NON-SELF-ADJOINT DIFFERENTIAL OPERATORS

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Abstract

A description is given of methods that have been used to analyze the spectrum of non-self-adjoint differential operators, emphasizing the differences from the self-adjoint theory. It transpires that even in cases in which the eigenfunctions can be determined explicitly, they often do not form a basis; this is closely related to a high degree of instability of the eigenvalues under small perturbations of the operator.

1. Introduction

In this review, we discuss the spectral behaviour of non-self-adjoint (nsa) linear operators acting in a Hilbert space. Many of our observations apply to operators in a Banach space, although modifications may be needed if the space is not reflexive. We are mainly interested in differential operators that have dense domains, but some of the initial observations are applicable to bounded operators, and even to $n \times n$ matrices for large enough n; we find that n = 32 is large enough to exhibit many of the phenomena described [73].

The theory of nsa differential operators is very much less unified than the self-adjoint theory. The latter is much easier to analyze because of the existence of the spectral theorem and the fact that one can often use variational methods to obtain tight bounds on eigenvalues, both numerically and theoretically. In addition, the self-adjoint theory has enormous importance in quantum mechanics; the properties of the Laplacian alone are of immense relevance to stochastic analysis and Riemannian geometry. Nevertheless, there are increasing numbers of problems in physics that require the analysis of nsa operators. The author came to these via the study of complex resonances of self-adjoint Schrödinger operators. If one uses the techniques of complex scaling, then these resonances turn into genuine eigenvalues of associated nsa Schrödinger operators. Such operators also arise in phenomenological models of nuclear scattering, in which an absorption term accounts for channels not explicitly included in the model. But there are many different sources of such problems, several of which are mentioned in the review; for a variety of others, see [28].

It has long been known by numerical analysts that the eigenvalues of nsa matrices may be very ill-conditioned. Since we do not wish to assume familiarity with this field, we summarize the ideas here. A generic $n \times n$ matrix A has distinct eigenvalues $\lambda_1, \ldots, \lambda_n$ and the corresponding eigenvectors v_1, \ldots, v_n form a basis in \mathbb{C}^n . The degree to which these eigenvectors point in different directions may be measured as follows. We may write $A = TDT^{-1}$, where D is the diagonal matrix whose entries are the eigenvalues of A and T is invertible. The number $\kappa = ||T|| ||T^{-1}||$ is called the condition number of T. We have $\kappa \ge 1$, with equality if and only if T is a unitary

matrix. In this case the eigenvectors of A (after normalization) form an orthonormal basis of \mathbb{C}^n and A is normal; that is, $AA^* = A^*A$. However, if A is a typical nsa matrix, then it is commonplace that any matrix T that diagonalizes A has a very large condition number; in practice, this is often of order 10^3 even for simple 32×32 matrices, and in theory it may be arbitrarily large. Although the eigenvectors form a basis, two of them may be very nearly parallel, with the result that the associated eigenvalues are very unstable under small perturbations of the matrix. A very simple example is given by

$$A_{i,j} = \begin{cases} 1, & \text{if } j = i+1, \\ \varepsilon, & \text{if } j = 1 \text{ and } i = n, \\ 0, & \text{otherwise,} \end{cases}$$

where $\varepsilon = 2^{-n}$ and n = 50.

Let us pursue this issue in more detail by examining individual eigenvalues. If we denote the eigenvector of A^* associated with the eigenvalue $\overline{\lambda_i}$ by \hat{v}_i , then (subject to a normalization) the sequences v_i and \hat{v}_i are biorthogonal in the sense that

$$\langle v_i, \hat{v}_j \rangle = \delta_{i,j}.$$

The spectral projection of A corresponding to the eigenvalue λ_i is given by

$$P_i f = \langle f, \hat{v}_i \rangle v_i,$$

one always has $||P_i|| \ge 1$, and in general

$$||P_i|| = ||v_i|| \, ||\hat{v}_i||.$$

If one normalizes the eigenvectors by $||v_i|| = ||\hat{v}_i|| = 1$ instead, then

$$||P_i|| = |\langle v_i, \hat{v}_i \rangle|^{-1}$$

and we see that the norm is large if the eigenvectors v_i and \hat{v}_i are nearly orthogonal. At the other extreme, P_i is an orthogonal projection, or has norm 1, if and only if $v_i = \hat{v}_i$.

Now let us pass to the case in which A is an unbounded closed linear operator with dense domain \mathcal{D} in the Hilbert space \mathcal{H} . The operator Af(x) = f'(x) acting in $L^2(0,1)$ subject to the initial condition f(0) = 0 has empty spectrum, and its inverse, the Volterra operator, has been much studied. In order to avoid such possibilities, we suppose in this section that A has compact resolvent operators, and for simplicity we also assume that its eigenvalues λ_n , $n = 1, 2, \ldots$, are all of multiplicity 1 in the sense that the associated spectral projections have rank 1. It is immediate that $\lim_{n\to\infty} |\lambda_n| = +\infty$. We finally suppose that the corresponding eigenvectors v_n form a complete set in the sense that their linear span is a dense subspace of \mathcal{H} . After normalization, the eigenvectors \hat{v}_m of A^* provide, together with v_n , a biorthogonal system in \mathcal{H} , and the spectral projections P_n of A are given by the same formulae as in the finite-dimensional case.

We say that $\{v_n\}$ forms a basis if every $f \in \mathcal{H}$ has a norm-convergent expansion

$$f = \sum_{n=1}^{\infty} P_n f = \sum_{n=1}^{\infty} \langle f, \hat{v}_n \rangle v_n. \tag{1}$$

By the uniform boundedness theorem, this is equivalent to the condition that the sequence of projections $Q_n = \sum_{r=1}^n P_r$ is uniformly bounded in norm. It implies that

there exists a constant k such that

$$||P_n|| = ||v_n|| \, ||\hat{v}_n|| \le k$$

for all n.

An even stronger condition is that $\{v_n\}$ form an unconditional basis, which means that every permutation of the sequence is a basis. It is a deep theorem of Lorch that this holds if and only if there exists a bounded invertible operator T such that $\{Tv_n\}$ is a complete orthonormal set in \mathcal{H} ; see [33]. In our context it is also equivalent to the condition that A is similar to a normal operator; this is rarely true, and we shall not consider it further.

