, \ldots, N) \tag{2.4}
\end{equation*}
$$

Being different from Kato-Temple's bounds, this method does not need any a priori information concerning eigenvalue distribution, although it does not give any lower bounds.

## Lehman's Bounds [3]

Concerning the lower bounds for eigenvalues, there is a Lehman's method as follows.
Let $\tilde{u}_{1}, \ldots, \tilde{u}_{N} \in \mathcal{D}(L)$ be linearly independent functions and suppose that $\Lambda_{N}<\nu \leq \lambda_{N+1}$ holds for a real number $\nu$, where $\Lambda_{N}$ denotes the Rayleigh-Ritz bound. Moreover define three $N \times N$ - matrices

$$
\begin{aligned}
& A_{3} \equiv\left(<L \widetilde{u}_{i} L \widetilde{u}_{j}>\right)_{i, j=1, \ldots, N}, \\
& B_{1} \equiv A_{1}-\nu A_{2} \\
& B_{2} \equiv A_{3}-2 \nu A_{1}+\nu^{2} A_{2},
\end{aligned}
$$

where $A_{1}$ and $A_{2}$ are the same matrices in Rayleigh-Ritz method. Then, for $N$ eigenvalues $\mu_{i}(i=1, \ldots, N)$ of the matrix eigenvalue problem

$$
\begin{equation*}
B_{1} x=\mu B_{2} x, x \in \mathbf{R}^{N} \backslash\{0\}, \tag{2.5}
\end{equation*}
$$

we have

$$
\begin{equation*}
\lambda_{N+1-i} \geq \nu+\frac{1}{\mu_{i}}(i=1, \ldots, N) \tag{2.6}
\end{equation*}
$$

This lower bound is also sharp, but it also has the same difficulty as Kato-Temple's method, i.e. it needs a priori information on the exact eigenvalue $\lambda_{N+1}$.

## Homotopy Method [19]

In order to overcome the difficulty to obtain a priori information on exact eigenvalues, the homotopy method was proposed by Plum in 1990 [19]. In his method a base problem is considered corresponding to the given problem, i.e. for the eigenvalue problem for $L$. Here the base problem is chosen so that the eigenvalue distribution of it is already obtained. Let $L_{0}$ be
an operator which corresponds to this base problem, then consider a homotopy which connects two operators $L$ and $L_{0}$ :

$$
L_{s} \equiv(1-s) L_{0}+s L, \quad s \in[0,1]
$$

Then starting from $s=0$ and making use of the continuity and monotonicity of eigenvalues on the parameter $s$, some eigenvalues for $L_{s}$ are enclosed in each step. Finally the first several eigenvalues of $L$ are enclosed when the parameter $s$ reached 1.

Besides these methods, there are the intermediate methods [1, 2], but all these methods are restricted to symmetric operators and cannot be applied to non-symmetric operators. Moreover, any eigenvectors are not enclosed by these methods. In the next section, we introduce our method which could be also applied to non-symmetric operators and also provides the eigenvector enclosures.

## 3 Enclosing and excluding method based on Nakao's theory

We have developed a method to enclose eigenvalues and eigenvectors for differential operators $[8,10]$, which was based on Nakao's verification methods for nonlinear differential equations $[15,16,17,18]$.

For example, we consider an eigenvalue problem:

$$
\left\{\begin{align*}
-\Delta u+q u & =\lambda u & \text { in } \Omega  \tag{3.1}\\
u & =0 & \text { on } \partial \Omega
\end{align*}\right.
$$

Here $\Omega$ is a bounded convex domain in $\mathbf{R}^{2}$ and let $q \in L^{\infty}(\Omega)$. We apply Nakao's method which is known as a numerical verification method for nonlinear problems, by normalizing the problem (3.1) as

$$
\text { find }(\widehat{u}, \lambda) \in H_{0}^{1}(\Omega) \times R \text { s.t. }
$$

$$
\left\{\begin{align*}
-\Delta \widehat{u}+(q-\lambda) \widehat{u} & =0  \tag{3.2}\\
\int_{\Omega} \widehat{u}^{2} d x & =1
\end{align*}\right.
$$

The basic idea of our method is as follows. Using the following compact map on $H_{0}^{1}(\Omega) \times \mathbf{R}$

$$
\begin{equation*}
F(\widehat{u}, \lambda) \equiv\left((-\Delta)^{-1}(\lambda-q) \widehat{u}, \lambda+\int_{\Omega} \widehat{u}^{2} d x-1\right) \tag{3.3}
\end{equation*}
$$

where $(-\Delta)^{-1}$ means the solution operator for Poisson equation with homogeneous boundary condition, we have the fixed point equation for $w=(\widehat{u}, \lambda)$

$$
\begin{equation*}
w=F(w) \tag{3.4}
\end{equation*}
$$

In actual computation we use a residual form, and apply the Newton-like method to the finite dimensional part of (3.4) and use a norm estimation for the infinite dimensional part. For details see $[8,10]$.

