Spectral inclusion and spectral exactness for singular non-selfadjoint Sturm-Liouville problems

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Abstract

We consider the effect of regularization by interval truncation on the spectrum of a singular non-selfadjoint Sturm-Liouville operator. We present results on spectral inclusion and spectral exactness for the cases where the singularity is in Sims Case II or Sims Case III. For Sims Case I we present a test for spectral inexactness, which can be used to detect when the interval truncation process is generating spurious eigenvalues. Numerical results illustrate the effectiveness of this test.

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1 Introduction

Over the last 30 years there has been considerable interest in numerical solution of singular Sturm-Liouville problems, and in particular in the development of automatic software for such problems: see, e.g., Bailey, Gordon and Shampine [2], Bailey, Garbow, Kaper and Zettl [3], Fulton and Pruess [9] and Marletta and Pryce [14]. The software described in these papers usually uses an interval truncation procedure to regularize problems posed either on infinite intervals, or on finite intervals with singular behaviour of the coefficients near at least one of the endpoints. Rigorous mathematical justification of the validity of the interval truncation process, however, did not appear (except for special cases) until the paper of Bailey, Everitt, Weidmann and Zettl [1] in 1993, which uses fundamental ideas from Reed and Simon [15] to develop conditions under which the spectra of a sequence of regularized problems can (a) provide approximations to the whole spectrum of the original singular eigenvalue problem (*spectral inclusion*); (b) *not* yield approximations to any points which are not in the spectrum of the original singular problem (*spectral exactness*). All of this work is for selfadjoint problems only.

Non-selfadjoint singular problems are also very important. They arise when the complex scaling method is used to find resonances of a selfadjoint problem (for a review see [12]) and also, more classically, in the study of hydrodynamic stability, where the spectra of the Orr-Sommerfeld and related equations are often studied over infinite intervals. Recent applications to the study of large disturbances in water waves are described by Chamberlain and Porter [5].

It is well known that the spectra of non-selfadjoint operators can be pathologically sensitive to perturbation of the operator. Matrix examples of such sensitivity are provided in the classic text of Wilkinson [20]. For a recent study in the context of non-selfadjoint Sturm-Liouville operators see Davies [6], and for a study in the context of general operators via *pseudospectra* see Trefethen [17]. Given this sensitivity, it seems important to ask: under what conditions can one expect the regularization process used for selfadjoint singular Sturm-Liouville operators to be successful for non-selfadjoint Sturm-Liouville operators? In particular, can one recover results on spectral inclusion and spectral exactness? If not, might one at least be able to recover results on pseudospectral inclusion and pseudospectral exactness, or develop a-posteriori tests for spectral exactness?

We seek to answer these questions in this paper, for singular second order non-selfadjoint Sturm-Liouville problems.

For selfadjoint problems a singular endpoint is either of *limit point* or of *limit circle* type. This is the Titchmarsh-Weyl theory and may be developed either using methods of complex analysis (see Titchmarsh [18]) or using the theory of deficiency indices for symmetric operators on Hilbert spaces (see, e.g., Dunford and Schwartz [7]). The analogous theory for non-selfadjoint problems is due to Sims [16] and to Brown, Evans, McCormack and Plum [4]. It is based on the Titchmarsh approach to the selfadjoint case, and will be very important in this paper. The other ingredient which we shall find useful is a non-selfadjoint analogue of the results of Reed and Simon on spectral inclusion and spectral exactness [15, theorems VIII.23-VIII.25], for which we shall use results from Harrabi [11] and Kato [13, p. 208].

2 A review of the Sims Classification

The problem which we consider concerns the spectral behavior of

$$\mathcal{M}[y] = \frac{1}{w}[-(py^{'})^{'} + qy] \quad \text{on} \ \ [a,b), \tag{1}$$

where as usual

(i) $w > 0$, $p \neq 0$ a.e. on $[a,b)$ and $w, 1/p \in L^1_{loc}[a,b)$;

(ii) p, q are complex-valued, $q \in L^1_{loc}[a,b)$ and

$$Q = \overline{co}\left\{\frac{q(x)}{w(x)} + rp(x) : x \in [a,b),\ 0 < r < \infty\right\} \neq \mathbb{C}. \tag{2}$$

These assumptions imply that a is a regular point of (1) and we shall assume that b is a singular point. By this we mean that either $b = +\infty$ or that $\int_a^b (w + \frac{1}{|p|} + \mid q \mid) dx = \infty$. Since we are assuming that Q does not occupy all of $\mathbb{C}$, it is known that its complement has either one or two connected components. For $\lambda_0 \in \mathbb{C}\backslash Q$ we denote by $K = K(\lambda_0)$ the nearest point in Q to λ_0 and by L the tangent to Q at K and arrange by translation and rotation through an angle η for L to coincide with the imaginary axis while λ_0 and Q are contained in the new left and right half planes respectively. That is, for all $x \in [a,b)$ and $r \in (0,\infty)$, we require by choice of K and η that

$$\Re[\{rp(x) + \frac{q(x)}{w(x)} - K\}e^{i\eta}] \geq 0 \tag{3}$$

and

$$\Re[(\lambda_0 - K)e^{i\eta}] < 0. \tag{4}$$

The set of all such *admissible* pairs (η, K) we call S and we also define

$$\Lambda_{\eta,K} = \{\lambda \in \mathbb{C} : \Re[(\lambda - K)e^{i\eta}] \leq 0\}.$$

In order to obtain from (1) a well posed eigenvalue problem we need to introduce boundary conditions at a and possibly at b. The conditions at a will be given in the form

$$y(a)\cos\alpha + py'(a)\sin\alpha = 0, \tag{5}$$

where the parameter α, which may be complex, will be subject to the condition

$$\Re[e^{i\eta}\cos\alpha\,\overline{\sin\alpha}] \leq 0. \tag{6}$$

This gives rise to a set $S(\alpha)$ which is defined as the subset of S in which (6) holds. We note that $\alpha = 0$ and $\alpha = \pi/2$ correspond to Dirichlet and Neumann boundary conditions respectively.

When $p = 1$ and q is real the classical theory of Weyl [19] and Titchmarsh [18] shows that if θ and ϕ are linearly independent solutions of (1) which satisfy

$$\begin{aligned} \phi(a,\lambda) &= \sin\alpha, \quad \theta(a,\lambda) = \cos\alpha, \\ p\phi^{'}(a,\lambda) &= -\cos\alpha, \quad p\theta^{'}(a,\lambda) = \sin\alpha, \end{aligned} \tag{7}$$

where α is now real, then there is a complex number $m(\lambda)$, a function of the strictly complex variable λ, such that

$$\psi = \theta + m\phi \tag{8}$$

lies in $L^2_w[a,b)$. When, up to constant multiples, ψ is the only solution of the differential equation which lies in $L^2_w[a,b)$, we say that (1) is in the limit point case at b. If however both θ and ϕ lie in $L^2_w[a,b)$ then we say that (1) is in the limit circle case at b. In this case an additional boundary condition at b is needed in order to make (1,5) into a well-posed eigenvalue problem. There is a one to one correspondence between this additional boundary condition and the choice of function $m(\cdot)$ in (8), in the sense that with an appropriate choice of boundary condition there exists a unique function $m(\cdot)$ such that eqn. (8) defines a solution ψ of the differential equation satisfying the boundary condition at $x = b$, while with an allowed choice of $m(\cdot)$ the function ψ defined in (8) can itself be used, for appropriate λ, to define the boundary condition at $x = b$ in the form $[y, \psi](b) = 0$, where $[f, g] := p(fg' - f'g)$ denotes the Wronsian of two functions f and g. It is known that the classification of limit point or limit circle is independent of the strictly complex parameter λ. The terminology of limit point or limit circle owes its origin to the method used to establish the existence and possible uniqueness of ψ in (8). It may be shown that the spectral points of any realisation of (1) as an operator in $L^2_w[a,b)$ may be charecterised by the behaviour in the limit as $\Im\lambda \to 0$ of the function $m(\lambda)$ associated with the boundary conditions defining the domain of the realisation.