Even if $\{v_n\}$ do not form a basis, it has been shown by Lidskii, Agranovich, Katznelson and others that for usa elliptic differential operators, one often has Abel-type convergence of the expansion (1) for a general $f \in \mathcal{H}$. This involves some adaptation of the formula

$$f = \lim_{t \to 0+} \sum_{n=1}^{\infty} e^{-\lambda_n^{\beta} t} \langle f, \hat{v}_n \rangle v_n,$$

where $\beta > 0$, depending on the particular features of the operator involved; see [5, 44]. If H = A + B, where B is a small perturbation of the non-negative self-adjoint operator A in a suitable sense, then considerably stronger basis-type theorems may be proved [4]; the examples discussed in this review are mostly *not* of this type.

There is another approach that is often numerically effective. Given $f \in \mathcal{H}$ and a finite set of eigenvectors v_1, \ldots, v_n , one may easily determine the 'minimum error' coefficients c_1, \ldots, c_n , defined as those that minimize $\varepsilon = ||g||$ in the expansion

$$f = \sum_{r=1}^{n} c_r v_r + g. \tag{2}$$

These coefficients depend upon n, and are quite different from the 'Fourier' coefficients determined by the adjoint eigenvectors. If the eigenvectors form a complete set, then $\varepsilon \to 0$ as $n \to \infty$.

Suppose that one wishes to solve the equation zh-Hh=f for h, given $z \notin \operatorname{Spec}(H)$ and $f \in \mathcal{H}$. If $\rho = \|(zI-H)^{-1}\|$ is too large, this is not possible stably. If $\rho = O(1)$, then using (2) one deduces quickly that

$$\left\|h - \sum_{r=1}^{n} c_r (z - \lambda_r)^{-1} v_r \right\| \leqslant \rho \varepsilon.$$

If iH is the generator of a contraction semigroup, then $Re(i\lambda_n) \leq 0$ for all n. Moreover,

$$e^{iHt}f = \sum_{r=1}^{n} c_r e^{i\lambda_r t} v_r + e^{iHt} g$$

for all $t \ge 0$, so

$$\left\| e^{iHt} f - \sum_{r=1}^{n} c_r e^{i\lambda_r t} v_r \right\| \leqslant \varepsilon,$$

again for all $t \ge 0$. In other words, the error is stable as a function of time. Of course, the condition that iH is the generator of a contraction semigroup is an extremely strong one, but it is applicable in the case of the complex harmonic oscillator discussed in [43, 66].

The set of eigenvalues of A is invariant under similarity transformations of the form $A \to TAT^{-1}$. Another such invariant is the asymptotic behaviour of $||P_n||$ as $n \to \infty$, where the eigenvalues are suitably ordered, for example so that $|\lambda_n|$ are in increasing order. We say that the spectral projections are *polynomially bounded* if there exist constants c and α such that

$$||P_n|| \leqslant cn^{\alpha}$$

for all n; clearly, α is then a similarity invariant of A. If no such constants exist, we say that A is spectrally wild.

If A is spectrally wild, then one cannot use expansions such as

$$(zI - A)^{-1}f = \sum_{n=1}^{\infty} (z - \lambda_n)^{-1} P_n f,$$

or often even

$$e^{At}f = \sum_{n=1}^{\infty} e^{\lambda_n t} P_n f$$

for all $f \in \mathcal{H}$, even if one knows that A is the generator of a strongly continuous one-parameter semigroup, because the right-hand side may not converge.

In this abstract context, Nath has shown that, given any complete minimal set of vectors $\{v_n\}_{n=1}^{\infty}$ in \mathcal{H} , there exists an unbounded closed operator A with compact resolvent for which these are precisely the eigenvectors. If $\{v_n\}_{n=1}^{\infty}$ is not an unconditional basis, then (4) below is not valid for this operator [49, 50]. The next issue to be faced is what one might reasonably expect for operators that arise in applied mathematics. We shall show that many typical nsa differential operators are spectrally wild.

The above analysis is closely related to the notion of pseudospectra, which we discuss in the next section. We describe a number of differential operators that have been analyzed in the last five years. Four techniques have been used to obtain the results that we describe: semigroup theory, perturbation theory, numerical ranges, and analytic function theory. Each of them has limitations, which we describe. By combining all four, we begin to get an idea of the huge variety of phenomena that are possible for nsa operators. At present, the subject has hardly moved beyond the foothills, but the clear message is that if one wishes to travel in this direction, one must give up any hope that theorems about self-adjoint operators will provide useful signposts: they regularly lead in quite the wrong direction. In practice, we have found that carefully chosen numerical computations provide surprising glimpses through the clouds that surround this subject, and guide one towards the theorems that might be proved.

2. Pseudospectra

If A is a bounded or unbounded linear operator on \mathcal{H} , one may define its pseudospectra $\operatorname{Spec}_{\varepsilon}(A)$ for $\varepsilon > 0$ to be the sets

$$\left\{z \in \mathbb{C} : \left\| (zI - A)^{-1} \right\| \geqslant \varepsilon^{-1} \right\}.$$

It is immediate that $z \in \operatorname{Spec}_{\varepsilon}(A)$ if and only if $z \in \operatorname{Spec}(A)$ or there exists $f \in \operatorname{Dom}(A)$ such that $\|(zI - A)f\| \le \varepsilon \|f\|$. Computation of the pseudospectra

amounts to producing a contour plot of the following function:

$$r_A(z) = \left\{ \begin{array}{l} \left\| (zI - A)^{-1} \right\|, & \text{if } z \notin \operatorname{Spec}(A), \\ \infty, & \text{otherwise.} \end{array} \right.$$

We refer to a forthcoming monograph [28, 29] on this subject, and to [74] for pictures of the pseudospectra of a variety of nsa differential operators arising in applied mathematics. Numerical computation of the pseudospectra by the obvious method is computationally very heavy, and much effort has been put into finding more efficient algorithms. We do not have the expertise to compare these, and we refer the reader to one recent approach to this problem [77, 75]. We also mention that r_Z is subharmonic and continuous on the complement of $\operatorname{Spec}(A)$, and another algorithm exploits this fact [31, 32].

