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PSEUDOSPECTRA OF THE CONVECTION-DIFFUSION OPERATOR*

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Abstract. The spectrum of the simplest 1D convection-diffusion operator is a discrete subset of the negative real axis, but the pseudospectra are regions in the complex plane bounded approximately by parabolas. Put another way, the norm of the resolvent is exponentially large as a function of the Péclet number throughout a certain approximately parabolic region. These observations have a simple physical basis, and suggest that conventional spectral analysis for convection-diffusion operators may be of limited value in some applications.

Key words. convection-diffusion operator, Péclet number, pseudospectra

AMS subject classifications. 35J25, 35P10, 47A10, 76R99

1. Introduction.

Figure 1 illustrates the phenomenon that is the subject of this paper. Let $\mathcal{L}$ denote the convection-diffusion operator[1]

$$\mathcal{L}u = u'' + u', \qquad u(0) = u(d) = 0, \tag{1.1}$$

acting in the Hilbert space $L^2[0,d]$.[2] For $d = 40$, the solid dots in the figure show the first 27 eigenvalues of $\mathcal{L}$, a set of numbers on the negative real axis. These eigenvalues are the points $\lambda \in \mathbf{C}$ where the resolvent of $\mathcal{L}$, $(\lambda I - \mathcal{L})^{-1}$, has a pole, which we may write as $\|(\lambda I - \mathcal{L})^{-1}\| = \infty$. This much is standard, but now consider the behavior of $\|(\lambda I - \mathcal{L})^{-1}\|$ at other points λ. Counting from the outside in, the figure plots the following contour lines in the complex λ-plane:

$$\|(\lambda I - \mathcal{L})^{-1}\| = 10^1,\ 10^2,\ 10^3, \ldots, 10^7$$

(§6 explains how these curves were computed). Outside the shaded region Π bounded by the dashed "critical parabola," $\|(\lambda I - \mathcal{L})^{-1}\|$ is small. Inside that region, however, it is huge, attaining values as great as 10^7 at points λ that are far from the eigenvalues. In fact, for any λ in the interior of the shaded region, $\|(\lambda I - \mathcal{L})^{-1}\|$ grows exponentially as $d \to \infty$.

It is common practice in applied mathematics to analyze an operator by investigating its spectrum. However, Fig. 1 shows that in the case of convection-diffusion

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[1] Convection-diffusion operators are often written with explicit convection and diffusion parameters, $\mathcal{N}U = \nu\partial^2 U/\partial\xi^2 + c\partial U/\partial\xi$, $U(0) = U(\delta) = 0$. The substitutions $x = c\xi/\nu$, $\mathcal{L} = \nu\mathcal{N}/c^2$, $d = \delta c/\nu$ reduce this problem to (1.1), and thus the results of this paper carry over to the more general case if d is replaced by the *Péclet number* dc/ν. For details see [31].

[2] To be precise, the domain of $\mathcal{L}$ is the subset of $L^2[0,d]$ of continuous functions on $[0,d]$ which satisfy the boundary conditions and possess a second derivative in $L^2[0,d]$. Similar remarks apply to the operators $\mathcal{L}^{[0,\infty)}$ and $\mathcal{L}^{(-\infty,\infty)}$ considered in §3.

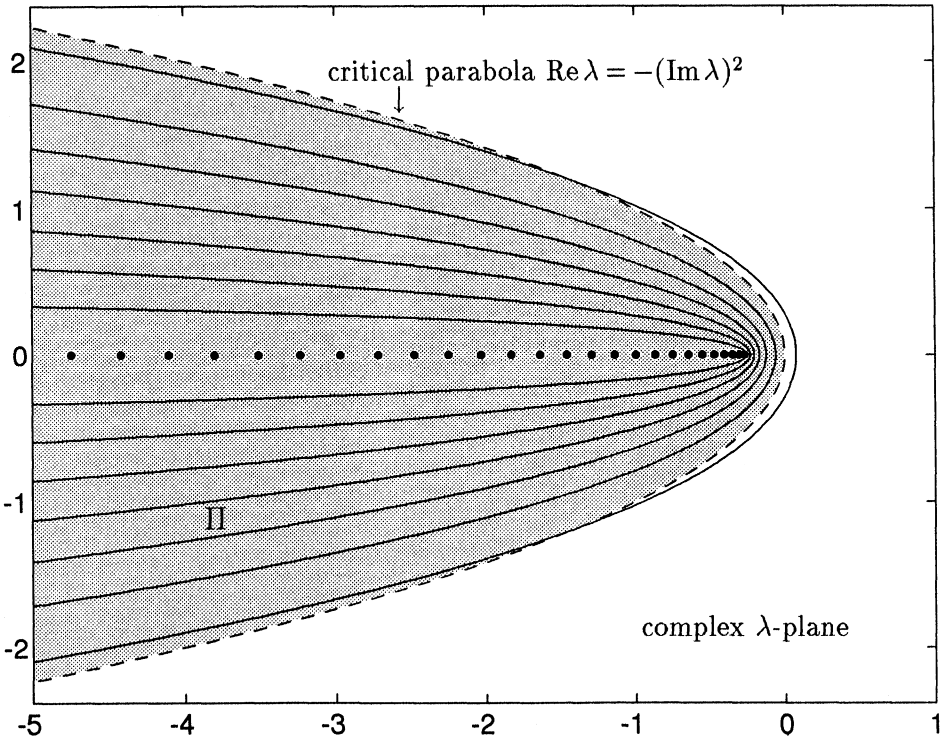

FIG. 1. *Contour plot of the resolvent norm surface* $\|(\lambda I - \mathcal{L})^{-1}\|$ *in the complex* λ*-plane* ($d = 40$). *The contours represent levels* $10^1, 10^2, \ldots, 10^7$, *and the dots are the eigenvalues. At each point* λ *in the interior of the region* Π *(shaded),* $\|(\lambda I - \mathcal{L})^{-1}\|$ *grows exponentially as* $d \to \infty$. *Equivalently, the figure can be interpreted as a depiction of* ϵ*-pseudospectra of* $\mathcal{L}$ *for* $\epsilon = 10^{-1}, 10^{-2}, \ldots, 10^{-7}$.

operators, there may be a great deal of structure in the surface $\|(\lambda I - \mathcal{L})^{-1}\|$ that is not revealed by the points where its height is infinite. This is a reflection of the fact that these operators are *nonnormal.* This means that they cannot be unitarily diagonalized, or to put it another way, their eigenfunctions are not orthogonal. For the convection-diffusion problem, the degree of nonnormality grows exponentially with d. It follows that any attempt to make quantitative estimates of the behavior of $\mathcal{L}$ by means of its eigenfunctions or eigenvalues is likely to lead to exponentially large constants. Such estimates are of little use when d is large, and have no content at all that is uniformly valid as $d \to \infty$.

This paper is devoted to an alternative analysis of convection-diffusion operators: the investigation of their *pseudospectra,* which are robust with respect to the limit $d \to \infty$. Here is the definition.

DEFINITION. *Let* $\mathcal{L}$ *be a closed linear operator in a Hilbert space* $\mathcal{H}$ *and let* $\epsilon \geq 0$ *be arbitrary. The* ϵ**-pseudospectrum** $\Lambda_\epsilon(\mathcal{L})$ *is the set of all* $\lambda \in \mathbf{C}$ *such that*

(i) $\|(\lambda I - \mathcal{L})^{-1}\| \geq \epsilon^{-1}$,

or equivalently,

(ii) *For any* $\epsilon' > \epsilon$, λ *belongs to the spectrum of* $\mathcal{L} + \mathcal{E}$ *for some bounded operator* $\mathcal{E}$ *in* $\mathcal{H}$ *with* $\|\mathcal{E}\| \leq \epsilon'$.