Our method is also applicable to non-symmetric operators. So far we have applied our enclosure method to enclose eigenpair of symmetric operators and to enclose real eigenvalues and corresponding eigenvectors of a non-symmetric operator. For details see $[9,11,12,13]$.

Moreover we have proposed a method to exclude an eigenvalue in a concrete interval, i.e. to prove that there is no eigenvalue in the interval. This could be done as follows.

Let $\Lambda$ be a narrow interval in which we want to exclude any eigenvalues. Then consider the linear equation

$$
\left\{\begin{align*}
-\Delta u+q u & =\Lambda u & \text { in } \Omega,  \tag{3.5}\\
u & =0 & \text { on } \partial \Omega .
\end{align*}\right.
$$

Since the equation (3.5) has a trivial solution $u \equiv 0$, if we could prove the uniqueness of the solution of (3.5) then the non-existance of eigenvalues in $\Lambda$ could be confirmed.

Now, we describe the manner how to validate the uniqueness of the solutions for (3.5). We consider the following second-order elliptic boundary value problem for a fixed $\lambda \in \Lambda$ :

$$
\left\{\begin{align*}
-\Delta u & =(\lambda-q) u & & \text { in } \Omega,  \tag{3.6}\\
u & =0 & & \text { on } \partial \Omega .
\end{align*}\right.
$$

Using the following compact map on $H_{0}^{1}(\Omega)$

$$
F(\lambda) u \equiv(-\Delta)^{-1}(\lambda-q) u
$$

we can rewrite (3.6) as follows:

$$
\begin{equation*}
F(\lambda) u=u \tag{3.7}
\end{equation*}
$$

Now, let $S_{h}$ be a finite dimensional subspace of $H_{0}^{1}(\Omega)$ dependent on $h(0<h<1)$. Usually, $S_{h}$ is taken to be a finite element subspace with mesh size $h$. Also, let

$$
P_{h 0}: H_{0}^{1}(\Omega) \longrightarrow S_{h}
$$

denote the $H_{0}^{1}$-projection defined by

$$
\left(\nabla\left(u-P_{h 0} u\right), \nabla v\right)_{L^{2}}=0 \quad \text { for all } v \in S_{h}
$$

We set

$$
\begin{aligned}
& N_{h 0}(\lambda) u \equiv P_{h 0} u-[I-F(\lambda)]_{h 0}^{-1}\left(P_{h 0} u-P_{h 0} F(\lambda) u\right), \\
& T(\lambda) u \equiv N_{h 0}(\lambda) u+\left(I-P_{h 0}\right) F(\lambda) u
\end{aligned}
$$

where we supposed that restriction to $S_{h}$ of the operator $P_{h 0}[I-F(\lambda)]: H_{0}^{1}(\Omega) \longrightarrow S_{h}$ has an inverse $[I-F(\lambda)]_{n 0}^{-1}$, and this can be checked in the actual computation. Then $T(\lambda)$ is a compact linear map on $H_{0}^{1}(\Omega)$ and following equivalence relation holds:

$$
\begin{equation*}
T(\lambda) u=u \Longleftrightarrow F(\lambda) u=u \tag{3.8}
\end{equation*}
$$

We have the following theorem:

Theorem 1. If there exists a non-empty, closed, bounded and convex set $U \subset H_{0}^{1}(\Omega)$ satisfying $T(\lambda) U \stackrel{\circ}{\subset} U$, then there exists a unique solution $u \in H_{0}^{1}(\Omega)$ of $F(\lambda) u=u$.

Here, $M_{1} \stackrel{\circ}{\subset} M_{2}$ implies $\bar{M}_{1} \subset \stackrel{\circ}{M}_{2}$ for any sets $M_{1}, M_{2}$.

Proof.

Consider $v$ satisfying $T(\lambda) v=v$. Since $T(\lambda)$ is a linear operator, for any $c \in \mathbf{R}$ we have

$$
\begin{equation*}
T(\lambda)(c v)=c T(\lambda) v=c v \tag{3.9}
\end{equation*}
$$

If $v \neq 0$, we can choose $\hat{c} \in R$ satisfying

$$
\hat{c} v \in \partial U
$$

But this contradicts with $T(\lambda) U \stackrel{\circ}{\subset} U$ and (3.9). Therefore $v=0$. That is, $u=0$ is a unique solution of $F(\lambda) u=u$.