One needs to be careful not to suppose that if $Af \simeq zf$, then z is close to the spectrum of A. One always has a bound of the type

$$||(zI - A)^{-1}|| \ge \operatorname{dist}(z, \operatorname{Spec}(A))^{-1},$$
 (3)

where dist(z, S) denotes the distance of z from S, with equality if A is normal. The existence of a reverse inequality of the form

$$||(zI - A)^{-1}|| \le k \operatorname{dist}(z, \operatorname{Spec}(A))^{-1}$$
 (4)

is a definite assumption, and the existence (but not the value) of k is a similarity invariant of A. If it holds, and z is an approximate eigenvalue in the sense that

$$||Af - zf|| < \varepsilon ||f||$$

for some non-zero $f \in Dom(A)$, then

$$dist(z, \operatorname{Spec}(A)) < k\varepsilon$$
.

The bound (3) can be re-expressed in more geometrical terms as the statement that $\operatorname{Spec}_{\varepsilon}(A)$ always contains the ε -neighbourhood of $\operatorname{Spec}(A)$. The failure of (4) is associated with the possibility that $\operatorname{Spec}_{\varepsilon}(A)$ may be much bigger than this ε -neighbourhood. For an example in which this occurs, we refer to Theorem 5 and the associated Figure 1.

There is a bound on the size of the pseudospectrum involving the numerical range

$$Num(A) = \{ \langle Af, f \rangle / \langle f, f \rangle : 0 \neq f \in Dom(A) \}$$

of A. Note that Num(A) is always a convex set [17]. The hypothesis of the following classical theorem is automatic for bounded operators, and also holds for many differential operators.

THEOREM 1. If the complement of Num(A) is connected and contains at least one point not in the spectrum of A, then

$$\operatorname{Spec}_{\varepsilon}(A) \subseteq \{z : \operatorname{dist}(z, \operatorname{Num}(A)) \leqslant \varepsilon\}$$

for every $\varepsilon > 0$.

There is an important theorem relating the pseudospectra to the stability of the spectrum under perturbations. It may be summarized by the statement that very large pseudospectra are always associated with eigenvalues that are very unstable with respect to perturbations. This is clearly of great importance to numerical

analysts: if a spectral problem is unstable enough, no numerical procedure can enable one to find the eigenvalues, whose significance therefore becomes a moot point.

Theorem 2 [63, Proposition 4.15]. Given $\varepsilon > 0$, one has

$$\operatorname{Spec}_{\varepsilon}(A) = \operatorname{cl}\left\{\bigcup_{\|B\| \leq \varepsilon} \operatorname{Spec}(A+B)\right\}$$

where 'cl' denotes the closure.

This theorem has been extended to some situations in which the perturbations are restricted more severely. We cannot describe all the variants possible, and the following is only representative; see also [31, 9, 41, 32]. If A is a closed densely defined operator on a Banach space \mathcal{B} , and D and E are bounded operators, then one may define the spectral value set, also called the structured pseudospectrum, by

$$\sigma(A, D, E, \varepsilon) = \bigcup_{\|S\| < \varepsilon} \operatorname{Spec}(A + DSE).$$

(It is also possible to allow certain classes of unbounded perturbations of a similar type.) The pseudospectrum arises by making the choice D = E = I, but other choices allow one to take account of conservation laws that the perturbed operator should satisfy. The analogue of the last theorem is more complicated because of the possibility that the perturbations do not affect certain parts of Spec(A).

THEOREM 3 [31, 32]. Under the above assumptions,

$$\sigma(A, D, E, \varepsilon) = \operatorname{Spec}(A) \cup \left\{ z \notin \operatorname{Spec}(A) : ||E(zI - A)^{-1}D|| > \varepsilon^{-1} \right\},\,$$

for any $\varepsilon > 0$. The two sets on the right-hand side are, respectively, closed and open.

In contrast with the situation with the pseudospectrum, the structured pseudospectrum may jump discontinuously as ε varies [9].

There is a close relationship between the resolvent norms and the norms of the spectral projections because of the formula

$$P_n = \frac{1}{2\pi i} \int_{\gamma_n} (zI - A)^{-1} \, \mathrm{d}z,\tag{5}$$

where γ_n is a sufficiently small circle with centre at the eigenvalue λ_n . Subject to (4), one concludes from (5) that $||P_n|| \le k$ for all n.

There is also a converse argument in finite dimensions. If $\dim(\mathcal{H}) = n < \infty$, then using

$$(zI - A)^{-1} = \sum_{i=1}^{n} (z - \lambda_i)^{-1} P_n,$$

we see that if $||P_i|| \le k$ for all i, then

$$||(zI - A)^{-1}|| \le kn \operatorname{dist}(z, \operatorname{Spec}(A))^{-1}.$$

Since k is frequently much larger than n, this often amounts to an equivalence between the stated resolvent norm estimates and the spectral projection estimates.

3. Classification of the spectrum

The classification of the spectrum of nsa operators into parts with particular properties is in a primitive state compared with the situation for self-adjoint operators. If H is similar to a self-adjoint or normal operator, then we may take over the powerful machinery of the spectral theorem. Such cases do arise, but they are very rare for differential operators.

One definition of the essential spectrum is that it is the set of $z \in \mathbb{C}$ such that A-zI is not a Fredholm operator. A closed operator B on \mathscr{H} is said to be Fredholm if Ker(B) is finite-dimensional and Ran(B) is closed with finite co-dimension in \mathscr{H} [17, p. 79]. The inessential spectrum of an operator may be much larger than the set of isolated eigenvalues of finite multiplicity, and may contain an entire region in the complex plane. We refer to [61, 37] for other inequivalent definitions and properties of the essential spectrum.

The following definition of the localized spectrum of an operator acting on $L^2(\mathbb{R}^n)$ is adapted from [24, 25], in which the idea is presented for $l^2(X)$, where X is a countable set provided with a metric. We say that $f \in L^2(\mathbb{R}^n)$ is of finite variance if ||f|| = 1 and also $||Qf|| < \infty$, where Q is the vector position operator $(Qf)_r(x) = x_r f(x)$ for $1 \le r \le n$. The expectation of f is then given by $E(f) = \langle Qf, f \rangle \in \mathbb{R}^n$, and the variance is given by

$$var(f) = \langle Q^2 f, f \rangle - \langle Q f, f \rangle^2.$$

We say that $z \in \operatorname{Spec}_{\operatorname{loc}}(H)$ if there exists a sequence f_n of unit vectors in $\operatorname{Dom}(H)$ such that $\lim_{n\to\infty} \|Hf_n - zf_n\| = 0$ and $\operatorname{var}(f_n)$ are uniformly bounded. There is no assumption about the expectations $E(f_n)$.