By convention we write $\|(\lambda I - \mathcal{L})^{-1}\| = \infty$ if $(\lambda I - \mathcal{L})^{-1}$ is unbounded or nonexistent, i.e., if λ is in the spectrum $\Lambda(\mathcal{L})$. An equivalent formulation of (ii) is to consider $\|\mathcal{E}\| \leq \epsilon$ and then take the closure of the resulting set.

In words: the pseudospectrum is the set of all points where the resolvent norm is large, or equivalently, which are spectral values of a slightly perturbed operator. Thus Fig. 1 depicts the boundaries of $\Lambda_{10^{-1}}(\mathcal{L}), \Lambda_{10^{-2}}(\mathcal{L}), \ldots, \Lambda_{10^{-7}}(\mathcal{L})$, illustrating that these sets are bounded approximately by parabolas. If $\mathcal{L}$ were normal, then for each ϵ, $\Lambda_\epsilon(\mathcal{L})$ would be just the union of the closed ϵ-balls about the eigenvalues.

The analysis of linear operators by means of the resolvent and its norm is an old technique [20], [22], [27]. The specific idea of considering the sets that we call pseudospectra was perhaps first introduced by H. J. Landau in 1975 [23], and has been subsequently employed by others including Varah [38], Demmel [6], and especially Godunov, Kostin, Malyshev, and their colleagues in Novosibirsk [13]. We and our coauthors have applied pseudospectra to problems in numerical linear algebra [12], [26], [34], the numerical solution of differential equations [8], [19], [30], and fluid dynamics [29], [37]. For introductions to these ideas, see [28], [32], [35], [36].

The results of this paper can be summarized as follows. Though the spectrum of $\mathcal{L}$ is a subset of the negative real axis, its pseudospectra are large regions in the left half-plane bounded approximately by parabolas. Any point λ at a distance $\operatorname{dist}(\lambda, \Pi)$ outside the critical parabola lies outside all of the pseudospectra $\Lambda_\epsilon(\mathcal{L})$ with $\epsilon < \operatorname{dist}(\lambda, \Pi)$, independently of d; equivalently, $\|(\lambda I-\mathcal{L})^{-1}\| \le 1/\operatorname{dist}(\lambda,\Pi)$ (Theorem 4). Any point λ inside the parabola is an ϵ-pseudo-eigenvalue for a value of ϵ that decreases exponentially as a function of d; equivalently, $\|(\lambda I-\mathcal{L})^{-1}\|$ grows exponentially as $d \to \infty$ (Theorem 5). Overall, although $\Lambda(\mathcal{L}) \not\to \Lambda(\mathcal{L}^{[0,\infty)})$ as $d \to \infty$, $\Lambda_\epsilon(\mathcal{L}) \to \Lambda_\epsilon(\mathcal{L}^{[0,\infty)})$ as $d \to \infty$ for every $\epsilon > 0$ (Theorem 6). Finally, the condition number of the basis of eigenfunctions of $\mathcal{L}$ grows exponentially as $d \to \infty$ (see (5.2)). Pseudospectra of finite-difference and spectral discretizations of the convection-diffusion operator are considered in §6, and §7 discusses some applications.

Convection-diffusion operators have a long history in applied mathematics. They are the canonical examples of non-self-adjoint operators, or after discretization, of nonsymmetric matrices. For $d \to \infty$, (1.1) becomes the simplest example of a singular perturbation problem, with a solution involving a boundary layer at $x = 0$. Such problems pose a natural challenge to analytical and numerical methods. Finite difference and finite element strategies for solving them, proposed as early as 1955, have been continuously refined since then [1]–[3], [5], [7], [39]. In recent years convection-diffusion equations have also assumed a new role in numerical analysis, emerging as favorite test problems for nonsymmetric iterative linear solvers and preconditioners [10], [11], [12], [15]. Our results imply that in any of these applications, when convection is dominant, predictions based on the exact spectrum are likely to be misleading, and numerical methods based on the exact spectrum are likely to be suboptimal.

2. Eigenfunctions and pseudo-eigenfunctions. If we ignore for the moment the matter of boundary conditions, the operator $\mathcal{L}$ multiplies the function $e^{\alpha x}$ by the factor $\lambda = \alpha^2 + \alpha$. Conversely, for each $\lambda \in \mathbf{C}$, there are two functions $e^{\alpha x}$ that $\mathcal{L}$ multiplies by λ, namely those given by the roots[3]

$$\alpha_\pm = -\tfrac{1}{2} \pm \tfrac{1}{2}\sqrt{1+4\lambda}\,. \tag{2.1}$$

For any λ and corresponding α_+ and α_-, the function

$$\phi(x) = \frac{e^{\alpha_+ x} - e^{\alpha_- x}}{\alpha_+ - \alpha_-} \tag{2.2}$$

[3] In the confluent case $\alpha_\pm = -\frac{1}{2}$, the second function becomes $xe^{-x/2}$. All of our results carry over continuously to this confluent point, so in the remainder of this paper, for simplicity, we shall ignore this case and speak as if α_+ and α_- are always distinct.

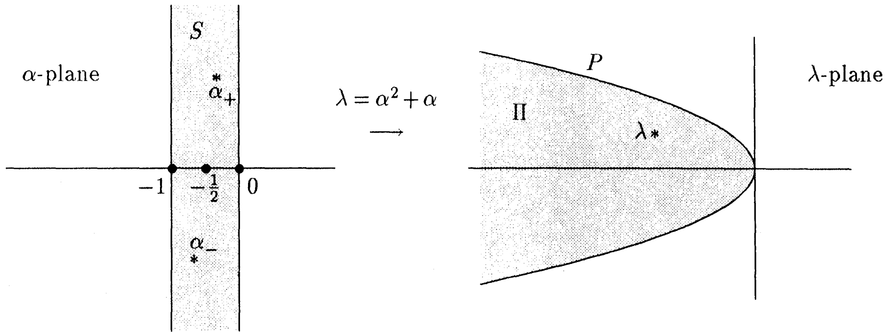

FIG. 2. *The algebra of the critical parabola. The value λ belongs to Π if and only if both of the corresponding values $\alpha_\pm$ lie in the left half-plane, or equivalently, if and only if either one lies in the strip S.*

satisfies the condition for an eigenfunction with eigenvalue λ in the interior of $[0, d]$ and the boundary condition at $x = 0$. It satisfies the boundary condition at $x = d$ too provided $e^{\alpha_+ d} = e^{\alpha_- d}$, that is, $(\alpha_+ - \alpha_-)d = 2\pi i n$ for some nonzero $n \in \mathbf{Z}$. By (2.1), this amounts to the condition $d\sqrt{1+4\lambda} = 2\pi i n$, and upon squaring we obtain the following eigenvalues.