By Theorem 1, if there exists a closed, bounded and convex set $U \subset H_{0}^{1}(\Omega)$ satisfying $T(\lambda) U \stackrel{\circ}{\subset} U$ for each $\lambda \in \Lambda$, then it means that we validated the uniqueness for the trivial solution $u=0$ of (3.5). We use an interval arithmetic to treat all $\lambda \in \Lambda$ in a computer.

Although we cannot take so wide interval as $\Lambda$ (usually $10^{-1} \sim 10^{-3}$, although it depends on each problem), by changing $\Lambda$ little by little we can cover a rather wide range which we want to prove the non-existence of eigenvalues. These enclosing and excluding methods will be able to be applied to the problem in $\mathbf{R}^{\mathbf{3}}$.

## 4 Spectral problem for 1-D Schrödinger operator

Now we describe an application to exclude eigenvalues in spectral gaps, i.e. we treat an operator which has the essential spectrum with band-gap structure.

We consider the following eigenvalue problem

$$
\begin{equation*}
L u \equiv-u^{\prime \prime}+q(x) u+s(x) u=\lambda u, \quad x \in \mathbf{R} \tag{4.1}
\end{equation*}
$$

where we assume that $q$ is a bounded, continuous and periodic function with a period $r>0$ and $s \in L^{\infty}(\mathbf{R})$ satisfies $s(x) \rightarrow 0(|x| \rightarrow \infty)$.

Some approach have been made to this kind of problem e.g. in [21] and [22], but they are the asymptotic results about the number of eigenvalues in spectral gaps in a limit case. Our aim is excluding an eigenvalue in some concrete interval between two essential spectra.

We can regard the operator $L$ as the selfadjoint operator $L: \mathcal{D}(L) \subset L^{2}(\mathbf{R}) \rightarrow L^{2}(\mathbf{R})$ defined on a suitable dense subspace $\mathcal{D}(L) \subset L^{2}(\mathbf{R})$; see [5] for details on the construction of this operator realizing the differential expression (4.1). The essential spectrum of $L$ could be obtained as follows.

At first the essential spectrum of the operator

$$
L_{0} u \equiv-u^{\prime \prime}+q(x) u
$$

is obtained using the result by Eastham [5].
Theorem 2. Let $q$ be a periodic function in $(0, r)$ and consider the following two eigenvalue problems:
I. Periodic eigenvalue problem:

$$
\left\{\begin{array}{l}
-u^{\prime \prime}+q(x) u=\lambda u  \tag{4.2}\\
u(0)=u(r), u^{\prime}(0)=u^{\prime}(r)
\end{array}\right.
$$

and
II. Semi-periodic eigenvalue problem:

$$
\left\{\begin{array}{l}
-u^{\prime \prime}+q(x) u=\mu u,  \tag{4.3}\\
u(0)=-u(r), u^{\prime}(0)=-u^{\prime}(r) .
\end{array}\right.
$$

Then for each eigenvalues $\left\{\lambda_{n}\right\},\left\{\mu_{n}\right\}$ we have

$$
\begin{equation*}
\lambda_{0}<\mu_{0} \leq \mu_{1}<\lambda_{1} \leq \lambda_{2}<\mu_{2} \leq \mu_{3} \leq \cdots, \tag{4.4}
\end{equation*}
$$

and the essential spectra of $L_{0}$ are obtained as

$$
\begin{equation*}
\left[\lambda_{2 m}, \mu_{2 m}\right],\left[\mu_{2 m+1}, \lambda_{2 m+1}\right] \quad m=0,1,2, \cdots . \tag{4.5}
\end{equation*}
$$

Moreover we are able to confirm that $L$ is a compact perturbation of $L_{0}$. Therefore essential spectra of $L$ and $L_{0}$ coincide. (cf. [7])

We try to exclude eigenvalues of $L$ in spectral gaps by the method proposed in $[8,10]$.
We first consider the case that $q(x)=a \cdot \cos (2 \pi x)$ for $a \in \mathbf{R}$. Then we obtain (approximate) $\left\{\mu_{i}\right\}$ and $\left\{\lambda_{i}\right\}$ for e.g. $a=5.0$ as follows:

$$
\begin{aligned}
\lambda_{0}(-0.624017) & <\mu_{0}(7.292924)<\mu_{1}(12.287917)<\lambda_{1}(39.425660) \\
& <\lambda_{2}(40.049607)<\mu_{2}(88.863540)<\cdots .
\end{aligned}
$$

The first spectral gap is ( $\mu_{0}, \mu_{1}$ ) and the second spectral gap is ( $\lambda_{1}, \lambda_{2}$ ) which is much narrow than the first spectral gap. Our first target is to exclude eigenvalue in the first spectral gap.