Theorem 4. If $H = -\Delta + V$ where V is relatively compact with respect to $-\Delta$, then its localized spectrum is the set of all of its eigenvalues whose corresponding eigenfunctions have finite variance.

The proof is analogous to that of [24, Theorem 7.2]. Note that there are theorems that prove under weak conditions that every eigenfunction decays exponentially, and therefore has finite variance. In spite of this example, the localized spectrum may be very different from the point spectrum if the potential does not decay at infinity. For applications of the localized spectrum to random nsa Schrödinger operators, see [24, 25].

4. Constant coefficient operators

One of the standard methods of analyzing the spectrum of a differential operator on $L^2(\mathbb{R})$ is to truncate it to a finite interval, then discretize and finally compute the spectrum of the matrix obtained. Such procedures can often be justified for self-adjoint operators by reference to the variational method, which may be used to prove that the eigenvalues computed are upper bounds to the true eigenvalues.

The situation with nsa operators is far less straightforward. In the following examples we prove that the very first step, the truncation procedure, may have the wrong asymptotic properties. No subsequent numerical procedure can possibly rectify this problem.

We first consider the convection-diffusion operator

$$H_n f(x) = -f''(x) - 2f'(x)$$

acting in $L^2([-n,n])$ subject to Dirichlet boundary conditions. A direct computation shows that the spectrum of H_n consists of the real eigenvalues $\lambda_m = 1 + \pi^2 m^2 / n^2$ where $m = 1, 2, \ldots$ We see immediately that $\lim_{n \to \infty} \operatorname{Spec}(H_n) = [1, \infty) \subseteq \mathbb{R}$. However, the limit operator H_∞ acting on $L^2(\mathbb{R})$ is also exactly soluble by the method of Fourier transforms, and its spectrum is the parabola $\{s^2 + 2is : s \in \mathbb{R}\}$. Thus the spectrum depends discontinuously on n as $n \to \infty$ [56, 74].

In this particular case, the problem can be resolved by using periodic boundary conditions instead of Dirichlet boundary conditions. However, there does not yet exist a procedure that is guaranteed to work in cases that are not exactly soluble, for example when one considers a similar operator with variable coefficients, for which none of the spectra concerned can be written down in closed form. One can at least predict the probable existence of such pathologies by finding the condition numbers of the eigenvalues. For the example given, one finds that these increase exponentially with n, a sure sign that one should not trust the truncation procedure.

If one considers such problems from the point of view of pseudospectra, their behaviour becomes much more regular [56, 74]. We refer the reader to [22] for details of the surprisingly complicated generalizations of the above results to constant coefficient differential operators of arbitrary order, and to [55] for other related results on constant coefficient differential operators. These may be viewed as the differential analogues of corresponding results for Toeplitz operators [10].

5. The harmonic oscillator

The general theory of second-order ordinary differential operators with complex coefficients is not a straightforward extension of that for the case of real coefficients. It is possible to generalize the Weyl limit-point, limit-circle classification for Sturm—Liouville equations to the case of equations with complex coefficients, yielding a classification into three types [8, 15, 67]. Many of the properties of the Titchmarsh—Weyl *m*-function may be extended to the non-self-adjoint context [15, 16, 67]. On the other hand, the following example shows that the nsa theory may have quite new characteristics.

We describe the harmonic oscillator with a complex coupling constant

$$Hf(x) = -f''(x) + cx^2 f(x)$$

acting in $L^2(\mathbb{R})$. For positive real c, this operator has been completely analyzed, so throughout this section we assume that Re(c) > 0 and Im(c) > 0. It has received considerable attention recently in the physics literature, as a model of an unstable optical resonator [43, 66]. In these papers, the non-orthogonality of its eigenfunctions and expansion problems associated with this were discussed, and the minimum error approximation discussed in the introduction was found to be efficient.

If one initially defines H on a Schwartz space \mathcal{S} , then the closure has compact resolvent. One may prove by direct computation or analytic continuation from the real case that the operator has eigenvalues $\lambda_n = c^{1/2}(2n+1)$ where $n=0,1,\ldots$, the corresponding eigenfunctions being Hermite functions that all lie in \mathcal{S} and form a complete set in $L^2(\mathbb{R})$. Boulton has proved in [12, 13] that the numerical range of H

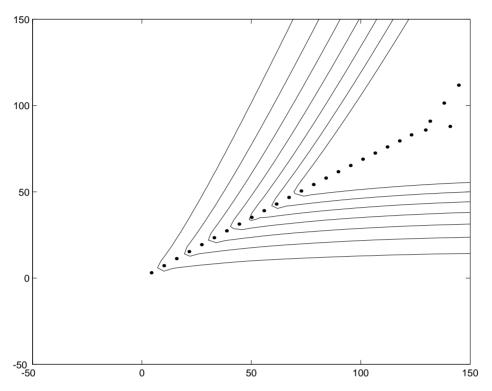


FIGURE 1. Harmonic oscillator eigenvalues and pseudospectra.

is given by the formula

$$Num(H) = \{s + tc : s > 0, t > 0, st \ge 1/4\}.$$

As one moves away from Num(H), the resolvent norm decreases to 0.

The first sign that the behaviour of these operators differs radically from those with c>0 comes from numerical computations of the norms of the spectral projections; these norms appear to increase exponentially as $n\to\infty$. This is a difficult computation, but for c=1+i one can carry it out for n up to 100 if one is willing to compute to a few hundred significant figures. The difficulty with a direct calculation is that one needs to evaluate certain extremely oscillatory integrals to high accuracy. Similar effects are obtained if one computes the pseudospectra of this operator numerically.

We now turn to what has been *proved* for this operator. The following theorem holds; see [20, 21].