Many of these notions may be carried over to the case when p, q and α are complex. In a seminal paper Sims [16] shows that when $p = w = 1$ and $\Im q \in \mathbb{C}_-$, where $\mathbb{C}_-$ denotes the strictly lower complex plane, then the limit point / limit circle classification of Weyl now gets replaced by a threefold classification. We shall discuss this in the more general setting of [4] which only requires (2), (3) and (4) to hold. Using a nesting circle method based on that of both Weyl and Sims, Brown et al. prove the following theorem.

Theorem 2.1 *[4] For $\lambda \in \Lambda_{\eta,K}$, $(\eta, K) \in S(\alpha)$ the following distinct cases are possible, the first two being sub-cases of the limit point case:*

- *Case I : there exists a unique solution of (1) satisfying*

$$\int_a^b \Re[e^{i\eta}\{p \mid y' \mid^2 + (q - Kw) \mid y \mid^2\}]dx + \int_a^b \mid y \mid^2 wdx < \infty; \tag{9}$$

and this is the only solution satisfying $y \in L^2_w[a,b)$;

- *Case II : there exists a unique solution of (1) satisfying (9), but all solutions of (1) lie in* $L^2_w[a,b)$*;*
- *Case III: all solutions of (1) lie in* $L^2_w[a,b)$ *and satisfy (9).*

It may also be shown that the classification is independent of λ *in the sense that*

(i) if all solutions of (1) satisfy (9) for some $\lambda^{'} \in \Lambda_{\eta,K}$ *(i.e. Case III) then all solutions of (1) satisfy (9) for all* $\lambda \in \mathbb{C}$*;*

(ii) if all solutions of (1) lie in $L^2_w[a,b)$ *for some* $\lambda^{'} \in \mathbb{C}$ *then all solutions of (1) satisfy* $y \in L^2_w[a,b)$ *for all* $\lambda \in \mathbb{C}$*.*

It is interesting to examine the case when p is real and non-negative. In this case for some $\eta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ and $K \in \mathbb{C}$ let

$$\theta_{K,\eta}(x) = \Re[e^{i\eta}(q(x) - Kw(x))] \geq 0 \;\; a.e. \; x \in (a,b). \tag{10}$$

Then the condition (9) in the Sims characterisation of (1) in Theorem 2.1 for $\lambda \in \Lambda_{\eta,K}$, $(\eta, K) \in S(\alpha)$, becomes

$$\cos\eta \int_a^b p \mid y' \mid^2 dx + \int_a^b \theta_{K\eta}(x) \mid y(x) \mid^2 dx + \int_\alpha^b \mid y(x) \mid^2 w(x) dx < \infty. \tag{11}$$

In this case the remark on the independence of the classification can be extended to the following:

(i) if for some $\lambda^{'} \in \mathbb{C}$ all the solutions of (1) satisfy (11), then for all $\lambda \in \mathbb{C}$ all solutions of (1) satisfy (11);

(ii) if for some $\lambda^{'} \in \mathbb{C}$ all the solutions of (1) satisfy one of

$$\cos\eta \int_a^b p \mid y' \mid^2 dx < \infty, \tag{12}$$

$$\int_a^b \theta_{K\eta} \mid y \mid^2 dx < \infty, \tag{13}$$

then the same applies for all $\lambda \in \mathbb{C}$.

We remark that Sim's analysis is the special case of the above when $\eta = \pi/2$, $K = 0$. This restriction overlooks the interesting features present in (11) when $\eta \in (-\frac{\pi}{2}, \frac{\pi}{2})$, namely, that the classification in Theorem 2.1 involves a weighted Sobolev space as well as $L^2_w[a,b)$. The paper [4] also examines the analytic behaviour of $m(\lambda)$ and the connection between this and the spectrum of M, an operator realisation of $\mathcal{M}$ in $L^2_w[a,b)$. This is sumarised in the following theorems, in which m denotes the unique function such that (8) defines a solution of (1) which either (i) lies in $L^2_w[a,b)$ (Sims Case I) or (ii) lies in $L^2_w[a,b)$ and satisfies the additional boundary condition at $x = b$ (Sims Cases II and III).

Theorem 2.2 *(Theorem 4.7, [4]) In Cases II and III,* λ_0 *is a pole of* m *of order* s *if and only if* λ_0 *is an eigenvalue of* M *of algebraic multiplicity* s*.*

Theorem 2.3 *(Theorem 4.13, [4]) Suppose that (2) is in Case I. Define*

$$Q(\alpha) = \bigcap_{(\eta,K)\in S(\alpha)} (\mathbb{C} \backslash \Lambda_{\eta,K}),$$

and let $Q_c(\alpha)$ denote the set $Q(\alpha)$ when the underlying interval is $[c,b)$ rather than $[a,b)$. Define

$$\begin{aligned} Q_c &:= \overline{co}\left\{\frac{q(x)}{w(x)} + rp(x) : x \in [c,b),\ r \in (0,\infty)\right\}, \\ Q_b &:= \cap_{c\in(a,b)} Q_c, \quad Q_b(\alpha) = \cap_{c\in(a,b)} Q_c(\alpha), \end{aligned}$$

Then $m(\lambda)$ is defined throughout $\mathbb{C}\backslash Q(\alpha)$ and has a meromorphic extension to $\mathbb{C}\backslash Q_b(\alpha)$, with poles only in $Q(\alpha)\backslash Q_b(\alpha)$. In addition λ is a pole of $m(\lambda)$ if and only if λ is an eigenvalue of M for $\lambda \notin Q_b(\alpha)$.

3 Tests for spectral inclusion and spectral exactness

In this section we prove a simple theorem (Theorem 3.1) which allows us to test a convergent sequence of eigenvalue approximations obtained from a sequence of truncated interval problems, in order to determine whether or not the limit of the sequence is truly an eigenvalue of our original problem. We also prove two additional results (Theorem 3.3 and Theorem 3.4) which give methods for determining whether or not the hypotheses of Theorem 3.1 are satisfied for a given problem. The second of these, Theorem 3.4, extends a convergence result in [4] from the complement of the numerical range of our singular operator into a set which is typically much larger.

Finally, we show how Theorem 3.3 and Theorem 3.4 allow us to develop a test for spectral inclusion, to ensure that there will be no eigenvalues of the original problem which remain unapproximated by the truncation process.

3.1 Spectral Exactness

We denote by $m(\cdot)$ the m-function developed in section 2; in Sims cases II and III, this corresponds to a particular choice of boundary condition at $x = b$. From Theorems 2.2 and 2.3 we know that the poles of m are the eigenvalues of a realization M of the differential operator $\mathcal{M}$ subject to a boundary condition of the form

$$(\cos\alpha)y(a) + (\sin\alpha)py'(a) = 0 \tag{14}$$

(and possibly an additional boundary condition at $x = b$).

We denote by L the operator, and by $\ell(\cdot)$ the Titchmarsh-Weyl function, when the boundary condition at $x = a$ is changed to

$$(\sin\alpha)y(a) - (\cos\alpha)py'(a) = 0, \tag{15}$$

but the boundary conditions at $x = b$ (where applicable) are left unchanged, the same as those for M.

The functions ℓ and m are related by the identity

$$m(\lambda)\ell(\lambda) = -1$$

(see [4, eqn. 5.17]).