### 4.1 Fixed Point Formulation

For a real number $\lambda \notin \sigma_{e s s}\left(L_{0}\right)$, consider a linear equation

$$
\begin{equation*}
(L-\lambda) u=0 \quad \text { on } \mathbf{R} . \tag{4.6}
\end{equation*}
$$

Since it is clear that (4.6) has a trivial solution $u=0$, if we validate the uniqueness of the solution of (4.6) by the method described below, it implies that any $\lambda$ is not an eigenvalue of $L$.

Since the inverse of $L_{0}-\lambda$ exists if $\lambda \notin \sigma_{\text {ess }}\left(L_{0}\right)$, we have

$$
\begin{aligned}
(L-\lambda) u=0 & \Leftrightarrow\left(L_{0}-\lambda\right) u+s u=0 \\
& \Leftrightarrow u=\left(\lambda-L_{0}\right)^{-1}(s u) .
\end{aligned}
$$

By Floquet Theory there exist fundamental solutions $\psi_{1}(x), \psi_{2}(x)$ of $L \psi=0$ s.t.

$$
\begin{equation*}
\psi_{1}(x)=e^{\mu x} p_{1}(x), \quad \psi_{2}(x)=e^{-\mu x} p_{2}(x), \tag{4.7}
\end{equation*}
$$

or

$$
\begin{equation*}
\psi_{1}(x)=e^{\mu x} p_{1}(x), \quad \psi_{2}(x)=e^{\mu x}\left(x p_{1}(x)+p_{2}(x)\right) \tag{4.8}
\end{equation*}
$$

where $\mu$ is the characteristic exponent and $p_{1}, p_{2}$ are $r$-periodic functions. In this paper we treat the case which allows to choose $\mu$ with positive real part. (In later estimations we use the same notation $\mu$ for its real part.)

Using those fundamental solutions we define the Green's function $G(x, y, \lambda)$ [5] for $-\infty<$ $x, y<\infty$ by

$$
G(x, y, \lambda)= \begin{cases}\psi_{1}(x) \psi_{2}(y) / W\left(\psi_{1}, \psi_{2}\right)(x) & (x \leq y)  \tag{4.9}\\ \psi_{2}(x) \psi_{1}(y) / W\left(\psi_{1}, \psi_{2}\right)(x) & (x \geq y)\end{cases}
$$

where $W\left(\psi_{1}, \psi_{2}\right)(x) \equiv \psi_{1}(x) \psi_{2}^{\prime}(x)-\psi_{1}^{\prime}(x) \psi_{2}(x)$ stands for the Wronskian.
Since by simple calculations we obtain that $W\left(\psi_{1}, \psi_{2}\right)(x)$ is the constant function, we express $W\left(\psi_{1}, \psi_{2}\right)(x)$ as $\xi$ and rewrite $G(x, y, \lambda)$ as

$$
G(x, y, \lambda)= \begin{cases}\psi_{1}(x) \psi_{2}(y) / \xi & (x \leq y)  \tag{4.10}\\ \psi_{2}(x) \psi_{1}(y) / \xi & (x \geq y)\end{cases}
$$

Using this Green's function we have [5]

$$
\begin{equation*}
\left(\lambda-L_{0}\right)^{-1} f=\int_{\mathbf{R}} G(x, y, \lambda) f(y) d y \tag{4.11}
\end{equation*}
$$

Consequently using a compact operator

$$
F_{\lambda} u \equiv \int_{\mathbf{R}} G(x, y, \lambda) s(y) u(y) d y
$$

on $H^{1}(\mathbf{R})$ we have a fixed point equation

$$
\begin{equation*}
u=F_{\lambda} u \tag{4.12}
\end{equation*}
$$

which is equivalent to $(L-\lambda) u=0$.

### 4.2 Projection and interpolation

Let $\Omega_{M} \equiv[-M, M]$ be a bounded interval on $\mathbf{R}$ and set $\widetilde{\Omega}_{M} \equiv \mathbf{R} \backslash \Omega_{M}$. For any $v \in H^{1}(\mathbf{R})$ we consider the following decomposition:

$$
\begin{equation*}
\left.v_{M}(x) \equiv v(x)\right|_{\Omega_{M}},\left.\tilde{v}_{M}(x) \equiv v(x)\right|_{\Omega_{M}} \tag{4.13}
\end{equation*}
$$

Defining the projections

$$
P_{M}: H^{1}(\mathbf{R}) \rightarrow H^{1}\left(\Omega_{M}\right)
$$

and

$$
\widetilde{P}_{M}: H^{1}(\mathbf{R}) \rightarrow H^{1}\left(\widetilde{\Omega}_{M}\right)
$$

as $P_{M}(v)=v_{M}$ and $\widetilde{P}_{M}(v)=\tilde{v}_{M}$, we decompose (4.12) into the bounded interval part and the remainder:

$$
\left\{\begin{array}{l}
P_{M} u=P_{M} F_{\lambda}(u),  \tag{4.14}\\
\widetilde{P}_{M} u=\widetilde{P}_{M} F_{\lambda}(u)
\end{array}\right.
$$