THEOREM 5. If $z = re^{i\theta}$ where $0 < \theta < \arg(c)$, then

$$\lim_{r \to \infty} \|(zI - H)^{-1}\| = \infty.$$

On the other hand, if $arg(c) < \theta < 2\pi$, then the value of the limit is 0.

The level curves of the resolvent norm are shown in Figure 1. Each contour represents an increase of the resolvent norm by a factor of 10, starting from the

outside contour, for which the norm is 1. The 'eigenvalues' in the top right-hand corner of the figure are spurious, either because the associated condition numbers are beyond the capacity of the software, or because the spectral instability makes them depend sensitively upon the particular discretization used.

A more detailed analysis of the behaviour of the resolvent norm within the sector $0 < \theta < \arg(c)$ was carried out by Boulton [12, 13]. He found that the resolvent norm remains bounded if $|z| \to \infty$ while z = x + iy satisfies $0 \le y < k$, for any k > 0. On the other hand, if $y = x^{\alpha}$ where $1/3 < \alpha \le 1$, then the resolvent norm diverges as $|z| \to \infty$; numerical computations by Embree and Boulton (separately) indicate that the constant 1/3 is optimal. Similar results hold in the neighbourhood of the other asymptote of the numerical range, namely $c[0,\infty)$. Returning to the study of the spectral projections, it has been proved that this operator is spectrally wild in the sense defined earlier [23].

The above operator may be analyzed in great detail because the eigenvalues, eigenfunctions, resolvent kernels and heat kernels may all be written down explicitly. However, many of the same conclusions hold for the anharmonic operator

$$Hf(x) = -f''(x) + c|x|^{\alpha}f(x), \tag{6}$$

where α is any positive real number. In particular, we have the following theorem.

Theorem 6. Let H be defined by (6) using quadratic form techniques. Then the eigenfunctions of H form a complete set for all $\alpha \ge 1$. Also, H is spectrally wild for all $\alpha > 0$ and all $c \notin \mathbb{R}$.

The first statement is a corollary of an old theorem of Keldysh and Lidskii, while the second is taken from [23]. In the following section we describe a much more general formulation of the problem.

6. The semi-classical limit

The results in the last section may be extended by using semi-classical methods. Consider the operator

$$H_h f(x) = -h^2 f''(x) + V(x) f(x),$$

where h > 0 and V is any smooth complex-valued potential on \mathbb{R} . We do not need to specify the full domain of H_h , but only to suppose that it contains $C_c^{\infty}(\mathbb{R})$. The following theorem shows that as $h \to 0$, the pseudospectrum of H_h expands to fill up the range of the complex classical Hamiltonian $H(p,q) = p^2 + V(q)$, p and q being restricted to taking real values. After a suitable space scaling, it includes Theorem 5.

THEOREM 7. Let $z = p^2 + V(q)$ for some $p, q \in \mathbb{R}$, and suppose that $\text{Im}(V'(q)) \neq 0$. For all m > 0, one has either $z \in \text{Spec}(H_h)$ or $\|(zI - H_h)^{-1}\| \geqslant h^{-m}$ for all sufficiently small h > 0.

The proof is entirely constructive: it depends upon writing down test functions in $C_c^{\infty}(\mathbb{R})$ that satisfy $H_h f_h = z f_h + O(h^m)$. The theorem is not restricted to one dimension. Zworski has commented that it is an immediate consequence of a theorem of Hörmander on pseudo-differential operators in several dimensions [78, 48, 42]. The exact rate at which the resolvent norms diverge can probably be determined

by the use of semi-classical techniques under suitable analyticity conditions on the symbol [48].

It has been suggested that the 'paradoxical' discrepancy between the spectrum and the pseuodspectrum in the semi-classical limit might be avoided by using a different space of functions—that is, by choosing the norm in a manner that is sympathetic to the operator concerned. This is a very interesting proposal, particularly for symbols that are holomorphic [48]. On the other hand, the basis for thinking that it would resolve the above problem is questionable. The spectrum of the Laplace–Beltrami operator on hyperbolic space acting in L^p depends upon p [18, pp. 178, 185]; this interesting fact becomes invisible if one argues that the space should be chosen to make the spectral theory as simple as possible, in which case one would only ever study L^2 . The fact that operators with the same symbol but acting in different Banach spaces may have different spectra has even been used to produce a numerical method of computing thresholds for the emergence of negative eigenvalues of Schrödinger operators [19].

If one does not assume that V is smooth, then Redparth has proved a more general version of the following theorem concerning the semi-classical limit of the pseudospectra [59, 60]. We assume that $H_h = -h^2\Delta + V$ on $L^2(\Omega)$, where h > 0, and that V is a complex-valued continuous function on the closure of the bounded region $\Omega \subseteq \mathbb{R}^n$, and we impose Dirichlet boundary conditions.

Theorem 8. Let Ψ denote the closed convex hull of

$$\Phi = \overline{\text{Ran}(V)} + [0, \infty).$$

Then $\operatorname{Num}(H_h) \subseteq \Psi$ *and*

$$\|(\lambda I - H_h)^{-1}\| \leq \operatorname{dist}(\lambda, \Psi)^{-1}$$

for all $\lambda \notin \Psi$. If $\lambda \in \Phi$, then $\|(\lambda I - H_h)^{-1}\| \to \infty$ as $h \to 0$. If, however, $\lambda \notin \Phi$, then $\limsup_{h \to 0} \|(\lambda I - H_h)^{-1}\| \leqslant \operatorname{dist}(\lambda, \Phi)^{-1}.$

Let us now turn to the behaviour of the spectrum itself in the semi-classical limit. We consider the operator

$$H_h f(x) = -h^2 f''(x) + V(x) f(x)$$

acting on $L^2(-1,1)$ subject to Dirichlet boundary conditions, where V(x) is a bounded complex-valued function. One might naïvely expect that as $h \to 0$ the spectrum of H_h would converge to that of the operator V of multiplication by the function V(x); in other words, that the spectrum of H_h converges to the closure of the set $\{V(x): -1 < x < 1\}$. This is completely wrong, even when V(x) = ix, for which H is relevant to the Orr-Sommerfeld problem, the Squire model for the Couette flow, and the Torrey equation [57, 65, 71]. Shkalikov [65] has proved that in this case the spectrum converges as $h \to 0$ to the (sideways Y-shaped!) set

$$Y = \left\{ -\lambda i + (1 - \lambda) / \sqrt{3} : 0 \le \lambda \le 1 \right\}$$
$$\cup \left\{ \lambda i + (1 - \lambda) / \sqrt{3} : 0 \le \lambda \le 1 \right\}$$
$$\cup \left\{ \lambda + 1 / \sqrt{3} : \lambda \ge 0 \right\}.$$

He has also has extended this result to a certain class of analytic potentials. In a

different direction, Redparth has extended it to all piecewise linear complex-valued potentials, jump discontinuities being permitted [58, 60]. In this case, the limit of the spectrum is a union of sideways Y-shaped sets, one for every interval of linearity of the potential.