Let $(b_n)_{n\in\mathbb{N}}$ be a sequence such that $b_n \nearrow b$ as $n \nearrow \infty$. Following [4, §2] we may construct a sequence M_n of regular operators defined on the intervals $[a, b_n]$. These operators M_n are still defined by $M_n y = \mathcal{M}y$ on their domains: it is the boundary conditions defining these domains which are of interest. At $x = a$ we keep the boundary condition (14). At $x = b_n$ we impose a boundary condition of the form

$$y(b_n)\cos\beta_n + py'(b_n)\sin\beta_n = 0. \tag{16}$$

The Titchmarsh-Weyl function m_n associated with M_n is then given in terms of the solutions θ and ϕ of (7) by

$$m_n(\lambda) = -\frac{\theta(b_n,\lambda)\cot\beta_n + p\theta'(b_n,\lambda)}{\phi(b_n,\lambda)\cot\beta_n + p\phi'(b_n,\lambda)}.$$

[4, eq. (2.6)]. We shall examine in Lemma 3.2, Theorem 3.3 and Theorem 3.4 below conditions on the β_n which ensure that, for λ in certain regions of $\mathbb{C}$,

$$m(\lambda) = \lim_{n\to\infty} m_n(\lambda). \tag{17}$$

Let L_n be a sequence of regular operators defined on the intervals $[a, b_n]$ with boundary condition (15) at $x = a$ and with the same boundary conditions (16) as the M_n at $x = b_n$, so that the associated Titchmarsh-Weyl functions $\ell_n(\cdot)$ satisfy

$$m_n(\lambda)\ell_n(\lambda) = -1.$$

By analogy with (17) we shall assume that in some appropriate regions of $\mathbb{C}$,

$$\ell(\lambda) = \lim_{n\to\infty} \ell_n(\lambda). \tag{18}$$

Theorem 3.1 *(Test for spectral inexactness) Suppose that $\mu \in \mathbb{C}$ has the following properties:*

1. *μ does not lie in the spectrum of M;*
2. *$m_n \to m$ and $\ell_n \to \ell$ uniformly on any compact annulus of sufficiently small outer radius surrounding μ.*

Then there are only two possibilities:

(a) *there exists a neighbourhood $\mathcal{N}$ of μ and $N \in \mathbb{N}$ such that no eigenvalue of M_n lies in $\mathcal{N}$ for any $n \geq N$;*

(b) *there exists a monotone increasing sequence $(n_j)_{j\in\mathbb{N}}$ of positive integers, and two associated sequences $(\lambda_j)_{j\in\mathbb{N}}$, $(\mu_j)_{j\in\mathbb{N}}$, such that*

$$\lambda_j \in \sigma(M_{n_j}), \quad \mu_j \in \sigma(L_{n_j}),$$

and $\lambda_j \to \mu$, $\mu_j \to \mu$ as $j \to \infty$.

A consequence of this theorem is that if a subsequence of eigenvalues of the regularized operators M_n converges to some point μ which is not an eigenvalue (spectral inexactness) then the L_n will also possess a subsequence of eigenvalues converging to the same point μ. Moreover, if subsequences of eigenvalues of M_n and of L_n converge to the same point then at least one of the subsequences is spectrally inexact, because the boundary conditions (14) and (15) ensure that M and L have no shared eigenvalues. Theorem 3.1 therefore gives us a test for spectral exactness: if only the M_n, and not the L_n, possess eigenvalues accumulating at μ, then μ must be an eigenvalue of M.

Proof of Theorem 3.1. Let A be any sufficiently small annulus surrounding μ and let Γ be a closed contour in A surrounding μ. For any function f which is meromorphic in a simply connected open set containing Γ we denote by $N_Z(f,\Gamma)$ the number of zeros of f inside Γ and by $N_P(f,\Gamma)$ the number of poles of f inside Γ. Rouché's Theorem gives

$$N_Z(m,\Gamma) - N_P(m,\Gamma) = \frac{1}{2\pi i}\int_\Gamma \frac{m'(\lambda)}{m(\lambda)} d\lambda.$$

In view of the identity $m(\lambda)\ell(\lambda) = -1$ we have $N_Z(m,\Gamma) = N_P(\ell,\Gamma)$ and $1/m = -\ell$, so we can write this

$$N_P(\ell,\Gamma) - N_P(m,\Gamma) = -\frac{1}{2\pi i}\int_\Gamma m'(\lambda)\ell(\lambda)d\lambda. \tag{19}$$

As μ does not lie in the spectrum of M, we have $N_P(m,\Gamma) = 0$ for all sufficiently small annuli A. Hence

$$N_P(\ell,\Gamma) = -\frac{1}{2\pi i}\int_\Gamma m'(\lambda)\ell(\lambda)d\lambda. \tag{20}$$

By arguments similar to those which gave (19) we have

$$N_P(\ell_n,\Gamma) - N_P(m_n,\Gamma) = -\frac{1}{2\pi i}\int_\Gamma m_n'(\lambda)\ell_n(\lambda)d\lambda.$$

The uniform convergence $m_n \to m$ implies uniform convergence of m_n' to m' (by the Cauchy integral representation of the derivative). Combined with the uniform convergence $\ell_n \to \ell$ this yields

$$N_P(\ell_n,\Gamma) - N_P(m_n,\Gamma) = -\frac{1}{2\pi i}\int_\Gamma m'(\lambda)\ell(\lambda)d\lambda$$

for all sufficiently large n. Combining this with (20) we have, for all sufficiently large n,

$$N_P(\ell,\Gamma) = N_P(\ell_n,\Gamma) - N_P(m_n,\Gamma). \tag{21}$$

In the case of possibility **(a)**, the sequence M_n does not have any eigenvalues converging spuriously to μ, which is a non-eigenvalue of M. Since eigenvalues of M_n are poles of m_n we have $N_P(m_n,\Gamma) = 0$ and (21) then shows that the sequence L_n is spectrally exact for L near μ. Thus we have spectral exactness near μ for both M and L. In the case that **(a)** is not true, then for some arbitrarily small annuli A and arbitrarily large $n \in \mathbb{N}$ we will have

$$N_P(m_n,\Gamma) = \text{no. of eigenvalues of } M_n \text{ inside } \Gamma > 0,$$

and, from (21),

$$N_P(\ell_n,\Gamma) - N_P(m_n,\Gamma) = N_P(\ell,\Gamma) \geq 0,$$

which shows that $N_P(\ell_n,\Gamma)$, the number of eigenvalues of L_n inside Γ, is at least 1. Thus L_n also has an eigenvalue close to μ. This gives possibility **(b)**. □

3.2 Conditions for m-function convergence

We now examine the hypotheses $m_n \to m$ and $\ell_n \to \ell$ of Theorem 3.1. Under what conditions do these hold?

We consider first Sims Cases II and III. The following result explains how to choose the boundary condition (16) to ensure that (17) and (18) hold.

Lemma 3.2 *Suppose that the differential equation is of Sims Case II or III. Let $\lambda' \in \Lambda_{\eta,K}$ be fixed. Express the boundary conditions at $x = b$ for M in terms of an L^2_w-solution $\psi(\cdot,\lambda') = \theta(\cdot,\lambda') + m(\lambda')\phi(\cdot,\lambda')$ of the differential equation $\mathcal{M}\psi = \lambda'\psi$, in the form*

$$[y, \psi(\cdot,\lambda')](b) = 0,$$

[4, eq. (4.11)] where $[\cdot,\cdot]$ denotes the usual Wronskian $[u,v] := p(uv' - u'v)$. Then appropriate boundary conditions (16) are given by choosing

$$(\cos\beta_n, \sin\beta_n) = const.(p\psi'(b_n,\lambda'), -\psi(b_n,\lambda')) \tag{22}$$

so that (16) is simply the condition $[y,\psi](b_n) = 0$.