THEOREM 1. *The spectrum of $\mathcal{L}$ is $\Lambda(\mathcal{L}) = \cup_{n>0}\{\lambda_n\}$, with*

$$\lambda_n = -\frac{1}{4} - \frac{\pi^2 n^2}{d^2}, \quad n = 1, 2, 3, \ldots. \tag{2.3}$$

Thus $\Lambda(\mathcal{L})$ is a discrete set of negative real numbers in the interval $(-\infty, -\frac{1}{4})$.[4] By (2.1), the eigenfunctions (2.2) can be written (after rescaling by a constant)

$$u_n(x) = e^{-x/2}\sin(\pi n x/d), \qquad n = 1, 2, 3, \ldots. \tag{2.4}$$

If $\mathcal{L}$ were purely a diffusion operator, the term $-\frac{1}{2}$ would be absent from (2.1), α_+ and α_- would be negatives of each other, and for every λ, one of $e^{\alpha_+ x}$ and $e^{\alpha_- x}$ would be decreasing as a function of x and the other would be increasing. For our problem, however, there are choices of λ for which both α_+ and α_- lie in the left half-plane and thus both $e^{\alpha_+ x}$ and $e^{\alpha_- x}$ are decreasing functions. For the eigenfunctions (2.4), this occurs with $\operatorname{Re}\alpha_+ = \operatorname{Re}\alpha_- = -\frac{1}{2}$. More generally, it occurs if and only if α belongs to the strip $S = \{\alpha \in \mathbf{C} : \; -1 \le \operatorname{Re}\alpha \le 0\}$, since if α is one solution of (2.1), the other is $-1-\alpha$. The corresponding region in the λ-plane is the image of S under the function $\lambda = \alpha + \alpha^2$, which we denote by Π:

$$\Pi = \{\lambda \in \mathbf{C} : \; \lambda = \alpha^2 + \alpha, \; -1 \le \operatorname{Re}\alpha \le 0\}. \tag{2.5}$$

The "critical parabola" that bounds Π is the image of the boundary of S under the same function, which we can represent simply by

$$P = \{\lambda \in \mathbf{C} : \; \lambda = \alpha^2 + \alpha, \; \operatorname{Re}\alpha = 0\} \tag{2.6}$$

[4]The calculation above does not prove Theorem 1 completely, but by more careful reasoning it can be shown that each number λ_n is a simple eigenvalue of $\mathcal{L}$ and that there are no other points in the spectrum.

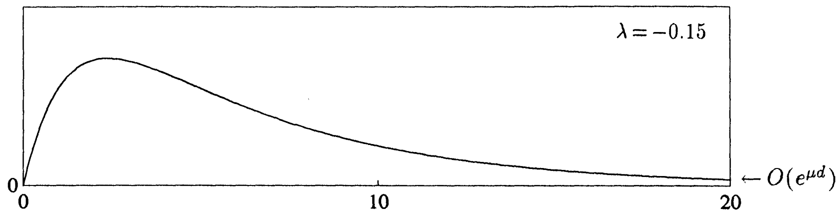

FIG. 3. *For any λ in the interior of Π, the function $\phi(x) = (e^{\alpha_+ x} - e^{\alpha_- x})/(\alpha_+ - \alpha_-)$ satisfies the eigenvalue condition and the boundary condition at $x = 0$, and it satisfies the boundary condition at $x = d$ up to an error that decreases exponentially with d. Thus $\phi(x)$ behaves nearly like an eigenfunction.*

since $\operatorname{Re}\alpha = -1$ maps onto the same parabola as $\operatorname{Re}\alpha = 0$. See Fig. 2.

Suppose now that λ is any complex number in the interior of Π, so that $\operatorname{Re}\alpha_+ < 0$ and $\operatorname{Re}\alpha_- < 0$. Then $\phi(x)$ decreases exponentially with x, so if d is reasonably large, the boundary condition $u(d) = 0$ is *nearly* satisfied, with an error of order $e^{\mu d}$, where $\mu = \max\{\operatorname{Re}\alpha_+, \operatorname{Re}\alpha_-\} = -\frac{1}{2} + \left|\operatorname{Re}\alpha_\pm + \frac{1}{2}\right|$ (Fig. 3). Thus $\phi(x)$ is "nearly an eigenfunction" of $\mathcal{L}$, though λ may be far from any of the exact eigenvalues.

3. The limiting case $d = \infty$. In the course of estimating the pseudospectra of $\mathcal{L}$, we shall make use of the analogous operators defined on the intervals $[0, \infty)$ and $(-\infty, \infty)$. Intuitively speaking, the boundary conditions become $u(0) = u(\infty) = 0$ and $u(-\infty) = u(\infty) = 0$, respectively. Since we are working in L^2 spaces, however, the boundary conditions at $\pm\infty$ need not be imposed explicitly. Thus the two operators in question are $\mathcal{L}^{[0,\infty)}$, acting in $L^2[0, \infty)$ with boundary condition $u(0) = 0$, and $\mathcal{L}^{(-\infty,\infty)}$, acting in $L^2(-\infty, \infty)$ with no boundary conditions.

$\mathcal{L}^{(-\infty,\infty)}$ is normal, and its spectrum and pseudospectra are easily determined. In the following theorem Δ_ϵ denotes the closed disk $\{\lambda \in \mathbf{C} : \ |\lambda| \le \epsilon\}$ and the sum of two sets A, $B \subseteq \mathbf{C}$ has the usual meaning: $A + B = \{\lambda \in \mathbf{C} : \ \lambda = \lambda_a + \lambda_b, \ \lambda_a \in A, \ \lambda_b \in B\}$.

THEOREM 2. *The spectrum of $\mathcal{L}^{(-\infty,\infty)}$ is $\Lambda(\mathcal{L}^{(-\infty,\infty)}) = P$, and for each $\epsilon \ge 0$, the ϵ-pseudospectrum is*

$$\Lambda_\epsilon(\mathcal{L}^{(-\infty,\infty)}) = P + \Delta_\epsilon. \tag{3.1}$$

Equivalently, for $\lambda \notin P$ the resolvent norm satisfies

$$\|(\lambda I - \mathcal{L}^{(-\infty,\infty)})^{-1}\| = \frac{1}{\operatorname{dist}(\lambda, P)}. \tag{3.2}$$

In words, $\Lambda_\epsilon(\mathcal{L}^{(-\infty,\infty)})$ is the parabola P together with a cushion of thickness ϵ. We shall not prove Theorem 2, as such results are standard; see [14] and [28].

On the semi-infinite interval, P is replaced by Π.

THEOREM 3. *The spectrum of $\mathcal{L}^{[0,\infty)}$ is $\Lambda(\mathcal{L}^{[0,\infty)}) = \Pi$, and for each $\epsilon \ge 0$, the ϵ-pseudospectrum is*

$$\Lambda_\epsilon(\mathcal{L}^{[0,\infty)}) = \Pi + \Delta_\epsilon. \tag{3.3}$$

Equivalently, for $\lambda \notin \Pi$ the resolvent norm satisfies

$$\|(\lambda I - \mathcal{L}^{[0,\infty)})^{-1}\| = \frac{1}{\operatorname{dist}(\lambda, \Pi)}. \tag{3.4}$$

Moreover, if $W(\mathcal{L}^{[0,\infty)})$ *denotes the numerical range of* $\mathcal{L}^{[0,\infty)}$*, then*

$$\mathrm{cl}\{W(\mathcal{L}^{[0,\infty)})\} = \Pi. \tag{3.5}$$

The numerical range $W(\mathcal{L}^{[0,\infty)})$ is defined as the set of Rayleigh quotients $(u, \mathcal{L}^{[0,\infty)}u)/(u,u)$ for u in the domain of $\mathcal{L}^{[0,\infty)}$, and $\mathrm{cl}\{\cdot\}$ denotes set closure.

Proof of Theorem 3. For any λ in the interior of Π, the function $\phi(x)$ of (2.2) satisfies both boundary conditions and belongs to $L^2[0,\infty)$. Thus $\phi(x)$ is an eigenfunction of $\mathcal{L}^{[0,\infty)}$ with eigenvalue λ. Since the spectrum is closed and contained in the closure of the numerical range [18, problem 214], this implies $\Pi \subseteq \Lambda(\mathcal{L}^{[0,\infty)}) \subseteq \mathrm{cl}\{W(\mathcal{L}^{[0,\infty)})\}$.