Let $\Pi$ be the piecewise linear interpolation operator on $\Omega_{M}$ and we further decompose the former part of (4.14) into the finite and infinite dimensional parts:

$$
\left\{\begin{align*}
\Pi P_{M} u & =\Pi P_{M} F_{\lambda}(u)  \tag{4.15}\\
(I-\Pi) P_{M} u & =(I-\Pi) P_{M} F_{\lambda}(u)
\end{align*}\right.
$$

Let $S_{h}\left(\Omega_{M}\right)$ denote the set of continuous and piecewise linear polynomials on $\Omega_{M}$ with uniform mesh $-M=x_{0}<x_{1}<\cdots<x_{N}=M$ and mesh size $h$. Due to Schultz [20] we have the following error estimation for $\Pi$ :

Lemma 1. If $f \in\left\{\varphi \in C^{2}\left(\Omega_{M}\right) \mid\left\|\varphi^{\prime \prime}\right\|_{\infty}<\infty\right\}$, then we have

$$
\begin{equation*}
\|f-\Pi f\|_{\infty} \leq \frac{1}{8} h^{2}\left\|f^{\prime \prime}\right\|_{\infty} \tag{4.16}
\end{equation*}
$$

### 4.3 Newton-like method and verification condition

Since we apply a Newton-like method only for the former part of (4.15), we define the following operator:

$$
\mathcal{N}_{\lambda}(u) \equiv P u-\left[I-F_{\lambda}\right]_{M}^{-1}\left(P u-P F_{\lambda}(u)\right)
$$

where $P \equiv \Pi P_{M}$.
Here we assumed that the restriction to $S_{h}\left(\Omega_{M}\right)$ of the operator $\Pi\left[I-F_{\lambda}\right]: S_{h}\left(\Omega_{M}\right) \rightarrow$ $S_{h}\left(\Omega_{M}\right)$ has the inverse $\left[I-F_{\lambda}\right]_{M}^{-1}$. The validity of this assumption can be numerically confirmed in actual computations.

We next define the operator

$$
T_{\lambda}: H^{1}\left(\Omega_{M}\right) \times H^{1}\left(\widetilde{\Omega}_{M}\right) \longrightarrow H^{1}\left(\Omega_{M}\right) \times H^{1}\left(\tilde{\Omega}_{M}\right)
$$

for $u_{M} \equiv P_{M} u$ and $\widetilde{u}_{M} \equiv \widetilde{P}_{M} u$ by

$$
T_{\lambda}\binom{u_{M}}{\widetilde{u}_{M}} \equiv\binom{\mathcal{N}_{\lambda}(u)+(I-\Pi) P_{M} F_{\lambda}(u)}{\widetilde{P}_{M} F_{\lambda}(u)}
$$

Then we have the following equivalence relation

$$
\binom{u_{M}}{\widetilde{u}_{M}}=T_{\lambda}\binom{u_{M}}{\widetilde{u}_{M}} \Longleftrightarrow u=F_{\lambda}(u) .
$$

Our purpose is to find a unique fixed point of $T_{\lambda}$ in a certain set $U \subset L^{\infty}\left(\Omega_{M}\right) \times L^{2}\left(\widetilde{\Omega}_{M}\right)$, which is called a 'candidate set'. Given positive real numbers $\gamma, \alpha_{M}$ and $\beta$ we define the corresponding candidate set $U$ by

$$
\begin{equation*}
U \equiv\binom{U_{M}+\left[\alpha_{M}\right]}{[\beta]} \tag{4.17}
\end{equation*}
$$

where

$$
\begin{equation*}
U_{M} \equiv\left\{v_{h} \in S_{h}\left(\Omega_{M}\right) \mid\left\|v_{h}\right\|_{L^{\infty}\left(\Omega_{M}\right)} \leq \gamma\right\} \tag{4.18}
\end{equation*}
$$

$$
\begin{align*}
& {\left[\alpha_{M}\right] \equiv\left\{v_{\perp}^{M} \in(I-\Pi)\left(H^{1}\left(\Omega_{M}\right)\right) \mid\left\|v_{\perp}^{M}\right\|_{L^{\infty}\left(\Omega_{M}\right)} \leq \alpha_{M}\right\}}  \tag{4.19}\\
& {[\beta] \equiv\left\{\widetilde{v} \in H^{1}\left(\widetilde{\Omega}_{M}\right) \mid\|\widetilde{v}\|_{L^{2}\left(\widetilde{\Omega}_{M}\right)} \leq \beta\right\}} \tag{4.20}
\end{align*}
$$

If the relation

$$
\begin{equation*}
\overline{T_{\lambda}(U)} \subset \operatorname{int}(U) \tag{4.21}
\end{equation*}
$$

holds, by the linearity of $T_{\lambda}$, there exists the unique fixed point $u \equiv 0$ of $T_{\lambda}$ in $U$, which implies that $\lambda$ is not an eigenvalue of $L$.