Proof Define $\psi_n(\cdot,\lambda') = \theta(\cdot,\lambda') + m_n(\lambda')\phi(\cdot,\lambda')$, in which m_n is chosen so that ψ_n satisfies (16) with β_n given by (22). From the definition of the β_n, the fact that ψ_n satisfies (16) may be written as

$$[\psi_n(\cdot,\lambda'),\psi(\cdot,\lambda')](b_n) = 0.$$

Substituting $\psi_n(\cdot,\lambda') = \theta(\cdot,\lambda') + m_n(\lambda')\phi(\cdot,\lambda')$ into this equation yields

$$m_n(\lambda') = -\frac{[\theta(\cdot,\lambda'),\psi(\cdot,\lambda')](b_n)}{[\phi(\cdot,\lambda'),\psi(\cdot,\lambda')](b_n)}. \tag{23}$$

In the identity $[\psi(\cdot,\lambda'),\psi(\cdot,\lambda')](b) = 0$, replace the first instance of $\psi(\cdot,\lambda')$ by $\theta(\cdot,\lambda')+m(\lambda')\phi(\cdot,\lambda')$, and hence obtain

$$m(\lambda') = -\frac{[\theta(\cdot,\lambda'),\psi(\cdot,\lambda')](b)}{[\phi(\cdot,\lambda'),\psi(\cdot,\lambda')](b)}. \tag{24}$$

Comparing (23) with (24) establishes (17) when $\lambda = \lambda'$:

$$\lim_{n\to\infty} m_n(\lambda') = m(\lambda'). \tag{25}$$

Now Brown et al. [4, Corollary 3.4, eqn. (3.4)] give a formula which allows us to extend this result to other values of λ:

$$m(\lambda) = \frac{m(\lambda') - (\lambda-\lambda')\int_a^b w(x)\theta(x,\lambda)\psi(x,\lambda')dx}{1 + (\lambda-\lambda')\int_a^b w(x)\phi(x,\lambda)\psi(x,\lambda')dx}. \tag{26}$$

This formula possesses the regular-interval analogue

$$m_n(\lambda) = \frac{m_n(\lambda') - (\lambda-\lambda')\int_a^{b_n} w(x)\theta(x,\lambda)\psi_n(x,\lambda')dx}{1 + (\lambda-\lambda')\int_a^{b_n} w(x)\phi(x,\lambda)\psi_n(x,\lambda')dx}. \tag{27}$$

These formulae hold at any point which is not an eigenvalue of M or of M_n, respectively. Moreover, since the equation is in Sims Case II or III, all of $\theta(\cdot,\lambda)$, $\theta(\cdot,\lambda')$, $\phi(\cdot,\lambda)$ and $\phi(\cdot,\lambda')$ lie in $L^2_w[a,b)$. Using $\psi_n(\cdot,\lambda') - \psi(\cdot,\lambda') = (m_n(\lambda') - m(\lambda'))\phi(\cdot,\lambda')$ it follows from (25) that $\psi_n(\cdot,\lambda') \to \psi(\cdot,\lambda')$ in $L^2_w[a,b)$. Hence, combining (26) and (27), we obtain the convergence

$$\lim_{n\to\infty} m_n(\lambda) = m(\lambda)$$

at any point λ which is not an eigenvalue of M. This establishes (17), and (18) is proved similarly. □

Of course, Theorem 3.1 requires more than just pointwise convergence, and so it is fortunate that the following stronger result holds.

Theorem 3.3 *Suppose that the problem is Sims Case II or Sims Case III at $x = b$ and let the hypotheses of Lemma 3.2 hold. Then for λ in any compact set $\mathcal{K} \subseteq \mathbb{C}$ not containing eigenvalues of M,*

$$\lim_{n\to\infty} m_n(\lambda) = m(\lambda), \tag{28}$$

the convergence being uniform over $\mathcal{K}$.

Proof That $m_n(\lambda) \to m(\lambda)$ pointwise on $\mathcal{K}$ has already been proved in Lemma 3.2. The uniformity of the convergence depends on having a uniform bound on the L^2_w norms of $\theta(\cdot,\lambda)$ and $\phi(\cdot,\lambda)$ for $\lambda \in \mathcal{K}$. This can be obtained by a standard variation of parameters argument, expressing the solutions in terms of $\theta(\cdot,\lambda')$ and $\phi(\cdot,\lambda')$: see Sims [16, section 3, Theorem 2] and also [4, Remark 2.2]. □

For the functions ℓ_n and ℓ, a result exactly analogous to Theorem 3.3 is clearly valid, the only difference being now that $\mathcal{K}$ must not contain eigenvalues of L.

We turn now to Sims Case I. In order to handle this case it is necessary to know more about the behaviour of the solutions of the differential equation. Suppose that for some $\lambda \in \mathbb{C}$, the differential equation possesses 'small' and 'large' solutions. We shall assume that the small solution is the (unique up to scalar multiples) square integrable solution $\psi(x, \lambda)$, and we denote the non-unique large solution by $\Upsilon(x, \lambda)$. By 'small' and 'large' we mean that these solutions satisfy the condition

$$\lim_{x \to b} \frac{\psi(x, \lambda)}{\Upsilon(x, \lambda)} = 0. \tag{29}$$

Clearly Υ is not unique: $\Upsilon + \psi$, for example, is also a 'large' solution in the sense of (29). The solutions θ and ϕ of (7) can clearly be written in terms of ψ and Υ:

$$\begin{aligned} \theta(x, \lambda) &= c_1 \psi(x, \lambda) + c_2 \Upsilon(x, \lambda), \\ \phi(x, \lambda) &= d_1 \psi(x, \lambda) + d_2 \Upsilon(x, \lambda), \end{aligned} \tag{30}$$

in which the constants c_1, c_2, d_1 and d_2 are given by

$$c_1 = \left((\cos \alpha) p \Upsilon'(a, \lambda) - (\sin \alpha) \Upsilon(a, \lambda) \right) / W, \quad c_2 = \left(-(\cos \alpha) p \psi'(a, \lambda) + (\sin \alpha) \psi(a, \lambda) \right) / W, \tag{31}$$

$$d_1 = \left((\sin \alpha) p \Upsilon'(a, \lambda) + (\cos \alpha) \Upsilon(a, \lambda) \right) / W, \quad d_2 = \left(-(\sin \alpha) p \psi'(a, \lambda) - (\cos \alpha) \psi(a, \lambda) \right) / W, \tag{32}$$

where $W = p(\psi \Upsilon' - \psi' \Upsilon)$ is the usual Wronskian. Suppose that m_n is defined by the requirment that the solution

$$\psi_n(\cdot, \lambda) = \theta(\cdot, \lambda) + m_n(\lambda) \phi(\cdot, \lambda)$$

satisfy the boundary condition $\psi_n(b_n, \lambda) = 0$. Then

$$m_n(\lambda) = -\frac{\theta(b_n, \lambda)}{\phi(b_n, \lambda)}. \tag{33}$$

Now combining (29) with (30) we have

$$\theta(b_n, \lambda) \sim c_2 \Upsilon(b_n, \lambda), \quad \phi(b_n, \lambda) \sim d_2 \Upsilon(b_n, \lambda)$$

for large n. Combining this with (33) yields

$$m_n(\lambda) \sim -\frac{c_2}{d_2}$$

for large n. Together with (31) and (32) this yields, for large n,

$$m_n(\lambda) \sim \frac{-(\cos \alpha) p \psi'(a, \lambda) + (\sin \alpha) \psi(a, \lambda)}{(\sin \alpha) p \psi'(a, \lambda) + (\cos \alpha) \psi(a, \lambda)} = m(\lambda), \tag{34}$$

the last equality in (34) being an immediate consequence of [4, Definition 4.10]. From these considerations the following result is clearly true.