We now establish the converse $W(\mathcal{L}^{[0,\infty)}) \subseteq \Pi$, which implies $\mathrm{cl}\{W(\mathcal{L}^{[0,\infty)})\} = \Lambda(\mathcal{L}^{[0,\infty)}) = \Pi$ and thus completes the proof of (3.5). By standard arguments to be found for example in [20], (3.5) is also equivalent to (3.4), and the equivalence of (3.4) and (3.3) follows from the definition of pseudospectra.

Let u be a function in the domain of $\mathcal{L}^{[0,\infty)}$ normalized by $\|u\| = 1$. By integration by parts we calculate

$$(u, \mathcal{L}^{[0,\infty)}u) = \int_0^\infty \bar{u}(x)(u'' + u')\,dx = -\int_0^\infty |u'(x)|^2 dx + \int_0^\infty \bar{u}(x)u'(x)dx.$$

The first term is real, and another integration by parts shows that the second is imaginary, so by the Cauchy-Schwarz inequality we have $\mathrm{Re}\,(u, \mathcal{L}^{[0,\infty)}u) = -\|u'\|^2$, $|\mathrm{Im}\,(u, \mathcal{L}^{[0,\infty)}u)| \le \|u\|\,\|u'\| = \|u'\|$. Therefore $\mathrm{Re}\,(u, \mathcal{L}^{[0,\infty)}u) \le -|\mathrm{Im}\,(u, \mathcal{L}^{[0,\infty)}u)|^2$, or by (2.6), $(u, \mathcal{L}^{[0,\infty)}u) \subseteq \Pi$. Thus $W(\mathcal{L}^{[0,\infty)}) \subseteq \Pi$, as claimed. □

4. Estimates of the pseudospectra. Our first theorem concerning the pseudospectra of $\mathcal{L}$ asserts that outside the parabolic region Π, the resolvent norm of $\mathcal{L}$ decreases inverse-linearly with constant 1 in the numerator—i.e., the "Kreiss constant" is 1 (cf. [8]).

THEOREM 4. *For each* $\epsilon \ge 0$*, the* ϵ*-pseudospectrum of* $\mathcal{L}$ *satisfies*

$$\Lambda_\epsilon(\mathcal{L}) \subseteq \Pi + \Delta_\epsilon. \tag{4.1}$$

Equivalently, for $\lambda \notin \Pi$ *the resolvent norm satisfies*

$$\|(\lambda I - \mathcal{L})^{-1}\| \le \frac{1}{\mathrm{dist}\,(\lambda, \Pi)}, \tag{4.2}$$

and the numerical range satisfies

$$W(\mathcal{L}) \subseteq \Pi. \tag{4.3}$$

Proof. By changing the upper limit of integration from ∞ to d in the proof of Theorem 3, we obtain (4.3), which implies (4.2) and equivalently (4.1). □

We now turn to the problem of estimating the resolvent norm inside Π. To motivate our estimates, note that the resolvent is the solution operator for the inhomogeneous problem

$$(\lambda I - \mathcal{L})u = f, \qquad u(0) = u(d) = 0 \tag{4.4}$$

for $f \in L^2[0,d]$. For each fixed λ and y, the Green's function $G(x,y)$ for this problem is the solution $u(x)$ corresponding to $f(x) = \delta(x-y)$, which can be written

$$G(x,y) = a\phi(x) + \phi([x-y]_+), \tag{4.5}$$

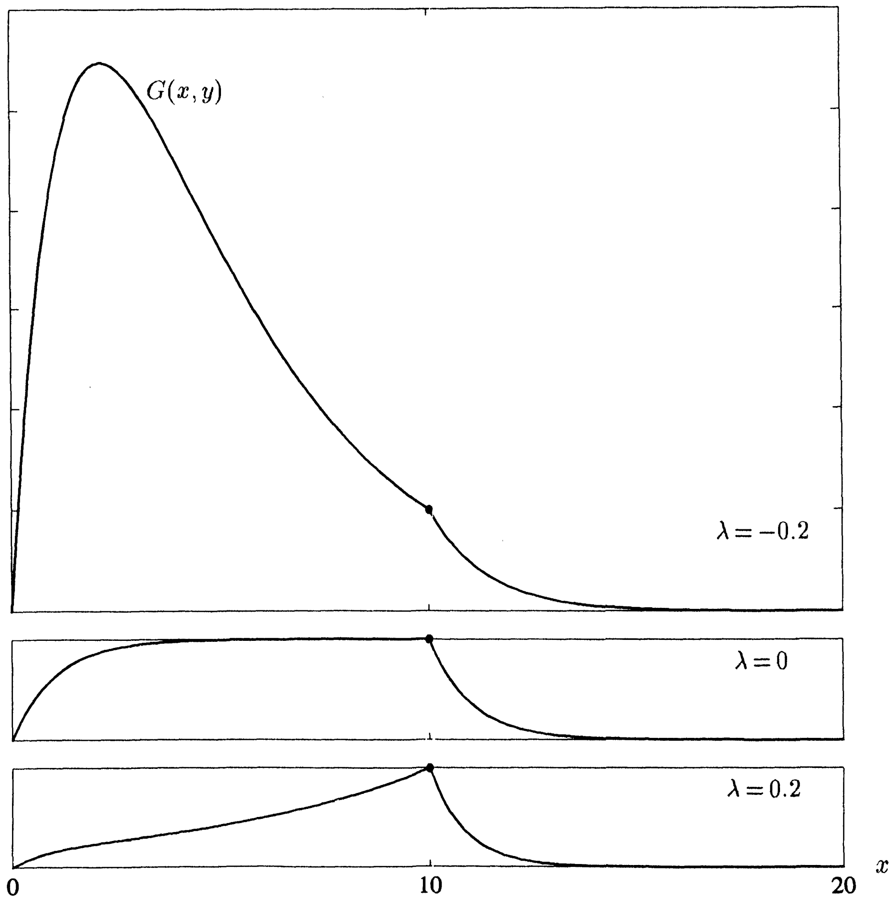

FIG. 4. *Green's functions $G(x,y)$ for three values of λ on the interval $[0,d]$, $d = 20$, $y = 10$, normalized by $G(y,y) = 1$. The value $\lambda = -0.2$ lies in the interior of Π, which explains the exponentially large lobe of $G(x,y)$ for $0 < x < y$ in the first plot.*

where $\phi(x)$ is the function (2.2) illustrated in Fig 3, $[x-y]_+$ denotes 0 for $x - y \le 0$ and $x - y$ for $x - y \ge 0$, and a is a constant. The term $\phi([x-y]_+)$ would be a solution to (4.4) if there were no right-hand boundary condition, and the term $a\phi(x)$ is a correction added to enforce that boundary condition. Figure 4 sketches $G(x,y)$ for $d = 20$, $y = 10$, and three values of λ. The figure reveals that in the case $\lambda = -0.2$, this correction term is exponentially large in $0 < x < y$.