By considering the bounded-unbounded parts and the finite-infinite dimensional parts, we have a sufficient condition for (4.21) as follows:

$$
\begin{align*}
\sup _{u \in U}\left\|\mathcal{N}_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)} & <\gamma,  \tag{4.22}\\
\sup _{u \in U}\left\|(I-\Pi) P_{M} F_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)} & <\alpha_{M},  \tag{4.23}\\
\sup _{u \in U}\left\|\widetilde{P}_{M} F_{\lambda}(u)\right\|_{L^{2}\left(\tilde{\Omega}_{M}\right)} & <\beta . \tag{4.24}
\end{align*}
$$

So in order to construct a suitable set $U$ which satisfies the condition (4.21), we find the positive real numbers $\gamma, \alpha_{M}$ and $\beta$ which satisfy the conditions (4.22)-(4.24). In what follows we consider the case $s(x)=c e^{-x^{2}} \quad(c \in \mathbf{R})$ as an example.

## Estimation for (4.22)

Note that we have

$$
\mathcal{N}_{\lambda}(u)=\left[I-F_{\lambda}\right]_{M}^{-1} P F_{\lambda}(u-P u) .
$$

Let $\left\{\varphi_{j}\right\}_{j=0}^{N}$ be a basis of $S_{h}\left(\Omega_{M}\right)$ and set $\mathcal{N}_{\lambda}(u)=\sum_{j=0}^{N} f_{j} \varphi_{j}$. We define the matrix $D=$ $\left(D_{i j}\right)_{0 \leq i, j \leq N}$ and the vector $\mathbf{r} \equiv\left(r_{j}\right)_{j=0}^{N}$ as

$$
\begin{equation*}
D_{i j} \equiv \delta_{i j}-\int_{-\infty}^{x_{i}} \frac{\psi_{2}\left(x_{i}\right) \psi_{1}(y)}{\xi} s(y) \varphi_{j}(y) d y-\int_{x_{i}}^{\infty} \frac{\psi_{1}\left(x_{i}\right) \psi_{2}(y)}{\xi} s(y) \varphi_{j}(y) d y \tag{4.25}
\end{equation*}
$$

$$
\begin{align*}
r_{i} \equiv \int_{-\infty}^{x_{i}} & \frac{\psi_{2}\left(x_{i}\right) \psi_{1}(y)}{\xi} s(y)(u(y)-P u(y)) d y \\
& +\int_{x_{i}}^{\infty} \frac{\psi_{1}\left(x_{i}\right) \psi_{2}(y)}{\xi} s(y)(u(y)-P u(y)) d y \tag{4.26}
\end{align*}
$$

Then $\mathbf{f} \equiv\left(f_{j}\right)_{j=0}^{N}$ is calculated as $D^{-1} \mathbf{r}$. Therefore we have the following estimation:

$$
\begin{equation*}
\sup _{u \in U}\left\|\mathcal{N}_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)} \leq \max _{0 \leq j \leq N}\left|f_{j}\right| . \tag{4.27}
\end{equation*}
$$

We may use the following estimation for $r_{i}$ :

$$
\begin{align*}
&\left|r_{i}\right| \leq \frac{c c_{p 1} c_{p 2}}{\xi}\left\{2 e^{\mu^{2} / 4} A_{\mu, M}\|u-P u\|_{L^{\infty}\left(\Omega_{M}\right)}\right. \\
&\left.+\frac{1}{\sqrt{2 \mu}} e^{-M^{2}-\mu M}\left(e^{-\mu x_{i}}+e^{\mu x_{i}}\right)\|u-P u\|_{L^{2}\left(\widetilde{\Omega}_{M}\right)}\right\} \tag{4.28}
\end{align*}
$$

where $c_{p 1} \equiv\left\|p_{1}\right\|_{L^{\infty}(\mathbf{R})}, c_{p 2} \equiv\left\|p_{2}\right\|_{L^{\infty}(\mathbf{R})}, A_{\mu, M} \equiv \max \left\{e^{-\mu M} \sqrt{\pi}, \frac{1}{\mu} e^{-\mu^{2} / 4}\right\}$.