Theorem 3.4 *Suppose that the differential equation is of Sims Case I type at $x = b$. Let $\mathcal{K} \subseteq \mathbb{C}$ be a compact set such that for $\lambda \in \mathcal{K}$ the square-integrable solution $\psi(x, \lambda)$ of the differential equation exists and is an analytic function of λ. Suppose moreover that there exists a second solution $\Upsilon(x, \lambda)$ such that*

$$\lim_{x \to b} \frac{\psi(x, \lambda)}{\Upsilon(x, \lambda)} = 0, \tag{35}$$

the limit being uniform with respect to $\lambda \in \mathcal{K}$. Suppose that the domains of the operators M_n are determined by the Dirichlet conditions $y(b_n) = 0$. Then we have the convergence

$$\lim_{n \to \infty} m_n(\lambda) = m(\lambda)$$

uniformly for $\lambda \in \mathcal{K}$.

Clearly a similar result holds for the functions $\ell_n(\lambda)$ and their convergence to the function $\ell(\lambda)$.

Remark The result of Theorem 3.4 will also hold if the domains of the M_n are defined by certain other boundary conditions at $x = b_n$. Suppose that a boundary condition

$$y(b_n)\cos\beta_n + y'(b_n)\sin\beta_n = 0$$

is imposed, where the β_n are complex numbers. Then it may be shown that the result continues to hold provided

$$\lim_{n\to\infty} \frac{\psi(b_n,\lambda)\cos\beta_n + \psi'(b_n,\lambda)\sin\beta_n}{\Upsilon(b_n,\lambda)\cos\beta_n + \Upsilon'(b_n,\lambda)\sin\beta_n} = 0, \qquad (36)$$

locally uniformly with respect to λ. In problems where $\psi'(x,\lambda)/\Upsilon'(x,\lambda) \to 0$ as $x \to b$, one would have to choose the β_n quite carefully for (36) to fail.

3.3 A simple test for spectral inclusion

In the selfadjoint case, spectral inclusion is usually very easy to prove. In fact, suppose T is a selfadjoint operator on a domain $D(T)$ in a Hilbert space H and let (T_n) be a sequence of operators with domains $(D(T_n))$ which converge pointwise to T on some set $\mathcal{C} \subseteq \cap_{m\in\mathbb{N}} \cup_{n\geq m} D(T_n)$:

$$\lim_{n\to\infty} \|T_n f - Tf\| = 0 \quad \forall f \in \mathcal{C}. \qquad (37)$$

Then provided $\mathcal{C}$ is a core of T – in other words, provided the set $(\mathcal{C}, T\mathcal{C})$ is dense in the graph of T – the sequence (T_n) will be spectrally inclusive for T: every eigenvalue of T will be the limit of some sequence $(\lambda^{(n)})$ in which $\lambda^{(n)}$ lies in the spectrum of T_n.

In the non-selfadjoint case a result of such generality does not seem to exist, although some of the results of Harrabi [11] come quite close. We shall examine some corollaries of Harrabi's work, as well as a standard result from Kato [13], in section 4 below. In this subsection, however, we shall show that spectral inclusion always holds in Sims Cases II and III, and in Sims Case I in those parts of the complex plane where Theorem 3.4 holds.

Theorem 3.5 *(Test for Spectral Inclusion) In the notation of Theorem 3.1, suppose that $\mu \in \mathbb{C}$ is an isolated eigenvalue of M. Suppose also that $m_n(\lambda) \to m(\lambda)$ as $n \to \infty$ uniformly on any compact annulus surrounding μ. Then there exists a sequence $(\lambda^{(n)})$ in which $\lambda^{(n)}$ lies in the spectrum of M_n, such that $\lim_{n\to\infty} \lambda^{(n)} = \mu$.*

Proof Given $\epsilon > 0$ sufficiently small, surround μ by an annulus A whose outer radius is at most ϵ and let Γ be a circular contour surrounding μ and contained in A. Since μ is a pole of m, we may assume by taking ϵ sufficiently small that A contains no zeros of m. The uniform convergence of m_n to m on A then guarantees that for all sufficiently large n, m_n is bounded away from zero in A, so $1/m_n$ also converges uniformly to $1/m$ in A. Moreover, Cauchy's integral representation of the derivative implies that m_n' converges uniformly to m' on A. Hence we have

$$\frac{1}{2\pi i}\int_\Gamma \frac{m_n'(\lambda)}{m_n(\lambda)} d\lambda \to \frac{1}{2\pi i}\int_\Gamma \frac{m'(\lambda)}{m(\lambda)} d\lambda \ \ (n \to \infty),$$

and the fact that both sides of this equation are integers gives

$$\frac{1}{2\pi i}\int_\Gamma \frac{m_n'(\lambda)}{m_n(\lambda)} d\lambda = \frac{1}{2\pi i}\int_\Gamma \frac{m'(\lambda)}{m(\lambda)} d\lambda \qquad (38)$$

for all sufficiently large n.

From the argument principle, if we let ν denote the algebraic multiplicity of μ as an eigenvalue – and hence as pole of m – we have

$$-\nu = \frac{1}{2\pi i}\int_\Gamma \frac{m'(\lambda)}{m(\lambda)}d\lambda. \tag{39}$$

Combining (38) and (39) shows that M_n also has eigenvalues of total algebraic multiplicity ν inside the contour Γ, for all sufficiently large n. □

In section 5 we shall give some examples in which the Eastham-Levinson asymptotics [8] allow us to verify the hypothesis (35) and hence apply the test for spectral exactness given in Theorems 3.1 and 3.5.

4 Pseudospectral inclusion and spectrum-of-sequence inclusion

In this section we consider a sequence (T_n) of operators on a Hilbert space H. Let T be some other operator on H. We denote by $D(T_n)$ the domain of T_n and by $D(T)$ the domain of T. We shall be interested in two different types of convergence of T_n to T: strong convergence, in which $T_nf \to Tf$ for each fixed f, and norm resolvent convergence, in which $\|(\lambda I - T_n)^{-1} - (\lambda I - T)^{-1}\| \to 0$. Strong convergence is usually observed when a problem of Sims Case I is regularized by a sequence of interval truncations, while the stronger property of norm resolvent convergence is observed when the problem being regularized is of Sims Case II or III. Strong convergence generally results in a very weak type of spectral approximation which is given by Theorem 4.3 below; in practice, for differential equation eigenvalue problems, this is probably not as useful a result as Theorem 3.5. Norm resolvent convergence, on the other hand, gives a spectral exactness result (Theorem 4.5) which Theorems 3.1 and 3.3 do not give: Theorems 3.1 and 3.3 do not preclude spectral inexactness in Sims Cases II and III, they merely give a test for spectral inexactness, whereas Theorem 4.5 precludes spectral inexactness.

The following definition is standard.

Definition 4.1 *A set $\mathcal{C} \subseteq D(T)$ is called a core of T if, for every $x \in D(T)$ and $\epsilon > 0$, there exists $x_\epsilon \in \mathcal{C}$ such that*

$$\|x - x_\epsilon\| < \epsilon, \quad \|Tx - Tx_\epsilon\| < \epsilon.$$

The following definition is also required.