For general functions $f(x)$ in (4.4), we can make an analogous decomposition of $u(x)$ into two terms. Assuming that λ is in the interior of Π, write

$$(\lambda I - \mathcal{L})^{-1} = R_\infty + R_d, \tag{4.6}$$

where R_∞ is the operator on $L^2[0,d]$ defined as follows: extend the data by zero to $L^2(-\infty,\infty)$, apply $(\lambda I - \mathcal{L}^{(-\infty,\infty)})^{-1}$, then restrict the result to $[0,d]$. By construction $\|R_\infty\| \le \|(\lambda I - \mathcal{L}^{(-\infty,\infty)})^{-1}\|$, so by (3.2) we have

$$\|R_\infty\| \le \frac{1}{\mathrm{dist}\,(\lambda, P)}. \tag{4.7}$$

This quantity is small compared with the exponentials of interest, and thus (4.6) and (4.7) effectively reduce the estimation of $\|(\lambda I - \mathcal{L})^{-1}\|$ to the estimation of $\|R_d\|$, which we can carry out with the aid of explicit representations of R_∞ and R_d. First, by integrating the term $\phi([x-y]_+)$ in (4.5) against $f(y)$, we obtain the formula $v(x) = \int_0^x \phi(x-y)f(y)\,dy$ for $v = R_\infty f$, or in particular,

$$v(d) = \int_0^d \phi(d-y)f(y)\,dy. \tag{4.8}$$

Since R_d is designed to enforce the boundary condition $(R_\infty f + R_d f)(d) = 0$, we have the formula $w(x) = -v(d)\,\phi(x)/\phi(d)$ for $w = R_d f$. Combining this with (4.8) gives

$$\|R_d\| \;=\; \sup_f \frac{\|w\|}{\|f\|} \;=\; \frac{\|\phi\|}{|\phi(d)|}\sup_f \frac{|v(d)|}{\|f\|}. \tag{4.9}$$

By the Cauchy–Schwarz inequality applied to (4.8), the second supremum in (4.9) is $\|\phi\|$, attained with $f(y) = \bar{\phi}(d-y)$, and thus we have

$$\|R_d\| = \frac{\|\phi\|^2}{|\phi(d)|}. \tag{4.10}$$

Estimates for $\|(\lambda I - \mathcal{L})^{-1}\|$ can now be obtained by combining (4.7) and (4.10) with the inequality

$$\|R_d\| - \|R_\infty\| \;\le\; \|(\lambda I - \mathcal{L})^{-1}\| \;\le\; \|R_d\| + \|R_\infty\|, \tag{4.11}$$

a consequence of (4.6).

The following theorem presents several estimates of this kind.

THEOREM 5. *Let λ be an arbitrary point in the interior of Π, with $\alpha_\pm$ and $\phi(x)$ defined by* (2.1) *and* (2.2), *and write $\alpha_+ - \alpha_- = \sqrt{1+4\lambda} = \sigma + i\tau$. Then*

$$\|(\lambda I - \mathcal{L})^{-1}\| \sim \frac{\|\phi\|^2}{\phi(d)} \tag{4.12}$$

and

$$\|\phi\|^2 \sim \frac{2}{(1-\sigma^2)(1+\tau^2)} \tag{4.13}$$

as $d \to \infty$. If in addition $\lambda \notin (-\infty, -\frac{1}{4}]$, then $\phi(d) \sim e^{\mu d}/|\alpha_+ - \alpha_-|$ and therefore

$$\|(\lambda I - \mathcal{L})^{-1}\| \sim \frac{2\,e^{-\mu d}\,(\sigma^2+\tau^2)^{1/2}}{(1-\sigma^2)(1+\tau^2)}, \tag{4.14}$$

where $\mu = \max\{\operatorname{Re}\alpha_+, \operatorname{Re}\alpha_-\} < 0$ as in §2.

Proof. By (4.7), $\|R_\infty\|$ is bounded independently of d as $d \to \infty$, whereas it follows from (4.10) that $\|R_d\|$ grows without bound. Therefore (4.12) follows from (4.10) and (4.11). Note that if $\lambda \in (-\infty, -\frac{1}{4})$, the terms on either side of (4.12) oscillate through ∞ between large positive and negative values each time d passes through a zero of $v(d)$ (making λ an eigenvalue of $\mathcal{L}$). Nevertheless, the ratio of the two converges to 1 as $d \to \infty$, as the "$\sim$" requires.

To derive (4.13), we carry out a straightforward computation [31] to find

$$\int_0^d |e^{\alpha_+ x} - e^{\alpha_- x}|^2\,dx \sim \int_0^\infty |e^{\alpha_+ x} - e^{\alpha_- x}|^2\,dx = \frac{2(\sigma^2+\tau^2)}{(1-\sigma^2)(1+\tau^2)}.$$

Since $\phi(x) = (e^{\alpha_+ x} - e^{\alpha_- x})/(\alpha_+ - \alpha_-)$ and $|\alpha_+ - \alpha_-|^2 = \sigma^2 + \tau^2$, this establishes (4.13). From here, the derivation of $\phi(d) \sim e^{\mu d}/|\alpha_+ - \alpha_-|$ and (4.14) is trivial. □

When d is reasonably large, the estimate (4.14) is a very good one. For example, if Fig. 1 is redrawn to plot contours of (4.14) instead of $\|(\lambda I - \mathcal{L})^{-1}\|$, all the curves except the outermost one ($\epsilon = 10^{-1}$) remain unchanged to plotting accuracy.

Theorems 4 and 5 imply that for each $\epsilon > 0$, $\Lambda_\epsilon(\mathcal{L})$ behaves continuously in the limit $d \to \infty$. The following theorem to this effect is analogous to Theorem 3.3 of [32].

THEOREM 6. *For each* $\lambda \in \mathbf{C}$,

$$\|(\lambda I - \mathcal{L})^{-1}\| \;\to\; \|(\lambda I - \mathcal{L}^{[0,\infty)})^{-1}\| \quad \textit{as } d \to \infty. \tag{4.15}$$

Proof. If λ is in the interior of Π, the right-hand side of (4.15) is ∞ by Theorem 3, and by Theorem 5, the left-hand side converges to ∞ as $d \to \infty$. Suppose on the other hand that λ is in the exterior of Π or on the boundary P. The right-hand side of (4.15) is now $1/\text{dist}(\lambda, \Pi)$, and by Theorem 4, the left-hand side is $\le 1/\text{dist}(\lambda, \Pi)$ for all d. To derive a reverse inequality, for any $\delta_1 > 0$ and $\delta_2 > 0$, let λ' be a point in the interior of Π with $|\lambda' - \lambda| < \text{dist}(\lambda, \Pi) + \delta_1$, and take d large enough so that $\|(\lambda' I - \mathcal{L})^{-1}\| > \delta_2^{-1}$. Then it is easily seen that there exists a perturbation $\mathcal{L}'$ with $\|\mathcal{L}' - \mathcal{L}\| < |\lambda' - \lambda| + \delta_2 < \text{dist}(\lambda, \Pi) + \delta_1 + \delta_2$ such that λ is in the spectrum of $\mathcal{L}'$, which implies $\|(\lambda I - \mathcal{L})^{-1}\| > 1/(\text{dist}(\lambda, \Pi) + \delta_1 + \delta_2)$. Taking $\delta_1 \to 0$ and $\delta_2 \to 0$ completes the proof. □

5. Symmetrizability and a further estimate. For each fixed d, the operator $\mathcal{L}$ is *symmetrizable:* similar by a diagonal similarity transformation to a self-adjoint operator with, of course, the same real eigenvalues. This is pointed out in Example III.6.11 of [20][5] and is also suggested by the form of the eigenfunctions (2.4).

