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NEW SUFFICIENT CONDITIONS IN THE GENERALIZED SPECTRUM APPROACH TO DEAL WITH SPECTRAL POLLUTION

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Abstract. In this work, we propose new sufficient conditions to solve the spectral pollution problem by using the generalized spectrum method. We give the theoretical foundation of the generalized spectral approach, as well as illustrate its effectiveness by numerical results.
Keywords: generalized spectrum, Schrödinger operator, eigenvalue approximation

Introduction

Spectral approximation for differential operators takes place in different applications in conjunction with the study of the mathematical modeling, as the case of Schrödinger operator in the quantum physics. Numerical discretization of these problems leads to spurious results, a phenomenon known as spectral pollution (see e.g. [1–5]). In this work, we establish new sufficient conditions to deal with the spectral pollution by using the generalized spectrum method. This method was introduced in [6], and recently was developed in [7].

Let T and S be two bounded operators defined on Banach space X, we define the generalized resolvent set by

$$re(T,S) = \{z \in \mathbb{C} : (T - zS) \text{ is bijective } \}.$$

The complementary of the generalized resolvent set is the generalized spectrum set, denoted by $sp(T,S)$. We say that λ is a generalized eigenvalue of (T,S) if there exists $u \in X \setminus \{0\}$ such that $Tu = \lambda Su$ (see [8]).

In [6], it is shown that the Schrödinger operator, say A, has a decomposition into two bounded operators, say T and S, that allows to express its spectrum in terms of generalized spectrum, i.e.

$$sp(A) = sp(T,S).$$

Through numerical approximation of the bounded operators T and S by sequences of bounded operators $(T_n)_{n\in\mathbb{N}}$ and $(S_n)_{n\in\mathbb{N}}$, we can prove that $\lim\limits_{n\to\infty} sp(T_n,S_n) = sp(T,S)$, where the limit is defined to satisfy the property U: if $T_n \to T$, $S_n \to S$, $\lambda_n \in sp(T_n, S_n)$ and $\lambda_n \to \lambda$, then $\lambda \in sp(T, S)$.

This propriety U is a natural extension of the classical case $S = I$ (see [9]).

In [6], the author showed that the Propriety U is valid under the norm convergence of $(T_n)_{n\in\mathbb{N}}$ and $(S_n)_{n\in\mathbb{N}}$ to T and S. In this work, we show that under the collectively compact convergence of $(T_n)_{n\in\mathbb{N}}$ and $(S_n)_{n\in\mathbb{N}}$ to T and S, the propriety U also takes place. Finally, our numerical application (see [7]) shows the coherence and effectiveness of the generalized spectrum method in comparison with other methods.

1. Generalized spectral approximation under collectively compact convergence

In this section, we prove that the propriety U can be obtained under the collectively compact convergence. Let X be a Banach space, we denote by $BL(X)$ the space of bounded linear operators acting on X. Let T and S be two operators in $BL(X)$. We assume that there exist $(T_n)_{n\in\mathbb{N}}$ and $(S_n)_{n\in\mathbb{N}}$ in $BL(X)$ such that

(B1) $T_n \xrightarrow{cc} T$,

(B2) $S_n \xrightarrow{cc} S$,

where $S_n \overset{cc}{\to} S$ stands for the collectively compact convergence, i.e. if the set

$$\bigcup_{n\geq n_0} \{S_n x - Sx : x \in X,\ \|x\|_X = 1\}$$

is relatively compact in X and for all $x \in X$, $S_n x \to Sx$ pointwisely.

In what follows, the pointwise convergence will be denoted by $\cdot \overset{p}{\to} \cdot$.

In this section, we state a set of lemmas which will be needed in the proofs of our main theorems.

Lemma 1.1. *If $T_n \overset{p}{\to} T$ and $S_n \overset{cc}{\to} S$, then for any bounded operator H in $BL(X)$,*

$$\|(T_n - T)H(S_n - S)\| \to 0.$$

P r o o f. Since $T_n \overset{p}{\to} T$, and the set

$$H(\bigcup_{n\geq n_0} \{Sx - S_n x : \|x\| = 1\}),$$

has compact closure, then $\|(T_n - T)H(S_n - S)\| \to 0$.