Definition 4.2 *The spectrum of the sequence (T_n), denoted $\sigma(\{T_n\})$, is the set*

$$\sigma(\{T_n\}) = \{\lambda \in \mathbb{C} \mid \lim_{n\to\infty} \|(\lambda I - T_n)^{-1}\| = +\infty\}.$$

Note that for selfadjoint operators, $\sigma(\{T_n\})$ can contain only points which are limit points of sequences of the form $(\lambda^{(n)})$ in which $\lambda^{(n)}$ lies in the spectrum $\sigma(T_n)$ of T_n:

$$\sigma(\{T_n\}) \subseteq \cap_{m\in\mathbb{N}}\overline{\cup_{n\geq m}\sigma(T_n)}. \tag{40}$$

To see this, let $\lambda \in \sigma(\{T_n\})$ and let $a_n := \|(\lambda I - T_n)^{-1}\|^{-1}$, so that $a_n \to 0$ as $n \to \infty$. By the spectral calculus for the selfadjoint operator T_n, given $\epsilon > 0$ there certainly exists a point of $\sigma(T_n)$ within distance $a_n + \epsilon$ of λ: in particular, choosing $\epsilon = \frac{1}{n}$ we can find $\lambda^{(n)} \in \sigma(T_n)$ such that $|\lambda - \lambda_n| < a_n + \frac{1}{n}$. Hence for any integer m,

$$\lambda \in \overline{\cup_{n\geq m}\sigma(T_n)}.$$

This proves (40). For the non-selfadjoint case the spectral calculus no longer holds (unless the T_n happen to be normal). The following result – a simple modification of a result of Harrabi [11] – thus provides for non-selfadjoint operators as close an analogue of the spectral inclusion result of Reed and Simon [15, Theorem VIII.24] as is possible, in general.

Theorem 4.3 *Let $\mathcal{C}$ be a core of T and suppose that*

$$\mathcal{C} \subseteq \cap_{m\in\mathbb{N}} \cup_{n\geq m} D(T_n),$$

so that if $f \in \mathcal{C}$ then $T_n f$ is defined for all sufficiently large n. Let

$$\sigma_a(T) := \{\lambda \in \mathbb{C} \mid \exists (x_n)_{n\in\mathbb{N}} \subseteq H \text{ such that } \|x_n\| = 1 \; \forall n \text{ and } \lim_{n\to\infty} \|(\lambda I - T)x_n\| = 0\}.$$

Suppose that for each $f \in \mathcal{C}$ we have $\lim_{n\to\infty} \|T_n f - Tf\| = 0$. Then

$$\sigma_a(T) \subseteq \sigma(\{T_n\}). \tag{41}$$

Proof Suppose that λ does not lie in $\sigma(\{T_n\})$. Then there exists $M \in \mathbb{R}^+$ and a monotone increasing sequence $(n_j)_{j\in\mathbb{N}}$ such that

$$\|(\lambda I - T_{n_j})^{-1}\| \leq M.$$

Now let $f \in \mathcal{C}$. Then $f = (\lambda I - T_{n_j})^{-1}(\lambda I - T_{n_j})f$, whence

$$\|f\| \leq M\|(\lambda I - T_{n_j})f\| \to M\|(\lambda I - T)f\| \text{ as } j \to \infty.$$

Since this holds for all $f \in \mathcal{C}$, it follows from Definition 4.1 that

$$\|f\| \leq M\|(\lambda I - T)f\| \quad \forall f \in D(T).$$

Hence λ does not lie in $\sigma_a(T)$, which proves the result. □

Because the result (40) does not hold, in general, for non-selfadjoint operators, it is not generally possible to replace $\sigma(\{T_n\})$ in (41) by $\overline{\cap_{m\in\mathbb{N}} \cup_{n\geq m} \sigma(T_n)}$. However, the following result concerning pseudospectra can be proved.

Theorem 4.4 *Let $\epsilon > \delta > 0$. Let*

$$\sigma_\epsilon(T_n) := \{\lambda \in \mathbb{C} \mid \|(\lambda I - T_n)^{-1}\| \geq \epsilon^{-1}\}, \tag{42}$$

$$\sigma_\delta(T) := \{\lambda \in \mathbb{C} \mid \|(\lambda I - T)^{-1}\| \geq \delta^{-1}\}. \tag{43}$$

Let $\mathcal{C}$ be a core of T satisfying the same hypotheses as in Theorem 4.3, and suppose that for all $f \in \mathcal{C}$ we have $\lim_{n\to\infty} \|T_n f - Tf\| = 0$. Then

$$\sigma_\delta(T) \subseteq \liminf_{n\to\infty} \sigma_\epsilon(T_n), \tag{44}$$

where

$$\liminf_{n\to\infty} \sigma_\epsilon(T_n) := \cup_{m\in\mathbb{N}} \cap_{n\geq m} \sigma_\epsilon(T_n).$$

Proof We start by defining

$$\sigma_\delta(\{T_n\}) := \{\lambda \in \mathbb{C} \mid \liminf_{n\to\infty} \|(\lambda I - T_n)^{-1}\| \geq \delta^{-1}\}. \tag{45}$$

Suppose that λ does not lie in $\sigma_\delta(\{T_n\})$. Then there exists $\gamma \in (0, \delta^{-1})$ and a monotone increasing sequence $(n_j)_{j\in\mathbb{N}}$ such that

$$\|(\lambda I - T_{n_j})^{-1}\| \leq \gamma < \delta^{-1}.$$

Let $f \in \mathcal{C}$, and write $f = (\lambda I - T_{n_j})^{-1}(\lambda I - T_{n_j})f$, giving

$$\|f\| \leq \gamma \|(\lambda I - T_{n_j})f\|.$$

Letting $j \to \infty$ gives

$$\|f\| \leq \gamma \|(\lambda I - T)f\| \tag{46}$$

Eqn. (46) holds for all $f \in \mathcal{C}$ and hence, since $\mathcal{C}$ is a core of T, for all $f \in D(T)$. In particular this implies that $\lambda I - T$ is invertible and

$$\|(\lambda I - T)^{-1} f\| \leq \gamma \|f\|$$

for all $f \in D(T)$. This implies that $\|(\lambda I - T)^{-1}\| \leq \gamma < \delta^{-1}$, and so λ does not lie in $\sigma_\delta(T)$. We have thus proved

$$\sigma_\delta(T) \subseteq \sigma_\delta(\{T_n\}). \tag{47}$$

The result will be proved if we can show that for $\delta < \epsilon$,

$$\sigma_\delta(\{T_n\}) \subseteq \liminf_{n\to\infty} \sigma_\epsilon(T_n). \tag{48}$$

To do this, suppose that μ does not lie in $\liminf_{n\to\infty} \sigma_\epsilon(T_n)$. By definition,

$$\liminf_{n\to\infty} \sigma_\epsilon(T_n) = \cup_{m\in\mathbb{N}} \cap_{n\geq m} \{\lambda \in \mathbb{C} \mid \|(\lambda I - T_n)^{-1}\| \geq \epsilon^{-1}\},$$

and so for each $m \in \mathbb{N}$, μ does not lie in

$$\cap_{n\geq m}\{\lambda \in \mathbb{C} \mid \|(\lambda I - T_n)^{-1}\| \geq \epsilon^{-1}\}.$$

In other words, there exists a subsequence $(T_{n_j})_{j\in\mathbb{N}}$ such that

$$\|(\mu I - T_{n_j})^{-1}\| < \epsilon^{-1}, \quad j \in \mathbb{N}.$$

Hence by definition,

$$\liminf_{n\to\infty} \|((\mu I - T_n)^{-1}\| \leq \epsilon^{-1} < \delta^{-1}.$$

From (45) we have clearly proved μ does not lie in $\sigma_\delta(\{T_n\})$. This establishes (48), and our proof is complete. □

Theorem 4.5 *Let $z \in \mathbb{C}$ be fixed. Suppose that $\|(zI - T_n)^{-1} - (zI - T)^{-1}\| \to 0$ as $n \to \infty$. Then*

$$\limsup_{n\to\infty} \sigma(T_n) \subseteq \sigma(T), \tag{49}$$

where $\limsup$ *is defined by*

$$\limsup_{n\to\infty} \sigma(T_n) = \cap_{m\in\mathbb{N}} \overline{\cup_{n\geq m} \sigma(T_n)}.$$

Proof Let $R_n = (zI - T_n)^{-1}$ and let $R = (zI - T)^{-1}$. Then $\|R_n - R\| \to 0$ as $n \to \infty$. From the results in Kato [13, IV, §3, p. 208] it follows that

$$\limsup_{n\to\infty} \sigma(R_n) \subseteq \sigma(R). \tag{50}$$

However the spectrum of R is related to the spectrum of T by

$$\lambda \in \sigma(T) \text{ if and only if } (z - \lambda)^{-1} \in \sigma(R).$$

[N.B. for our applications, ∞ will be an accummulation point of $\sigma(T)$ and so 0 will lie in $\sigma(R)$.] A similar relationship holds between $\sigma(T_n)$ and $\sigma(R_n)$. Thus (50) implies (49). □

We shall now show that in Sims Cases II and III, the hypotheses of Theorem 4.5 are satisfied by taking $T_n = M_n$ and $T = M$, where M_n and M are the operators of Theorem 3.1. Thus Theorem 4.5 will supercede Theorem 3.1 in Sims Cases II and III as a guarantee that spectral inexactness is impossible provided the boundary conditions are correct. Spectral inclusion still holds by Theorem 3.5. Combining all these results will show that in Sims Cases II and III, provided we generate the M_n using the boundary conditions described for these cases in Lemma 3.2, we have spectral inclusion and spectral exactness (Theorem 4.7 below).