To carry out the symmetrization we define $u(x) = e^{-x/2}v(x)$, which implies $u' = e^{-x/2}(-\frac{1}{2}v + v')$, $u'' = e^{-x/2}(\frac{1}{4}v - v' + v'')$, and therefore $\mathcal{L}u = u'' + u' = e^{-x/2}(v'' - \frac{1}{4}v)$. Thus if we define $\mathcal{K}v = v'' - \frac{1}{4}v$, $\mathcal{M}v = e^{-x/2}v$, then we have

$$\mathcal{L} = \mathcal{M}\mathcal{K}\mathcal{M}^{-1}. \tag{5.1}$$

Here $\mathcal{K}$ is a self-adjoint operator and $\mathcal{M}$ is a diagonal operator with $\|\mathcal{M}\| = 1$, $\|\mathcal{M}^{-1}\| = e^{d/2}$, and consequently

$$\kappa(\mathcal{M}) = \|\mathcal{M}\|\,\|\mathcal{M}^{-1}\| = e^{d/2}. \tag{5.2}$$

The notation $\kappa(\mathcal{M})$ comes from numerical analysis, where $\|\mathcal{M}\|\|\mathcal{M}^{-1}\|$ is interpreted as a condition number. On the face of it $\kappa(M)$ is just the condition number of the symmetrizing transformation M, but a little thought shows that it is also equal to the condition number of the basis of eigenfunctions (2.4) if they are normalized to satisfy $\|u_n\| = 1$, for these eigenfunctions are related by the same transformation M to an orthonormal set of eigenfunctions of $\mathcal{K}$, namely the suitably normalized sine functions.

Since $\mathcal{K}$ is self-adjoint, its resolvent norm is

$$\|(\lambda I - \mathcal{K})^{-1}\| = \frac{1}{\text{dist}(\lambda, \Lambda(\mathcal{K}))} = \frac{1}{\text{dist}(\lambda, \Lambda(\mathcal{L}))}.$$

[5] A good deal of information about convection-diffusion operators can be found in [20]. See §III.2.3 and Examples III.5.32, III.6.11, III.6.20, and VIII.1.19.

On the other hand the resolvents of $\mathcal{L}$ and $\mathcal{K}$ are related by

$$(\lambda I - \mathcal{L})^{-1} = (\lambda I - \mathcal{M}\mathcal{K}\mathcal{M}^{-1})^{-1} = \mathcal{M}(\lambda I - \mathcal{K})^{-1}\mathcal{M}^{-1}.$$

Combining these formulas yields the following new bound.

THEOREM 7. *For any $d > 0$ and $\lambda \in \mathbf{C}$,*

$$\|(\lambda I - \mathcal{L})^{-1}\| \;\le\; \frac{e^{d/2}}{\operatorname{dist}(\lambda, \Lambda(\mathcal{L}))} \;\le\; \frac{e^{d/2}}{|\operatorname{Im}\lambda|}. \tag{5.3}$$

It is interesting to compare this result with Theorem 5. That theorem, as well as Fig. 1 and our discussion up to this point, suggested that the pseudospectra of $\mathcal{L}$ are bounded approximately by parabolas. Theorem 7 reveals that although this may be true in a large part of the λ-plane, it cannot be true as $|\lambda| \to \infty$. Instead, for any fixed ϵ and d, $\Lambda_\epsilon(\mathcal{L})$ is contained in a strip of finite (though typically large) width:

$$\Lambda_\epsilon(\mathcal{L}) \;\subseteq\; \{\lambda \in \mathbf{C} : \; |\operatorname{Im}\lambda| \le \epsilon\, e^{d/2}\}. \tag{5.4}$$

With hindsight we can see that this deviation from a parabola was foreshadowed in the presence of the algebraic factors $O(|\lambda|^{-1/2})$ in (4.14), and is visible in Fig. 1.

Because of the equivalence of conditions (i) and (ii) in the definition of pseudospectra, (5.3) can be interpreted as a statement about the sensitivity of $\Lambda(\mathcal{L})$: if $\mathcal{L}$ is perturbed to $\mathcal{L} + \mathcal{E}$, each eigenvalue changes by at most $e^{d/2}\|\mathcal{E}\|$. In numerical analysis this bound is known as the *Bauer–Fike theorem.* To see how close it is to sharp, one can calculate the (absolute) condition number of an individual eigenvalue λ_n, equal to the inverse of the absolute value of the inner product of the corresponding normalized eigenfunctions of $\mathcal{L}$ and its adjoint. This calculation shows that the condition numbers are $\sim e^{d/2}/d$ for fixed d as $n \to \infty$, so (5.4) is sharp up to a factor asymptotic to d.

6. Finite difference and spectral discretizations. Pseudospectra of differential operators can be computed numerically by finite difference, finite element, or spectral methods. In future work we hope to prove convergence of some of these numerical approximations. Here, we shall just present two examples.

The simplest finite-difference discretizations of (1.1) involve 3-point approximations to the first and second derivatives. In practice it may be better to use an irregular grid in the convection-dominated case, but for simplicity, consider the regular grid $x_j = jh$, $h = d/N$, $j = 0, 1, \ldots, N$ for some $N > 1$ and the centered difference approximations $u''(x_j) \approx (v_{j+1} - 2v_j + v_{j-1})/h^2$, $u'(x_j) \approx (v_{j+1} - v_{j-1})/2h$, with $v_j \approx u(x_j)$. With this discretization and our homogeneous boundary conditions, $\mathcal{L}$ is approximated by the tridiagonal Toeplitz matrix $L^{(N)}$ of dimension $N-1$ with entries $L^{(N)}_{jj} = -2h^{-2}$, $L^{(N)}_{j,j\pm1} = h^{-2} \pm (2h)^{-1}$.

Figure 5 plots numerically computed pseudospectra of $L^{(N)}$ for $d = 40$ and $N = 30$. The parameters and contour lines are the same as in Fig. 1, and the reader should compare these figures. Evidently $\Lambda_\epsilon(L^{(N)})$ approximates $\Lambda_\epsilon(\mathcal{L})$ well near the origin of the λ-plane, corresponding to smooth modes that are well resolved by the discretization. For larger λ the approximation deteriorates quickly and it is clear that one would have to take $N \gg 200$ to achieve a good match throughout the region displayed. As it happens, quite a bit is known about the pseudospectra of Toeplitz matrices [32]. In particular, the fact that the pseudospectra $\Lambda_\epsilon(L^{(N)})$ approximate

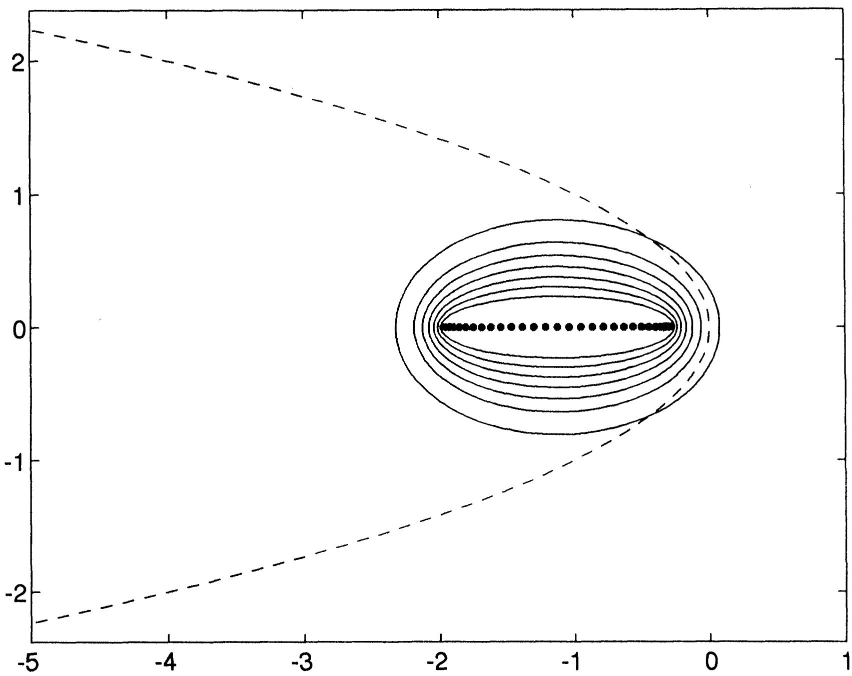

FIG. 5. *A finite-difference approximation to Fig.* 1 *with* $N = 30$.