□

Lemma 1.2. *Let $T, \widetilde{T}, S, \widetilde{S} \in BL(X)$, and let $z \in re(T, S)$ be such that*

$$\| \left[\left((T - \widetilde{T}) - z(S - \widetilde{S}) \right) (T - zS)^{-1} \right]^2 \| < 1.$$

Then $z \in re(\widetilde{T}, \widetilde{S})$, and

$$\|(\widetilde{T} - z\widetilde{S})^{-1}\| \leq \frac{\|(T - zS)^{-1}\| \left[1 + \| \left((T - \widetilde{T}) - z(S - \widetilde{S}) \right) (T - zS)^{-1} \|\right]}{1 - \| \left[\left((T - \widetilde{T}) - z(S - \widetilde{S}) \right) (T - zS)^{-1} \right]^2 \|}.$$

P r o o f. We denote $\widetilde{E}=(T-\widetilde{T})(T-zS)^{-1}$, $\widetilde{F}=(S-\widetilde{S})(T-zS)^{-1}$, then

$$\widetilde{T}-z\widetilde{S}=[I-(\widetilde{E}-z\widetilde{F})](T-zS).$$

So, by using the second Neumann expansion (see, [9]), we obtain that

$$\begin{aligned}(\widetilde{T}-z\widetilde{S})^{-1} &= (T-zS)^{-1}\sum_{k=0}^{\infty}(\widetilde{E}-z\widetilde{F})^{2k} \\ &\quad +(T-zS)^{-1}\sum_{k=0}^{\infty}(\widetilde{E}-z\widetilde{F})^{2k+1} \\ &= (T-zS)^{-1}\left[I+(\widetilde{E}-z\widetilde{F})\right]\sum_{k=0}^{\infty}\left[(\widetilde{E}-z\widetilde{F})^{2}\right]^{k}. \\ \|(\widetilde{T}-z\widetilde{S})^{-1}\| &\leq \frac{\|(T-zS)^{-1}\|\left(1+\|\widetilde{E}-z\widetilde{F}\|\right)}{1-\|(\widetilde{E}-z\widetilde{F})^{2}\|}.\end{aligned}$$

□

P r o p o s i t i o n 1.1. *If (B1) and (B2) are obtained, then for each* $z\in re(T,S)$, z *belongs to* $re(T_n,S_n)$ *for big enough* n.

P r o o f. Let $z\in re(T,S)$, for big enough n we consider

$$T_n-zS_n=[I-(\widetilde{E}_n-z\widetilde{F}_n)](T-zS),$$

where $\widetilde{E}_n=(T-T_n)(T-zS)^{-1}$ and $\widetilde{F}_n=(S-S_n)(T-zS)^{-1}$. Firstly, we have

$$(\widetilde{E}_n-z\widetilde{F}_n)^{2}=(\widetilde{E}_n)^2+(z\widetilde{F}_n)^2-z\widetilde{E}_n\widetilde{F}_n-z\widetilde{F}_n\widetilde{E}_n.$$

So, according to lemma 1.1, we find $\|(\widetilde{E}_n-z\widetilde{F}_n)^{2}\|\to 0$. Thus, by applying lemma 1.2, we obtain that $z\in re(T_n,S_n)$ for big enough n.

□

The following theorem shows that the property U is valid under the collectively compact convergence.

Theorem 1.1. *Under (B1) and (B2), if for each* n *big enough,* $\lambda_n\in sp(T_n,S_n)$ *and* $\lambda_n\to\lambda$, *then* $\lambda\in sp(T,S)$.

P r o o f. Assume that $\lambda\notin sp(T,S)$, knowing that $sp(T,S)$ is closed (see e.g. [6]), there exists $r>0$ such that the ball $B(\lambda,r)$ is contained in $re(T,S)$. Hence according to proposition 1.1, $B(\lambda,r)$ is contained also in $re(T_n,S_n)$ for n big enough. On the other hand, we have $\lambda_n\to\lambda$. Thus there exists n_0 such that for any $n\geq n_0$, $\lambda_n\in B(\lambda,r)\subset re(T_n,S_n)$ which forms the contradiction.

□

2. Numerical application

As an example, for which the numerical results are available by other approaches, we consider the following problem from [10], which is also studied in [1].

We consider the unbounded operator A defined in $L^2(0,+\infty)$ by the differential equation

$$-u'' + x^2 u = 0, \quad u(0) = 0.$$

This is the harmonic oscillator problem with domain

$$D(A) = H^2(0,\infty) \bigcap \left\{ u \in L^2(0,\infty) : \quad \int_0^\infty x^2 \, |u|^2 dx < +\infty \right\}.$$

First, according to the theory of pseudo spectrum for self-adjoint operators (see [6, 7, 11]) we can find

$$sp(A) = \bigcup_{a>0} sp(A_a), \tag{2.1}$$

where A_a is the Schrödinger operator which has the same formula as A in $L^2(0,a)$, but with the Dirichlet condition at the point a. The domain of A_a is given by

$$D(A_a) = H^2(0,a) \bigcap H_0^1(0,a).$$

Let $a > 0$, we denote by L_a the Laplacian operator defined on $L^2(0,a)$ by

$$L_a u = -u'', \quad D(L) = H^2(0,a) \bigcap H_0^1(0,a).$$

P r o p o s i t i o n 2.2. *L_a is invertible and its inverse is the bounded operator S_a defined by*

$$S_a u(x) = \int_0^a G_{\{0,a\}}(x,y) u(y) dy, \quad u \in L^2(0,a),$$

where

$$G_{\{0,a\}}(x,y) = \begin{cases} \frac{x(a-y)}{a} & 0 \le x \le y \le a, \\ \frac{y(a-x)}{a} & 0 \le y \le x \le a. \end{cases}$$

P r o o f. See [12].