Theorem 4.6 *Consider a differential expression of Sims Case II or Case III type at $x = b$. Let M be a realization of this expression through analytic continuation of an m-function which is a limit of functions $m_n(\cdot)$ for realizations M_n of the differential operator defined on intervals $[a, b_n]$, $b_n \nearrow b$ as $n \nearrow \infty$, as described in Lemma 3.2. Let $\psi_n(x, \lambda)$ be the solution of the differential equation defined by*

$$\psi_n(x, \lambda) = \theta(x, \lambda) + m_n(\lambda)\phi(x, \lambda),$$

and let the $G_n(x, y, \lambda)$ be the Green's functions given by

$$G_n(x, y, \lambda) = \begin{cases} -\phi(x, \lambda)\psi_n(y, \lambda), & a < x < y < b, \\ -\psi_n(x, \lambda)\phi(y, \lambda), & a < y < x < b. \end{cases}$$

Let $R_n(\lambda)$ be the extension to $L^2_w[a, b)$ of $(\lambda I - M_n)^{-1}$ defined by

$$(R_n(\lambda)f)(x) = \int_a^{b_n} G_n(x, y, \lambda)f(y)w(y)dy, \quad f \in L^2_w[a, b).$$

(see [4, eqn. (4.2)]). Fix $z \in \mathbb{C}$ and suppose that z does not lie in the spectrum of M or of any of the M_n for sufficiently large n. Let $R = (zI - M)^{-1}$. Then $\|R(z) - R_n(z)\| \to 0$ as $n \to \infty$.

Proof From [4, eqn. (4.2)] we know that

$$(R(z)f)(x) = \int_a^b G(x, y, z)f(y)w(y)dy,$$

in which $\psi(x, z) = \theta(x, z) + m(z)\phi(x, z)$. Thus

$$(R(z) - R_n(z))f)(x) = \int_{b_n}^b G(x, y, z)f(y)w(y)dy + \int_a^{b_n} (G(x, y, z) - G_n(x, y, z))f(y)w(y)dy.$$

Because the differential equation is of Sims Case II or Case III, we know that both $\theta(\cdot, z)$ and $\phi(\cdot, z)$ lie in $L^2_w[a, b)$. This implies that

$$\int_a^b w(x)dx \int_a^b w(y)G(x, y, z)^2 dy < +\infty, \quad \int_a^b w(x)dx \int_a^b w(y)G_n(x, y, z)^2 dy < +\infty.$$

In particular, therefore,

$$\lim_{n\to\infty} \int_a^b w(x)dx \int_{b_n}^\infty |G(x, y, z)|^2 w(y)dy = 0.$$

The bound

$$\begin{aligned} \|R(z) - R_n(z)\|^2 \quad &\leq \quad 2\int_a^b w(x)dx \int_{b_n}^b |G(x, y, z)|^2 w(y)dy \\ &\quad +2\int_a^b w(x)dx \int_a^b w(y)dy|G(x, y, z) - G_n(x, y, z)|^2 \end{aligned}$$

now yields

$$\lim_{n\to\infty}\|R(z)-R_n(z)\|^2 \le 2\lim_{n\to\infty}\int_a^b w(x)dx\int_a^b w(y)dy|G(x,y,z)-G_n(x,y,z)|^2.$$

We now use the formulae

$$G(x,y,z)-G_n(x,y,z)=\begin{cases} -(m(z)-m_n(z))\phi(x,z)\phi(y,z), & a<x<y<b,\\ -(m(z)-m_n(z))\theta(y,z)\phi(y,z), & a<y<x<b,\end{cases}$$

to obtain

$$\lim_{n\to\infty}\|R(z)-R_n(z)\|^2 \le 2\left(\lim_{n\to\infty}|m_n(z)-m(z)|^2\right)\left(\int_a^b w(\xi)|\theta(\xi,z)|^2d\xi\right)\left(\int_a^b w(\xi)|\phi(\xi,z)|^2d\xi\right).$$

Since $\lim_{n\to\infty}|m_n(z)-m(z)|=0$, this proves the result. □

Theorem 4.7 *(Spectral Inclusion and Spectral Exactness for Sims Cases II and III). Let M_n and M be as in Theorem 4.6. Then*

(a) *for every λ in the spectrum of M, there exists a convergent sequence $(\lambda^{(n)})_{n\in\mathbb{N}}$, with $\lambda^{(n)}$ in the spectrum of M_n, whose limit is λ;*

(b) *if $(\lambda^{(n)})_{n\in\mathbb{N}}$ is a convergent sequence with limit λ and $\lambda^{(n)}$ lies in the spectrum of M_n for each n, then λ lies in the spectrum of M.*

Proof By Theorem 4.6, the hypotheses of Theorem 4.5 are satisfied. This immediately gives (b). Turning to (a), we observe that the hypotheses of Theorem 3.3 are satisfied. The result of Theorem 3.3 allows us to use Theorem 3.4, which in turn allows us to use Theorem 3.5. The conclusion of Theorem 3.5 is precisely (a). □

5 Examples

We illustrate the results of the preceding sections with some numerical examples.

Example 1 An equation of the form

$$-y''+c^2y=\lambda w(x)y,\quad x\in[0,\infty),$$

in which $\Re(c)\neq 0$ and $w(x)=\exp(-3|\Re(c)|x)$, is easily checked to be in Sims Case II at infinity. Letting $v(x)=\exp(-|\Re(c)|x)$ we can define an operator M by $(My)(x)=w(x)^{-1}\{-y''+c^2y\}$ for $y\in D(M)$, where the boundary conditions for $D(M)$ are

$$y(0)=0,\quad [y,v](\infty)=0.$$

The corresponding operator L has domain $D(L)$ specified by the boundary conditions

$$y'(0)=0,\quad [y,v](\infty)=0.$$

For the operators M_n and L_n on finite intervals $[0,b_n]$ the boundary conditions at the origin will be the same as for M and L respectively, while the boundary condition (22) at $x=b_n$ will be given, according to Lemma 3.2, by

$$[y,v](b_n)=0.$$

Using the code described in [10] we computed the eigenvalues of the operators M_n and L_n in the box with corners 100, $100(1+i)$, $100i$, 0. The results, shown in Table 1, indicate that the eigenvalues of the M_n and of the L_n converge to distinct points in the box, and so our test for spectral exactness suggests that the operator M has eigenvalues close to $94.4890 + i28.8595$ and $24.21335 + i14.11108$, while L has eigenvalues close to $3.1163595 + i5.808222$ and $51.51888 + i21.3277$. Of course, this is what we would expect for a Sims Case II problem, by Theorem 4.7.