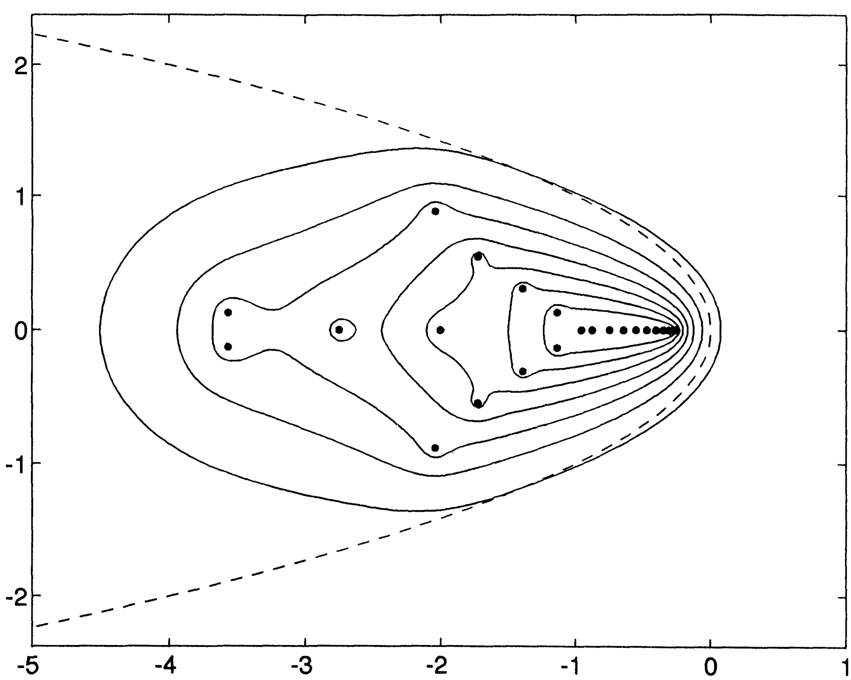

FIG. 6. *A Chebyshev spectral approximation to Fig.* 1 *with* $N = 30$. *Six real eigenvalues lie off-scale to the left of the figure.*

ellipses is related to the fact that the symbol of a tridiagonal Toeplitz matrix maps circles about the origin onto ellipses.

Better approximations to $\Lambda_\epsilon(\mathcal{L})$ can be achieved with spectral methods. In Fig. 6, the same pseudospectra are plotted for the case of a spectral collocation approximation $L_{\rm sp}^{(N)}$ based on the Chebyshev grid $x_j = \frac{1}{2}d(1+\cos(j\pi/N))$, $j=0,1,\ldots,N$. It is obvious at a glance that the approximation $\Lambda_\epsilon(L_{\rm sp}^{(N)}) \approx \Lambda_\epsilon(\mathcal{L})$ is accurate over a larger region of the λ-plane than in the finite-difference case. Indeed it appears to be "spectrally accurate" over a sizable portion of the plane. Note that this effect happens automatically when the differential operator is discretized; in no sense is the discretization an explicit attempt to capture pseudospectra.

The exact spectrum of $L_{\rm sp}^{(N)}$ is complicated, and in fact, there are three real pairs of additional eigenvalues off-scale to the left of Fig. 8, with absolute values approximately 7, 17, and 95. The eigenvalues of spectral discretization matrices are of some importance, for the location of the outlying eigenvalues may determine the allowable step size in discretization of time-dependent problems. A comparison of Fig. 8 with Fig. 1 suggests, however, that the location of the higher eigenvalues in the spectrum is almost an accidental matter, with the essential approximation phenomenon taking place in the pseudospectra. There is a natural reason for this. If a discrete operator approximates a continuous operator to a certain accuracy τ, it is reasonable to expect that the ϵ-pseudospectra with $\epsilon \geq O(\tau)$ may be approximated meaningfully, at least in regions near eigenvalues whose eigenfunctions are well resolved by the grid. There is little reason to expect accurate approximations "below the level of truncation error," i.e., for $\epsilon \ll \tau$ and in particular $\epsilon = 0$.

We can now explain how Fig. 1 was computed. Experiments indicate that for each λ, both $\|(\lambda I - L^{(N)})^{-1}\|$ and $\|(\lambda I - L_{\rm sp}^{(N)})^{-1}\|$ converge to the correct value $\|(\lambda I - \mathcal{L})^{-1}\|$ as $N \to \infty$. To produce Fig. 1 we used spectral discretizations $L_{\rm sp}^{(N)}$ and chose values of N adaptively for each λ until convergence to four relative digits seemed to be achieved. The largest value of N required for the range of λ in Fig. 1 was 72, with a more typical value being 32. See [31] for details.

7. Applications. In this final section we briefly examine applications of the pseudospectra of $\mathcal{L}$, and relatedly, some of the limitations of spectral analysis for convection-diffusion problems.

One application of spectral analysis is to simplify a problem by expressing it in the basis of eigenmodes, where the equation becomes diagonal. The limitation of this idea for convection-diffusion problems is apparent from (5.2): the basis of eigenmodes is exponentially ill-conditioned. If a function of norm $O(1)$ is expanded in this basis, then as a rule the expansion coefficients will be of order $e^{d/2}$, and the time evolution will be largely determined by the evolving patterns of cancellation among these coefficients. This is an indication that the eigenfunction basis is a poor one. It may be simpler and more natural to work with a basis chosen for its approximation properties, unrelated to eigenmodes. If $e^{d/2}$ is greater than the inverse of machine precision on the computer, one will be forced to do so, or else the computation will fail because of rounding errors.

Another application of spectral analysis is the estimation of norms of evolution processes. Suppose one wishes to study energy growth or decay for the time-dependent linear problem

$$u_t = \mathcal{L}u, \qquad u(0) = u_0. \tag{7.1}$$

The solution is $u(t) = e^{t\mathcal{L}}u_0$, with norm governed by the quantity $\|e^{t\mathcal{L}}\|$. We naturally expect that $\|e^{t\mathcal{L}}\|$ should be related to the *spectral abscissa* of $\mathcal{L}$, $\alpha(\mathcal{L}) =$

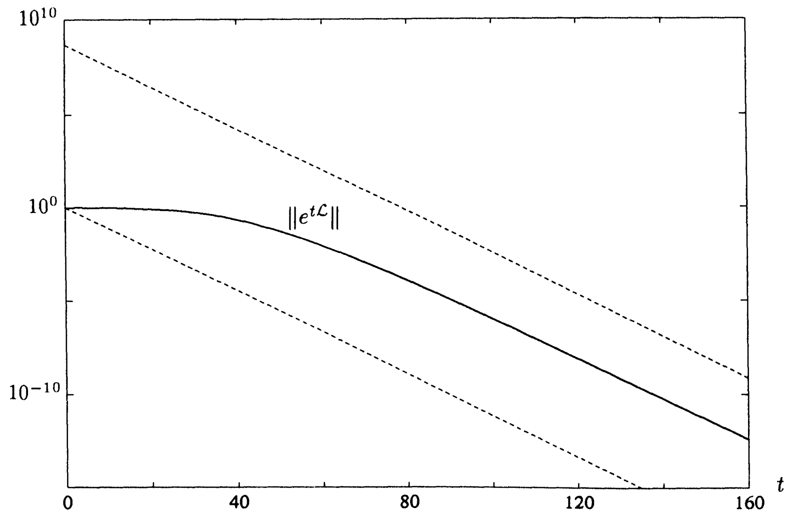

FIG. 7. *Comparison of $\|e^{t\mathcal{L}}\|$ with upper and lower bounds* (7.3) *based on the spectrum. Spectral information is meaningful asymptotically as $t \to \infty$, but fails to capture the transient.*