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In the particular case

$$V_{\delta}(x) = \begin{cases} i(x+\delta), & \text{if } x > 0, \\ i(x-\delta), & \text{if } x < 0, \end{cases}$$

the limit of the spectrum as $h \to 0$ is the union of two sideways Y-shaped curves, however small $\delta > 0$ may be. Although $H_{h,\delta} \to H_{h,0}$ in the resolvent norm sense as $\delta \to 0$, the limits $\delta \to 0$ and $h \to 0$ do not commute as far as the spectrum is concerned [58, 60].

We mention in passing that the wave equation with a damping term can also be reduced to a nonlinear eigenvalue problem for a Schrödinger operator with a purely imaginary potential, namely finding $\lambda \in \mathbb{C}$ for which

$$(-\Delta - \lambda^2 + 2ia(x)\lambda)f(x) = 0;$$

see [68] for the spectral asymptotics of the real parts of the eigenvalues. There is a rich theory of such quadratic operator pencils, which can be reduced to nsa linear eigenvalue problems for systems [46, 64].

7. Perturbation methods

One may sometimes obtain bounds on the location of the spectrum of an nsa operator by considering it as a perturbation of a self-adjoint operator. In this section we describe an example of this type. We develop the ideas in one space dimension, although partial analogues in higher dimensions exist [3, 49]. Let

$$Hf(x) = -f''(x) + V(x)f(x),$$

where V is a potential that is sufficiently regular locally, and vanishes at infinity in a suitable sense. Under such conditions, one may show that $(zI-H)^{-1}-(zI-H_0)^{-1}$ is compact, where H_0 is the operator obtained by setting $V \equiv 0$. The spectrum of H is therefore equal to $[0,\infty)$ together with a finite or countable set of eigenvalues of finite multiplicity, which can only accumulate on $[0,\infty)$. Our goal is to find bounds on the possible locations of such eigenvalues. As well as having intrinsic interest, such an enterprise considerably reduces the task of computing the eigenvalues numerically.

The simplest case to be considered is when $V \in L^1(\mathbb{R})$. One then has the following theorem, where the bound is optimal of its type.

Theorem 9. Every eigenvalue z of H lies within the disc

$$\left\{z \in \mathbb{C} : |z| \leqslant \|V\|_1^2 / 4\right\}. \tag{7}$$

The first problem to be resolved is the proper definition of H. If one makes the stronger assumption that $V \in L^1 \cap L^2$, then V is a relatively compact perturbation of H_0 , and H and H_0 have the same domain. In the general case, H has to be defined as a quadratic form sum, or using the theory of Kato class potentials.

The constant on the right-hand side of (7) is optimal under the conditions stated. However, the theorem does not allow one to treat the simple case $V(x) = -c|x|^{-\alpha}$, where $c \in \mathbb{C}$ and $0 < \alpha < 1$. Starting from the case in which c = 1 and then scaling,

one may show that if $|\arg(c)| < \pi(2-\alpha)/2$, the eigenvalues of this operator are of the form

 $\lambda_n = c^{2/(2-\alpha)} \mu_n,$

where μ_n , n = 1, 2, ..., is an increasing sequence of negative numbers converging to 0

A more sophisticated theory, allowing one to treat slowly decaying potentials, has been developed in [27]. The basic assumption there is that for all $\varepsilon > 0$, one may write V = W + X, where $||X||_{\infty} \le \varepsilon$ and $||W||_1 \le C_{\varepsilon}$. Explicit bounds on the positions of the eigenvalues depend upon the form of the function C_{ε} . Typical of the results in [27] is the following theorem. Qualitatively, it states that the eigenvalues of H are confined to a region around the real axis, which gets narrower as their real part (energy) increases. Even if $V \in L^1$, the theorem may provide much better estimates than Theorem 9 near the origin.

THEOREM 10. If $V \in L^p(\mathbb{R})$ where $1 , and <math>z = -\lambda^2$ is an eigenvalue of H where $\lambda = \lambda_1 + i\lambda_2$, $\lambda_1 > 0$ and $\lambda_2 \in \mathbb{R}$, then $\lambda_1 \leq (k/2)^{q/(q+1)}$ and

$$|\lambda_2| \leqslant \sqrt{k^2 \lambda_1^{-2/q} / 4 - \lambda_1^2},$$

where $k = ||V||_p (2/q)^{1/q}$ and 1/p + 1/q = 1.

Even if V is smooth and rapidly decaying, the condition numbers of the eigenvalues of H may be very large. In a series of papers, Aslanyan and the author have studied examples that arise by applying the complex scaling technique to determine the resonances of certain self-adjoint Schrödinger operators that have high barriers delaying the escape of an initially trapped state. Sophisticated techniques are needed to evaluate the highly oscillatory integrals that arise in the computations [3, 6, 7]. We do not pursue this here, since the theory of resonances would need a separate review, and is in a very incomplete state.

It might be expected, on the basis of the self-adjoint case, that the number of eigenvalues of such nsa Schrödinger operators would be finite under moderate decay rate conditions. The actual situation is rather surprising; see [52, 53, 54].

THEOREM 11. Suppose that

$$|V(x)| \leqslant c_1 \exp[-c_2|x|^{\alpha}] \tag{8}$$

for all $x \in \mathbb{R}$ and some positive c_1 , c_2 . Then if $\alpha = 1/2$, the operator H has only a finite number of eigenvalues. On the other hand, for any α satisfying $0 < \alpha < 1/2$, there exists a potential V satisfying (8) for which it has an infinite number of eigenvalues, converging to some point in $(0, \infty)$.