Note that these eigenvalue problems can be formulated as compact perturbations of selfadjoint eigenvalue problems, although it is not immediately clear how one might use this to obtain spectral inclusion and/or exactness results.

n	b_n	Eigenvalues of M_n	Eigenvalues of L_n
1	5	24.21311+i14.10915 94.4880+i28.8342	3.1163619+i5.808222 51.51912+i21.3277
2	10	24.21334+i14.11103 94.4891+i28.8584	3.1163595+i5.808219 51.51879+i21.3274
3	15	24.21333+i14.11106 94.4888+i28.8590	3.1163591+i5.808221 51.51875+i21.3276
4	20	24.21335+i14.11108 94.4890+i28.8595	3.1163595+i5.808222 51.51888+i21.3277

Table 1: Example 1 on intervals $[0, b_n]$, using code of [10] with $TOL = 10^{-7}$.

Example 2 We consider the (now rather infamous) rotated harmonic oscillator problem

$$-y'' + c^2x^2y = \lambda y, \quad x \in [0,\infty), \quad y(0) = 0, \quad c \in \mathbb{C},\ \Re(c) > 0,$$

(see Davies [6]). This problem is of Sims Case I at infinity and its eigenvalues are given by

$$\lambda_k = c(4k+3) \quad k = 0, 1, 2, \cdots.$$

It is known that the higher index eigenvalues are very ill-conditioned (when c^2 is not positive). Denoting by M the operator associated with this problem, this ill-conditioning may be explained by the fact that $\|(M - zI)^{-1}\|$ is extremely large in very large neighbourhoods of these eigenvalues, making it numerically difficult to determine the precise location of the poles of $\|(M - zI)^{-1}\|$, which are the eigenvalues.

On the other hand, it is easy to verify that the hypotheses of Theorem 3.4 are satisfied for this problem, so Theorem 3.1 still gives a valid test for spectral inexactness.

One might expect that this would be of rather academic interest, given that the operators M_n and L_n on the truncated intervals $[0, b_n]$ will themselves have very ill-conditioned higher index eigenvalues. To some extent this is correct. However, in Table 5 we show the result of truncating the interval to $[0, 20]$ and locating all the eigenvalues in a rectangle in the complex plane with bottom right-hand corner $\lambda = 100$ and top left-hand corner $\lambda = 90i$. The boundary conditions used were $y(0) = 0 = y(20)$ for the M_n problem and $y'(0) = 0 = y(20)$ for the L_n problem. The spurious eigenvalues are marked with asterisks. One can see quite clearly that these eigenvalues distinguish themselves by being almost invariant under the change of boundary condition at the origin. Indeed, in all but one case the relative differences are less than the tolerance which was used in the computations (10^{-5}). There is also a problem with 'missing' eigenvalues in this table: M_n ought to have an eigenvalue close to $73 + i50$ and

L_n ought to have an eigenvalue close to $77 + i55$, both of which are missing. Thus the ill-conditioning of these problems may induce spectral inexactness, for which we seem to be able to test by changing the boundary conditions, but it can also cause a lack of spectral inclusion, which is rather more difficult to spot.

Eigenvalues of M_n	Eigenvalues of L_n
4.3278454 + i 3.1193175	1.4426265 + i 1.0397661
10.098296 + i 7.2784044	7.2130633 + i 5.1988778
15.868726 + i 11.437476	12.983488 + i 9.3579536
21.639117 + i 15.596455	18.753885 + i 13.517014
27.409413 + i 19.755403	24.524267 + i 17.676070
33.179628 + i 23.914366	30.294667 + i 21.835034
38.949823 + i 28.073359	36.065062 + i 25.993830
44.720108 + i 32.232282	41.835242 + i 30.152542
50.490469 + i 36.391057	47.605269 + i 34.311200
56.260702 + i 40.549373	53.375120 + i 38.469967
62.032125 + i 44.715888	59.146275 + i 42.628491
67.763082 + i 48.620308	64.868061 + i 46.792270
70.791811 + i 54.525167*	70.836011 + i 54.242901*
76.994286 + i 49.224379	71.821431 + i 49.862180
72.268485 + i 64.384873*	72.268524 + i 64.384384*
73.809759 + i 74.921450*	73.809759 + i 74.921449*
75.474904 + i 86.054406*	75.474905 + i 86.054405*
87.360734 + i 47.089232	82.109895 + i 48.176485
98.348465 + i 44.849646	92.771537 + i 45.977747

Table 2: Testing for spectral inexactness on the rotated harmonic oscillator

Example 3 Consider the problem of locating resonances of the equation

$$-y'' + 16x^2 \exp(-x)y = \lambda y, \quad y'(0) = 0, \quad x \in [0, \infty). \tag{51}$$

Using the 'complex scaling' method, the resonances of this problem are of the form $\mathrm{e}^{-2i\theta}\mu_\theta$ where μ_θ is an eigenvalue of the non-selfadjoint problem

$$-z'' + 16x^2\mathrm{e}^{2i\theta} \exp(-x\mathrm{e}^{i\theta})z = \mu z, \quad z'(0) = 0, \quad x \in [0, \infty), \tag{52}$$

(see Hislop and Segal [12]). The rotation angle $\theta > 0$ must be such that the function $x \mapsto 16x^2\mathrm{e}^{2i\theta} \exp(-x\mathrm{e}^{i\theta})$ lies in $L^1[0, \infty)$, and in particular therefore $\theta < \pi/2$. Resonances have the property that $\mathrm{e}^{-2i\theta}\mu_\theta$ is independent of θ, so in general not all eigenvalues of (52) yield resonances: one should carry out the computations for at least two different values of θ to identify resonances.

In addition to the complications caused by the fact that some eigenvalues of (52) do not correspond to resonances, we have the additional problem that (52) is a singular problem and must be regularized by interval truncation. This truncation process might introduce spurious eigenvalues, not corresponding to eigenvalues of (52), which we need to be able to detect. Theorem 3.1 gives a way to do this.

Using a rotation angle $\theta = 1.1$ and a truncated interval $[0, 100]$ with boundary condition $y(100) = 0$ we computed both the eigenvalues of the equation in (52) with $y'(0) = 0$ and the eigenvalues for the same equation but with the boundary condition $y(0) = 0$ using the code of [10]. We asked the code to find, in the μ plane, all the eigenvalues in the box with corners $(-0.01, 0.01)$, $(-0.01, 5)$, $(-10, 5)$, $(-10, 0.01)$, with a tolerance of 10^{-6}. The results, rotated back into the λ plane via $\lambda = e^{-2i\theta}\mu$, are shown in Table 5.

Alleged resonances with $y(0) = 0 = y(100)$ on $[0, 100]$	Alleged resonances with $y'(0) = 0 = y(100)$ on $[0, 100]$
2.429823932+i 2.95502902	2.429823937 +i 2.95502903
3.869964809-i 0.74439879	3.869964804 -i 0.74439879
0.554661821+i 0.66915540	0.554661961 +i 0.66915556
	2.861786706 -i 1.6×10^{-6}

Table 3: Testing for spurious resonances due to interval truncation

Of the four alleged resonances found with $y'(0) = 0$, three are virtually unchanged when the boundary condition is changed to $y(0) = 0$. Theorem 3.1 indicates that these are probably spurious. This is obvious for the two which have positive imaginary parts, as resonances lie in the lower half plane by definition; however, without Theorem 3.1 it would not have been obvious for the alleged resonance at $3.8699648 - i0.7443988$. For this problem we believe that the only genuine resonance found, for boundary condition $y'(0) = 0$, is the one at $2.861786706 - i1.6 \times 10^{-6}$. In fact, of the four alleged resonances this is the only one which is invariant under a change of the rotation angle θ; however, in general it is not clear that a spurious resonance generated by interval truncation would always fail to be invariant under change of θ.

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