## Estimation for (4.23)

Using Lemma 1 we have

$$
\begin{equation*}
\left\|(I-\Pi) P_{M} F_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)} \leq \frac{h^{2}}{8}\left\|\frac{d^{2}}{d x^{2}} P_{M} F_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)}=\frac{h^{2}}{8}\left\|P_{M} \frac{d^{2}}{d x^{2}} F_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)} . \tag{4.29}
\end{equation*}
$$

Setting $f \equiv F_{\lambda}(u)=-\left(L_{0}-\lambda\right)^{-1}(s u)$ we have

$$
\begin{aligned}
\left(L_{0}-\lambda\right) f & =-s u \\
-f^{\prime \prime}+(q-\lambda) f & =-s u \\
f^{\prime \prime} & =(q-\lambda) f+s u
\end{aligned}
$$

Therefore we obtain

$$
\begin{align*}
\left\|P_{M} \frac{d^{2}}{d x^{2}} F_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)} & =\left\|P_{M}(q-\lambda) F_{\lambda}(u)+P_{M}(s u)\right\|_{L^{\infty}\left(\Omega_{M}\right)}  \tag{4.30}\\
& \leq\|q-\lambda\|_{L^{\infty}\left(\Omega_{M}\right)}\left\|P_{M} F_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)}+c\left(\gamma+\alpha_{M}\right)
\end{align*}
$$

Here we can estimate $\left\|P_{M} F_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)}$ as follows:

$$
\begin{align*}
\left\|P_{M} F_{\lambda}(u)\right\|_{L^{\infty}\left(\Omega_{M}\right)} \leq \frac{c c_{p 1} c_{p 2}\{ }{\xi}\{ & 2 e^{\mu^{2} / 4} A_{\mu, M}\|u\|_{L^{\infty}\left(\Omega_{M}\right)} \\
& \left.+\frac{1}{\sqrt{2 \mu}} e^{-M^{2}-\mu M}\left(e^{-\mu x_{i}}+e^{\mu x_{i}}\right)\|u\|_{L^{2}\left(\tilde{\Omega}_{M}\right)}\right\} \tag{4.31}
\end{align*}
$$

## Estimation for (4.24)

Due to [5] we have the following point-wise estimation for $f \in L^{2}(\mathbf{R})$ :

$$
\begin{equation*}
\left|\left(L_{0}-\lambda\right)^{-1} f(x)\right| \leq \frac{c_{p 1} C_{p 2}}{\xi}\left\{G_{1}(x)+G_{2}(x)\right\} \tag{4.32}
\end{equation*}
$$

where $G_{1}$ and $G_{2}$ are defined by

$$
\begin{align*}
G_{1}(x) & \equiv e^{-\mu x} \int_{-\infty}^{x} e^{\mu y}|f(y)| d y,  \tag{4.33}\\
G_{2}(x) & \equiv e^{\mu x} \int_{x}^{\infty} e^{-\mu y}|f(y)| d y \tag{4.34}
\end{align*}
$$

We use the $L^{2}$-estimation in $\widetilde{\Omega}_{M}$ based on the following estimations:

$$
\begin{align*}
\left\|G_{1}\right\|_{L^{2}(-\infty,-M)} & \leq \frac{1}{\mu}\|f\|_{L^{2}(-\infty,-M)},  \tag{4.35}\\
\left\|G_{2}\right\|_{L^{2}(-\infty,-M)} & \leq \frac{1}{2 \mu}\|f\|_{L^{2}(-\infty,-M)}+\sqrt{\frac{1}{4 \mu^{2}}\|f\|_{L^{2}(-\infty,-M)}^{2}+\frac{1}{2 \mu} G_{2}^{2}(-M)} \tag{4.36}
\end{align*}
$$

We could obtain the analogous estimations for $\left\|G_{1}\right\|_{L^{2}(M, \infty)}$ and $\left\|G_{2}\right\|_{L^{2}(M, \infty)}$. By considering the case of $f(x)=s(x) u(x)$ we can derive some concrete estimation which we need in the actual computations. For example we can estimate $G_{1}(M)$ as follows:

$$
G_{1}(M) \leq e^{-\mu M} c\left\{e^{\mu^{2} / 4} \sqrt{\pi}\left(\gamma+\alpha_{M}\right)+e^{-M^{2}} \frac{1}{\sqrt{2 \mu}} e^{-\mu M} \beta\right\}
$$

Concerning how to obtain the fundamental solutions $\psi_{1}$ and $\psi_{2}$ for $\left(L_{0}-\lambda\right) \psi=0$, see [14].

| $M$ | $N$ | $\gamma$ | $\alpha_{M}$ | $\beta$ |
| :--- | :--- | :--- | :--- | :--- |
| 1 | 40 | $3.728040 \times 10^{-5}$ | $4.145585 \times 10^{-7}$ | $1.397699 \times 10^{-4}$ |

Table 1: Results of verification

### 4.4 Numerical examples

We consider the case $q(x)=5.0 \cos 2 \pi x$ and $s(x)=0.2 e^{-x^{2}}$. The computations were carried out on the DELL Precision WorkStation 340 (Intel Pentium4 2.4GHz) using MATLAB (Ver. 7.0.1).