$\sup_{\lambda\in\Lambda(\mathcal{L})} \operatorname{Re}\lambda$, whose value we know from Theorem 1: $\alpha(\mathcal{L}) = -1/4 - \pi^2/d^2$. However, a precise connection between $\|e^{t\mathcal{L}}\|$ and $\alpha(\mathcal{L})$ again requires the introduction of the exponentially large factor $\kappa(M)$. In general we have

$$e^{t\alpha(\mathcal{L})} \leq \|e^{t\mathcal{L}}\| \leq \kappa(M)e^{t\alpha(\mathcal{L})}, \tag{7.2}$$

hence for the convection-diffusion operator in particular,

$$e^{-t/4-t\pi^2/d^2} \leq \|e^{t\mathcal{L}}\| \leq e^{d/2-t/4-t\pi^2/d^2}. \tag{7.3}$$

Figure 7 plots the three quantities of (7.3) for the case $d = 40$. What we see is a great difference between the transient and the asymptotic behavior of $\|e^{t\mathcal{L}}\|$. In the transient phase, of length $O(d)$, $\|e^{t\mathcal{L}}\|$ is nearly constant. Only after that does the curve bend around to match the slope predicted by the spectrum. Physically, it is easy to see the explanation for this behavior. A broad pulse that begins at the upstream end of the interval may convect downstream with relatively little diffusion for a time period $O(d)$, decaying rapidly only when it nears the downstream end.

This gap between transient and asymptotic behavior can be captured better if one considers the pseudospectra of $\mathcal{L}$ as well as the spectra. One has the following relationships:

(7.4a) $\|e^{t\mathcal{L}}\|$ for $t \to \infty$ $\leftrightarrow$ $\Lambda_\epsilon(\mathcal{L})$ for $\epsilon \to 0$,

(7.4b) $\|e^{t\mathcal{L}}\|$ for $t \to 0$ $\leftrightarrow$ $\Lambda_\epsilon(\mathcal{L})$ for $\epsilon \to \infty$,

(7.4c) $\|e^{t\mathcal{L}}\|$ for finite t $\leftrightarrow$ $\Lambda_\epsilon(\mathcal{L})$ for finite ϵ.

The first of these statements is the association just discussed between the asymptotic behavior of $\|e^{t\mathcal{L}}\|$ as $t \to \infty$ and the spectral abscissa of $\mathcal{L}$. The second can be justified by the equation

$$e^{t\beta(\mathcal{L})-o(t)} \leq \|e^{t\mathcal{L}}\| \leq e^{t\beta(\mathcal{L})} \tag{7.5}$$

as $t \to 0$, where $\beta(\mathcal{L})$ is the the *numerical abscissa* of $\mathcal{L}$, i.e., the largest real part of the numerical range, which is very close to 0. It can be shown that the numerical range is determined by the behavior of $\Lambda_\epsilon(\mathcal{L})$ in the limit $\epsilon \to \infty$, and this implies (7.4b). Finally, (7.4c) can be made precise in various ways with the aid of the integral

$$e^{t\mathcal{L}} = \frac{1}{2\pi i}\int_\Gamma e^{t\lambda}(\lambda I - \mathcal{L})^{-1}\,d\lambda, \tag{7.6}$$

where Γ is any contour enclosing $\Lambda(L)$. From (7.6) one can derive bounds on $\|e^{t\mathcal{L}}\|$ that depend on the location of the pseudospectra in the complex plane; an example is the Kreiss Matrix Theorem. We shall not give details here, but refer the reader to [8], [22], [29], [37], [40].

All of these remarks apply to the purely linear, constant-coefficient problem (7.1). Another limitation of spectral analysis is that as a rule it is not robust with respect to the introduction of complications such as nonlinearity, variable coefficients, or inhomogeneous forcing data. If (7.1) is modified in any of these ways, the effect will typically be that the transient part of Figure 7 remains approximately unchanged, but the long-time part of the figure—precisely the part related to eigenvalues—may change entirely. For a discussion of these matters, see [19], and for their application to the physical problem of hydrodynamic stability, see [37].

We close with a discussion of a different type of application of the ideas of this paper. Suppose we wish to solve a linear system of equations $L^{(N)}u = f$ by a nonsymmetric Chebyshev iteration of the kind investigated by Manteuffel [24], where $L^{(N)}$ is a discrete approximation to $\mathcal{L}$ as considered in §6. Such an iteration depends upon a pair of parameters $a, b \in \mathbf{C}$, which define an interval with respect to which a family of Chebyshev polynomials $\{p_n\}$ is implicitly constructed. The lemniscates $|p_n(z)| =$ const. of these polynomials approximate ellipses with foci a, b.

The conventional view is that a and b should be chosen so that the spectrum $\Lambda(L^{(N)})$ lies in one of these ellipses that is in an appropriate sense as small as possible. This view is supported by the estimate analogous to (7.2),

$$\frac{\|r_n\|}{\|r_0\|} \le \|p_n\|_{\Lambda(L^{(N)})}\kappa(M), \tag{7.7}$$

where $\|r_n\|/\|r_0\|$ denotes the ratio of the nth to the initial residual norms, $\|p_n\|_{\Lambda(L^{(N)})}$ is the supremum of $|p_n(z)|$ for $z \in \Lambda(L^{(N)})$, and $\kappa(M)$ is the condition number of a transformation that makes $L^{(N)}$ diagonal or self-adjoint. The trouble with (7.7) is that $\kappa(M)$ may be very large. An alternative bound can be based on the norm of p_n on a pseudospectrum, rather than the spectrum. For any $\epsilon > 0$ we have

$$\frac{\|r_n\|}{\|r_0\|} \le \|p_n\|_{\Lambda_\epsilon(L^{(N)})}\frac{\ell_\epsilon}{2\pi\epsilon}, \tag{7.8}$$

where ℓ_ϵ denotes the arc length of $\partial\Lambda_\epsilon(L^{(N)})$; the proof is by a contour integral analogous to (7.7) [26]. When $\kappa(M)$ is large and ϵ is not too small, a comparison of (7.7) and (7.8) suggests that when $L^{(N)}$ is far from normal, the parameters of a nonsymmetric matrix iteration may be more appropriately based on the pseudospectra than on the spectrum. Experiments confirm this prediction [34].

A related example is the phenomenon of direction-dependent convergence considered in [4], [11], [18]: a Gauss–Seidel or SOR iteration for a convection-diffusion problem may converge in far fewer steps if one sweeps with the convection rather than against it. This effect cannot be explained on the basis of spectra alone, which are ty ically independent of the sweep direction, but the explanation becomes clear when o looks at the pseudospectra. A similar gap between spectra and pseudospectra ari in the study of the numerical stability of discrete methods for convection-diffusi equations [9], [16], [25], [30].

It is a curious phenomenon that choices of iteration parameters based on ada tive or automatic estimates of the spectrum $\Lambda(L^{(N)})$, such as those constructed the Manteuffel algorithm, are often more reliable than the above observations see to suggest. The same is true of choices based on certain kinds of a priori analysis $\Lambda(L^{(N)})$, as in [21]. The explanation is that most approximate techniques for estim ing spectra are robust enough that that they actually estimate pseudospectra instea whether or not that that was the intention of their authors. Most numerical metho based on estimates of spectra of nonsymmetric matrices would become less reliable those estimates could be replaced by exact spectral information.

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