□

Let T_a be the bounded operator defined on $L^2(0,a)$ to itself by

$$T_a u(x) = u(x) + \int_0^a G_{\{0,a\}}(x,y) y^2 u(y) dy, \quad \forall x \in [0,a].$$

Theorem 2.2. $sp(A) = \bigcup_{a>0} sp(T_a, S_a)$, P r o o f. According to equality (2.1), we only need to show that $sp(A_a) = sp(T_a, S_a)$ for $a > 0$. Let λ be an eigenvalue of A_a with eigenvector $u \in D(A_a) \setminus \{0\}$, by applying S_a to $A_a u = \lambda u$ we get

$$T_a u = \lambda S_a u,$$

which implies that λ is a generalized eigenvalue of the couple (T_a, S_a) with eigenvector $u \in L^2(0, a) \setminus \{0\}$. Inversely, let λ be a generalized eigenvalue of the couple (T_a, S_a) with eigenvector $u \in L^2(0, a) \setminus \{0\}$, i.e. $T_a u = \lambda S_a u$, so

$$u = \lambda S_a u - S_a(v\, u) \Rightarrow u = S_a(\lambda u - v\, u),$$

where $v(x) = x^2$. Since $\lambda u - vu \in L^2(0, a)$, we find $u \in D(L_a) = D(A_a)$, then

$$u + S_a(v\, u) = \lambda S_a u \Rightarrow L_a u + v\, u = \lambda u.$$

$\square$

Now, we use numerical methods to approach the operators T_a and S_a. We begin by the Nyström method then the Sloan method and the Kantorovich method.

1. Nyström method: We define a subdivision of $[0, a]$ for $n \geq 2$ by

$$h_n = \frac{a}{n-1},\ x_i = (i-1)h_n,\ 1 \leq i \leq n.$$

Let $T_{a,n}$ and $S_{a,n}$ be approximation of T_a and S_a respectively, according to the Nyström method (see [13]),

$$\begin{aligned} T_{a,n} u_n(x) &= u_n(x) + \sum_{i=1}^{n} w_i G_{\{0,a\}}(x, x_i) x_i^2 u_n(y_i), \\ S_{a,n} u_n(x) &= \sum_{i=1}^{n} w_i G_{\{0,a\}}(x, x_i) u_n(x_i), \end{aligned}$$

where $\{w_i\}_{i=1}^n$ are real weights such that $\sup\limits_{n\geq 2} \sum\limits_{i=1}^{n} |w_i| < \infty$.

Then, we get the matrix generalized eigenvalue problem, $A = \lambda_n B$ where

$$A(i,j) = I(i,j) + w_i G_{\{0,a\}}(x_j, x_i) x_i^2, \quad B(i,j) = w_i G_{\{0,a\}}(x_j, x_i),$$

$I_{n\times n}$ represents the identity matrix. Finally, we use the function ”eig” in Matlab to calculate the generalized eigenvalue of the couple (A, B).

Note that in this case of using the Nyström method, the collectively compact convergence takes place (see [13]).

2. Sloan method: By using the previous subdivision of $[0,a]$, we define the approximate operators $\widetilde{T}_{a,n}$ and $\widetilde{S}_{a,n}$ of T_a and S_a respectively, by using the Sloan method (see [9]), i.e. for all $x\in[0,a]$,

$$\begin{aligned}\widetilde{T}_{a,n}u_n(x) &= \sum_{i=1}^{n}u_n(x_i)e_i(x)+\sum_{i=1}^{n}w_{1,i}(x)u_n(x_i),\\ \widetilde{S}_{a,n}u_n(x) &= \sum_{i=1}^{n}w_{2,i}(x)u_n(x_i),\end{aligned}$$

where

$$w_{1,i}(x)=\int_0^a G_{\{0,a\}}(x,y)y^2e_i(y)dy,\ w_{2,i}(x)=\int_0^a G_{\{0,a\}}(x,y)e_i(y)dy,\ \ 1\le i\le n,$$

and for $2\le i\le n-1$,

$$\begin{aligned}e_i(x) &= \begin{cases}1-\dfrac{|x-x_i|}{h_n}, & x_{i-1}\le x\le x_{i+1}\\ 0, & otherwise.\end{cases}\\ e_1(x) &= \begin{cases}\dfrac{x_2-x}{h_n}, & x_1\le x\le x_2\\ 0, & otherwise.\end{cases}\\ e_n(x) &= \begin{cases}\dfrac{x-x_{n-1}}{h_n}, & x_{n-1}\le x\le x_n\\ 0, & otherwise.\end{cases}\end{aligned}$$