In case of taking the $\lambda$ in (4.6) as an interval $\Lambda=[8.0,8.1]$, we could obtain the results in Table 1. Finally we could verify the non-existence of eigenvalues in the interval [7.2, 10.8].

## References

[1] Bazley, N. W., and Fox, D. W., A Procedure for Estimating Eigenvalues, Journal of Mathematical Physics, 3, No. 3 (1962), pp. 469-471.
[2] Beattie, C., and Goerisch, F., Methods for computing lower bounds to eigenvalues of self-adjoint operators, Numerische Mathematik, 72 (1995), pp. 143-172.
[3] Behnke, H., and Goerisch, F., Inclusions for Eigenvalues of Selfadjoint Problems, In: J.Herzberger(eds.), Topics in Validated Computations-Studies in Computational Mathematics, Elsevier, Amsterdam, 1994.
[4] Chatelin, F., Spectral Approximation of Linear Operators, Academic Press, New York, 1983.
[5] Eastham, M. S. P., The Spectral Theory of Periodic Differential Equations, Scottish Academic Press (1973).
[6] Kato, T., On the upper and lower bounds of eigenvalues, Journal of the Physical Society of Japan, 4 (1949), pp. 334-339.
[7] Kato, T., Perturbation Theory for Linear Operators, Springer, Berlin Heidelberg 1966, 1976.
[8] Nakao, M. T., Yamamoto, N., and Nagatou, K., Numerical Verifications for eigenvalues of second-order elliptic operators, Japan Journal of Industrial and Applied Mathematics, 16, No. 3 (1999), pp. 307-320.
[9] Nagatou, K., Yamamoto, N., and Nakao, M. T., An approach to the numerical verification of solutions for nonlinear elliptic problems with local uniqueness, Numerical Functional Analysis and Optimization, 20, $5 \& 6$ (1999), pp. 543-565.
[10] Nagatou, K., A numerical method to verify the elliptic eigenvalue problems including a uniqueness property, Computing, 63 (1999), pp. 109-130.
[11] Nagatou, K., and Nakao, M. T., An enclosure method of eigenvalues for the elliptic operator linearlized at an exact solution of nonlinear problems, a special issue of Linear Algebra and its Applications on LINEAR ALGEBRA IN SELF-VALIDATING METHODS, 324/13 (2001), pp. 81-106.
[12] Nagatou, K., Nakao, M. T., and Wakayama, M., Verified numerical computations for eigenvalues of non-commutative harmonic oscillators, Numerical Functional Analysis and Optimization, 23, 5 \& 6 (2002), pp. 633-650.
[13] Nagatou, K., A computer-assisted proof on the stability of the Kolmogorov flows of incompressible viscous fluid, Journal of Computational and Applied Mathematics, 169/1 (2004), pp. 33-44.
[14] Nagatou, K., Validated computations for fundamental solutions of linear ordinary differential equations, to appear in Inequalities and Applications.
[15] Nakao, M.T., A numerical approach to the proof of existence of solutions for elliptic problems, Japan Journal of Applied Mathematics 5 (1988), pp. 313-332.
[16] Nakao, M.T., A numerical approach to the proof of existence of solutions for elliptic problems II, Japan Journal of Applied Mathematics 7 (1990), pp. 477-488.
[17] Nakao, M.T. and Yamamoto, N., Self-validating methods (in Japanese), Nihonhyoron-sha, 1998.
[18] Nakao, M.T., Numerical verification methods for solutions of ordinary and partial differential equations, Numerical Functional Analysis and Optimization 22 (3\&4) (2001), pp. 321-356.
[19] Plum, M., Eigenvalue inclusions for second-order ordinary differential operators by a numerical homotopy method, Journal of applied mathematics and physics (ZAMP), 41 (1990), pp. 205-226.
[20] Schultz, M. H., Spline Analysis, Prentice-Hall, London (1973).
[21] Schmidt, K. M., Critical Coupling Constants and Eigenvalue Asymptotics of Perturbed Periodic Sturm-Liouville Operators, Commun. Math, Phys. 211 (2000), pp. 465-485.
[22] Sobolev, A. V., Weyl Asymptotics for the Discrete Spectrum of the Perturbed Hill Operator, Advances in Soviet Mathematics, Vol. 7 (1991), pp. 159-178.
[23] Yamamoto, N., and Nakao, M. T., Numerical verifications for solutions to elliptic equations using residual iterations with a high order finite element, Journal of Computational and Applied Mathematics 60 (1995) pp. 271-279.