The case $\alpha = 1$ is much easier, and is due to Naimark.

8. The numerical range

We consider spectral bounds of an operator $H = -\Delta + V$, acting in $L^2(\mathbb{R}^n)$, which are obtained by using the numerical range. We assume that |V| is relatively compact with respect to $-\Delta$ in the sense of quadratic forms, and we define H to be the quadratic form sum of $-\Delta$ and V; necessary and sufficient conditions on V for this

to hold may be found in [47]. H then has the form domain $Quad(H) = W^{1,2}(\mathbb{R}^n)$ and the associated sectorial form

$$Q(f) = \int_{\mathbb{R}^n} \left(|\nabla f|^2 + V|f^2| \right) \, \mathrm{d}x.$$

The numerical range Num(H) of H is a convex set contained in a sector of the complex plane and containing the spectrum of H, which consists of \mathbb{R}^+ together with a discrete set of eigenvalues of finite multiplicity whose only limit points lie in \mathbb{R}^+ .

Bounds on Num(H) yield bounds on Spec(H) that have the advantage that they utilize information about the phase of V rather than just of its absolute value. The results to be described are sometimes better and sometimes worse than those of the last section.

The standard method of computing the numerical range of matrices may also be used for the differential operator H. For each angle θ such that $-\pi/2 < \theta < \pi/2$, one considers the self-adjoint operator

$$H_{\theta} = \operatorname{Re}(e^{-i\theta}H) = -\cos(\theta)\Delta + V_{\theta},$$

where $V_{\theta} = \text{Re}(e^{-i\theta}V)$. Let λ_{θ} denote the bottom of the spectrum of H_{θ} , and let v_{θ} denote the associated normalized eigenvector in the case where λ_{θ} is an eigenvalue. One may compute λ_{θ} numerically by variational methods, but there are also highly developed methods of obtaining general bounds on the value of λ_{θ} .

LEMMA 12. The numerical range of H is contained within each of the half planes $\{(x,y):x\cos(\theta)+y\sin(\theta)\geq\lambda_{\theta}\}$. If λ_{θ} is an eigenvalue of H_{θ} , then $\langle Hv_{\theta},v_{\theta}\rangle$ lies on the edge of the associated half-plane, and also in the numerical range. If λ_{θ} is an eigenvalue for all θ such that $-\pi/2 < \theta < \pi/2$, then the curve $\theta \to \langle Hv_{\theta},v_{\theta}\rangle$ is the boundary of the numerical range.

Important further information about the location of the eigenvalues of H can be obtained if V satisfies a standard dilation analyticity condition. Following [3], we assume that the potential V_z is an analytic function of z with continuous boundary values on the domain $D = \{z \in \mathbb{C} : 0 \le \arg(z) \le \alpha\}$ for some $\alpha > 0$, and that V_z is relatively compact with respect to $-\Delta$ in the sense of quadratic forms for all relevant z. We also suppose that $V_z(x) = V(zx)$ for all z > 0 and $x \in \mathbb{R}^n$. The following theorem is classical, and is due to Aguilar, Balsev, Combes, Simon and others.

THEOREM 13. If one puts

$$H_{\theta}f(x) = -e^{-2i\theta}\Delta f(x) + V_{e^{i\theta}}(x)f(x)$$

for all θ such that $0 \le \theta \le \alpha$, then the spectrum of H_{θ} consists of $e^{-2i\theta}\mathbb{R}^+$ together with eigenvalues whose only limit points lie in this set. The eigenvalues λ that satisfy $0 < \arg(\lambda) < 2\pi - 2\alpha$ are independent of θ for $0 \le \theta \le \alpha$. Hence any such eigenvalue λ of H satisfies

$$\lambda \in \bigcap_{0 \le \theta \le \alpha} \operatorname{Num}(H_{\theta}).$$

The above theorem often enables one to conclude that H has no eigenvalues with large real parts. How much one can say depends upon the particular potential V, but the following corollary is representative.

COROLLARY 14. If $|V_z(x)| \le c$ for all $x \in \mathbb{R}^n$ and all $z \in D$, then every eigenvalue λ of H such that $\operatorname{Im}(\lambda) > 0$ satisfies $-c \le \operatorname{Re}(\lambda) \le c/\sin(2\alpha)$ and $0 < \operatorname{Im}(\lambda) \le c$. The only possible limit point of such eigenvalues is 0.

The proof depends upon the fact that the numerical range of H_{α} is contained in the set $\left\{z: \operatorname{dist}(z, \mathrm{e}^{-2i\alpha} \mathbb{R}^+) \leqslant c\right\}.$

9. ODE systems

If A is an operator on a Hilbert space \mathcal{H} , and Num(A) is contained in the left-hand half plane \mathbb{C}_{-} (that is, A is dissipative), and if any one z satisfying Re(z) > 0 lies in the resolvent set of A, then every such z lies in the resolvent set and Spec(A) $\subseteq \mathbb{C}_{-}$; see [17]. From the theory of strongly continuous one-parameter semigroups, one then concludes that

$$\|\mathbf{e}^{At}\| \leqslant 1$$

for all $t \ge 0$. In such a situation, one says that the evolution associated with A is stable.

Unfortunately, the fact that the spectrum of A lies in \mathbb{C}_- is not sufficient for stability. Indeed it is quite possible for A to have its spectrum in \mathbb{C}_- but for $\|\mathbf{e}^{At}\|$ to increase exponentially fast as $t \to \infty$. This phenomenon has been known at an abstract level for a long time, but examples involving naturally arising differential operators are more recent.

Another surprising fact is that quite simple differential operators with discrete spectrum and compact resolvents may have a numerical range equal to \mathbb{C} . This section is devoted to a discussion of ODE systems—that is, differential operators acting on the space of L^2 functions $f: [\alpha, \beta] \to \mathbb{C}^n$, where $2 \le n < \infty$. Such operators arise in a variety of contexts, for example statistical dynamics of hot fluids [72], and have properties that are quite different from those of scalar-valued ODEs.

The following example has been analyzed in detail by Boulton [12, 14].