Then, we get the matrix generalized eigenvalue problem $\widetilde{A}=\lambda_n\widetilde{B}$, where

$$\widetilde{A}(i,j)=I(i,j)+w_{1,i}(x_j),\ \ \widetilde{B}(i,j)=w_{2,i}(x_j).$$

Finally, we use the function "eig" in Matlab to calculate the generalized eigenvalue of the couple $(\widetilde{A},\widetilde{B})$.

Note that on the case of the Sloan projection method, the collectively compact convergence also takes place (see [9]).

3. Kantorovich method: By using again the previous subdivision of $[0,a]$, we apply the Kantorovich projection method (see [9]), we get for all $x\in[0,a]$

$$u_n(x)+\sum_{i=1}^{n}\left(\int_0^a G_{\{0,a\}}(x_i,y)y^2u_n(y)dy\right)e_i(x)=\lambda_n\sum_{i=1}^{n}\left(\int_0^a G_{\{0,a\}}(x_i,y)u_n(y)dy\right)e_i(x). \quad (2.2)$$

Multiplying first by $G_{\{0,a\}}(x_j,x)x^2$ then by $G_{\{0,a\}}(x_j,x)$ and integrating over $[0,a]$ the equation (2.2), this leads to the matrix generalized eigenvalue problem

$$\begin{bmatrix}\widetilde{A}+I_{n\times n} & O_{n\times n}\\ \widetilde{B} & I_{n\times n}\end{bmatrix}\begin{bmatrix}\beta_1\\ \beta_2\end{bmatrix}=\lambda_{2n}\begin{bmatrix}O_{n\times n} & \widetilde{A}\\ O_{n\times n} & \widetilde{B}\end{bmatrix}\begin{bmatrix}\beta_1\\ \beta_2\end{bmatrix},$$

Table 1. The numerical results for a=5

Nystrom	Sloan	Kantorovich	results of [10]
2.9998027	3.0001972	3.0001972	2.9621125
6.9990159	7.0009887	7.0009887	6.8083144
10.9977898	11.0026039	11.0026039	10.5272610
15.0013776	15.0103317	15.0103317	14.1401140
19.0656824	19.0806050	19.0806050	17.8348945

where

$$\beta_1(j) = \int_0^a G_{\{0,a\}}(x_j, y)y^2 u_n(y)dy,\ \beta_2(j) = \int_0^a G_{\{0,a\}}(x_j, y)u_n(y)dy,\ 1 \leq j \leq n,$$

and $(\widetilde{A}, \widetilde{B})$ are the same matrices presented in the Sloan method. Finally, we use again the function "eig" in Matlab to calculate the generalized eigenvalue of

$$\left(\begin{bmatrix} \widetilde{A} + I_{n\times n} & O_{n\times n} \\ \widetilde{B} & I_{n\times n} \end{bmatrix}, \begin{bmatrix} O_{n\times n} & \widetilde{A} \\ O_{n\times n} & \widetilde{B} \end{bmatrix}\right)$$

In this case of the Kantorovich projection method, the norm convergence takes place (see [9]).

We fix $n = 200$ to approach the eigenvalues in our example by using the three numerical methods, we compare our results with those in [10]. Table (3.) shows the numerical results.

3. Conclusion

Our study shows the efficiency of the generalized spectrum method, from both theoretical and numerical points of view. This technique appears to be a computationally attractive tool for resolving the spectral pollution. We resolved it by treating the analytical question, to find the bounded operators T and S representing the spectrum proprieties of the Schrödinger operator in the theory of generalized spectrum.

As perspective, we will try to answer this question in more complicated case, for two dimensions and then for three dimensions, where the geometry of the domain and the boundary conditions, will form the main part of the problem. We will also try to generalize this method to other unbounded operators.

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НОВЫЕ ДОСТАТОЧНЫЕ УСЛОВИЯ ОБОБЩЕННОГО СПЕКТРАЛЬНОГО ПОДХОДА ДЛЯ РЕШЕНИЯ СПЕКТРАЛЬНОГО ЗАГРЯЗНЕНИЯ

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Аннотация. В этой работе мы предлагаем новые достаточные условия для решения задачи спектрального загрязнения с использованием метода обобщенного спектра. Мы приводим теоретическую основу обобщенного спектрального подхода, а также иллюстрируем его эффективность на численных результатах.
Ключевые слова: обобщенный спектр; оператор Шрёдингера; аппроксимация собственных значений

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