EXAMPLE 15. Let H act in $L^2((\alpha, \beta), \mathbb{C}^2)$ according to the formula

$$Hf(x) = Af''(x),$$

where f is a twice differentiable function with two components ϕ and ψ , and A is a constant, invertible 2×2 matrix. One imposes Dirichlet boundary conditions on ϕ , and Neumann boundary conditions on ψ .

The operator H has discrete spectrum, and Boulton gives a complete classification of the surprisingly complicated way in which the spectrum depends upon the choice of A. We cannot reproduce his results here, but mention that even if A is a real matrix, one has to break the analysis down into five independent cases. Among the possibilities is that H may have only real eigenvalues, but may not be similar to a self-adjoint operator [12, 14]. There is no obvious relationship between the spectrum of A and that of H in general.

Following on from the above, the author has investigated a family of nsa elliptic systems of first order on a finite interval $[\alpha, \beta]$. These are of the form

$$Hf(x) = A(x)f'(x),$$

where $f : [\alpha, \beta] \to \mathbb{C}^n$, A(x) are invertible $n \times n$ matrices for each x, and one imposes a general boundary condition of the form $Sf(\alpha) + Tf(\beta) = 0$. Certain n-component second-order systems are also considered in [26]. If A(x) is piecewise constant, it is possible to give a detailed spectral analysis of the operators concerned. While this condition is highly restrictive, almost all of the properties discovered have no self-adjoint analogues: for example, the leading term of the spectral asymptotics depends on the boundary conditions, and is usually not given by Weyl's formula [26].

Theorem 16. Under certain conditions on the piecewise constant coefficients A(x), and on the boundary conditions at α and β , the eigenvalues λ_n of H are precisely the zeros of an analytic function of the form

$$F(z) = \sum_{r=1}^{R} \delta_r e^{z\overline{\gamma_r}}.$$

Generically, the number N(E) of eigenvalues such that $|\lambda_n| \leq E$ is of the form

$$N(E) = b(K)E/2\pi + O(1)$$

as $E \to \infty$, where b(K) is the length of the boundary of the polygon

$$K = \overline{\text{conv}}\{\gamma_r : 1 \le r \le R\}.$$

The eigenvalues themselves are asymptotic to certain lines perpendicular to the edges of K.

The above theorem covers only the generic case in which no γ_r lie within the edges of K. If this does happen, then the asymptotic distribution of the eigenvalues depends upon whether the edges are divided into parts whose lengths have rational or irrational ratios [12, 14, 26].

10. Analytic function theory

Many of the nsa spectral problems that have been analyzed to date depend upon determining the zeros of some analytic function. In very special cases, the analytic function may be written down in closed form, but mostly it is computed numerically. One way of determining the zeros of such a function f(z) is to produce either a contour plot of |f(z)|, or plots of both Re(f(z)) and Im(f(z)) on the same diagram. Alternatively, one may use Rouche's theorem to count the number of zeros inside a square contour, and then steadily subdivide the region enclosed by the contour until the zeros are determined. An advantage of this method is that one need not compute the integrals accurately, because one knows beforehand that they must take integral values [1].

The numerical implementation of these ideas for ordinary differential operators or systems may be far from straightforward. In principle, one needs only to compute a transfer function and then insert the relevant boundary conditions, but this may not be numerically feasible. Modifications to the scheme have been developed and implemented in code; see [1, 2, 6, 62].

There is one serious problem associated with this method. If f(z) is a meromorphic function and we put

$$g(z) = f(z)\frac{z - a}{z - b},$$

where a and b are very close to each other, then f(z) and g(z) are almost equal except when z is very close to a and b. It may not be possible to distinguish between the two functions numerically, and one may therefore miss some of the eigenvalues of the operator. One might hope that such problems would not occur, but they are very common when one has eigenvalues that are highly unstable. Indeed, several routine methods of computing complex eigenvalues collapse for exactly this reason when confronted with highly unstable eigenvalues. We do not see how to avoid such problems without devising quite different methods of approach.

It is not obvious how to apply analytic function theory methods in higher dimensions. We have, however, been able to use them to find resonances for deformed cylinders, by rewriting the problem as a one-dimensional *system*, for which a transfer function can be computed. Another possibility is to study the relative determinant or scattering matrix of the operator with respect to some other, better understood, operator [40, 48]. Most of the progress that has been made on the asymptotics of resonances depends ultimately on theorems about the distributions of zeros of analytic functions [69, 70].

11. Random nsa Schrödinger operators

In this section we mention a closely related problem, for which only the discretized version has so far been studied in detail. This is the theory of random nsa Schrödinger operators in one dimension. The operators concerned are of the form

$$Hf(n) = e^{\gamma} f(n+1) + e^{-\gamma} f(n-1) + V(n)f(n),$$

where V is a random, real-valued, bounded potential. If $\gamma = 0$, the operator is self-adjoint, and is known as the Anderson model; the two- and three-dimensional versions of this model are of great importance to the properties of materials. The nsa problem has only recently been studied by physicists [38, 39, 51, 30], and some of their very interesting numerical results have now been proved, principally by Goldsheid and Khoruzhenko [34, 35].

The standard approach to this problem is to start on a finite interval $\{-n,n\}$, and to examine the almost sure limit of the spectrum as n increases. Goldsheid and Khoruzhenko proved that the spectrum converges almost surely to a set of curves whose topological structure depends upon the values of the parameters defining the potential. It turns out that this is quite different from what one gets by analyzing the spectrum of the operator on $l^2(\mathbb{Z})$ directly, in which case the spectrum is the union of certain quite complicated regions in the complex plane [24, 25]. Once again, the spectrum depends discontinuously on n as $n \to \infty$. The spectrum of the operator on $l^2(\mathbb{Z})$ does not depend nearly so heavily on the probability law used to generate the potential. Which of the two types of spectrum one gets depends upon whether extremely rare large deviations of the potential from its typical form should be allowed to affect it or not. If one works on $l^2(\mathbb{Z})$ directly, then their effect is dominant, but if one first computes the spectrum for finite n and then lets $n \to \infty$, the effect of such fluctuations is eliminated almost surely. If one considers the pseudospectrum instead of the spectrum, then the limit as $n \to \infty$ should be continuous. These issues have been explored in detail for an exactly soluble model by Trefethen, Contedini and Embree [76]. This field is developing very rapidly, as may be seen from the forthcoming papers [11] and [36].

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