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Approximate diagonalization of variable-coefficient differential operators through similarity transformations

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ABSTRACT

Approaches to approximate diagonalization of variable-coefficient differential operators using similarity transformations are presented. These diagonalization techniques are inspired by the interpretation of the Uncertainty Principle by Fefferman, known as the *SAK* Principle, that suggests the location of eigenfunctions of self-adjoint differential operators in phase space. The similarity transformations are constructed using canonical transformations of symbols and anti-differential operators for making lower-order corrections. Numerical results indicate that the symbols of transformed operators can be made to closely resemble those of constant-coefficient operators, and that approximate eigenfunctions can readily be obtained.

1. Introduction

In this paper, we consider the problem of approximating eigenvalues and eigenfunctions of an mth order differential operator $L(x, D)$ defined on the space $C_p^n[0, 2\pi]$ consisting of functions that are m times continuously differential and 2π-periodic. The operator $L(x, D)$ has the form

$$L(x, D)u(x) = \sum_{\alpha=0}^{m} a_\alpha(x)D^\alpha u, \quad D = \frac{1}{i}\frac{d}{dx}, \tag{1}$$

with spatially-varying coefficients a_α, $\alpha = 0, 1, \dots, m$. We will assume that the operator $L(x, D)$ is self-adjoint and positive definite. In Section 6, we will drop these assumptions, and also discuss problems with more than one spatial dimension.

Our goal is to develop an algorithm for preconditioning a differential operator $L(x, D)$ to obtain a new operator $\tilde{L}(x, D) = UL(x, D)U^{-1}$ that, in some sense, more closely resembles a constant-coefficient operator. This would facilitate the solution of PDE involving $L(x, D)$ through spectral methods such as the Fourier method, or Krylov subspace spectral (KSS) methods [1,2]. To accomplish this task, we will rely on ideas summarized by Fefferman in [3].

The structure of the paper is as follows. Section 2 reviews the Uncertainty Principle and Fefferman's related *SAK* principle, and demonstrates how accurately it applies to constant- and variable-coefficient differential operators on a bounded domain. Section 3 reviews Egorov's Theorem to motivate the construction of similarity transformations of pseudodifferential operators via analysis of their symbols. Section 4 reviews symbolic calculus and then introduces *anti-differential operators*, which will be used to homogenize lower-order coefficients of differential operators. The application of the rules of symbolic calculus to anti-differential operators will be presented. Section 5 shows how simple canonical transformations can be used for local homogenization of a symbol in phase space. Section 6 contains the development of unitary similarity transformations based on anti-differential operators for iterative homogenization of lower-order coefficients of pseudodifferential operators. While this work is focused on operators in one space dimension, discussion of generalization

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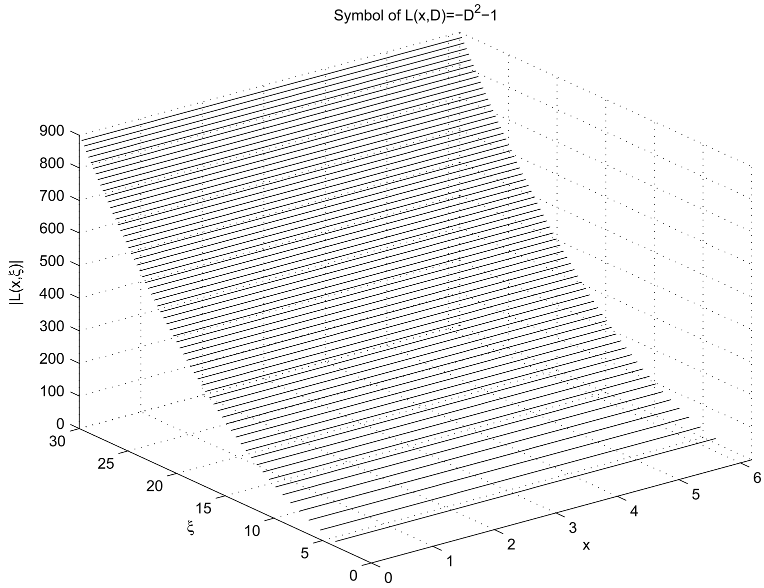

Fig. 1. Symbol of a constant-coefficient operator $A(x, D) = -D^2 - 1$.

to higher space dimensions is included. Section 7 discusses the practical implementation of the transformations presented in Sections 5 and 6. Section 8 presents numerical results illustrating the effect of these transformations and demonstrating the accuracy of approximate eigenfunctions that they produce. Concluding remarks are made in Section 9.

2. The uncertainty principle

The uncertainty principle says that a function ψ, mostly concentrated in $|x - x_0| < \delta_x$, cannot also have its Fourier transform $\hat{\psi}$ mostly concentrated in $|\xi - \xi_0| < \delta_\xi$ unless $\delta_x\delta_\xi \geq 1$. Fefferman describes a sharper form of the uncertainty principle, called the *SAK* principle, which we will now describe.

Assume that we are given a self-adjoint differential operator

$$A(x, D) = \sum_{|\alpha| \leq m} a_\alpha(x) \left(\frac{1}{i}\frac{\partial}{\partial x}\right)^\alpha, \tag{2}$$

with symbol

$$A(x, \xi) = \sum_{|\alpha| \leq m} a_\alpha(x)(\xi)^\alpha = e^{-i\xi x} A(x, D) e^{i\xi x}. \tag{3}$$

The *SAK* principle, which derives its name from the notation used by Fefferman in [3] to denote the set

$$S(A, K) = \{(x, \xi) | A(x, \xi) < K\}, \tag{4}$$

states that the number of eigenvalues of $A(x, D)$ that are less than K is approximately equal to the number of distorted unit cubes that can be packed disjointly inside the set $S(A, K)$. Since $A(x, D)$ is self-adjoint, the eigenfunctions of $A(x, D)$ are orthogonal, and therefore the *SAK* principle suggests that these eigenfunctions are concentrated in disjoint regions of phase space defined by the sets $\{S(A, \lambda) | \lambda \in \lambda(A)\}$.

We consider only differential operators defined on the space of 2π-periodic functions. We therefore use a modified definition of the set $S(A, K)$,

$$S(A, K) = \{(x, \xi) | 0 < x < 2\pi, |A(x, \xi)| < |K|\}. \tag{5}$$

The absolute values are added because symbols of self-adjoint operators are complex when the leading coefficient is not constant.

In the case of a constant-coefficient operator $A(x, D)$, the sets $S(A, K)$ are rectangles in phase space. This simple geometry of a constant-coefficient symbol is illustrated in Fig. 1. The eigenfunctions of $A(x, D)$, which are the functions $\hat{e}_\xi(x) = \exp(i\xi x)$, are concentrated in frequency, along the lines $\xi = $ constant. Fig. 2 shows the volumes of the sets $S(A, \lambda_j)$ for selected eigenvalues $\lambda_j, j = 1, \ldots, 32$, of $A(x, D)$. The eigenvalues are obtained by computing the eigenvalues of a matrix of the form

$$A_h = \sum_{\alpha=0}^{m} A_\alpha D_h^\alpha \tag{6}$$

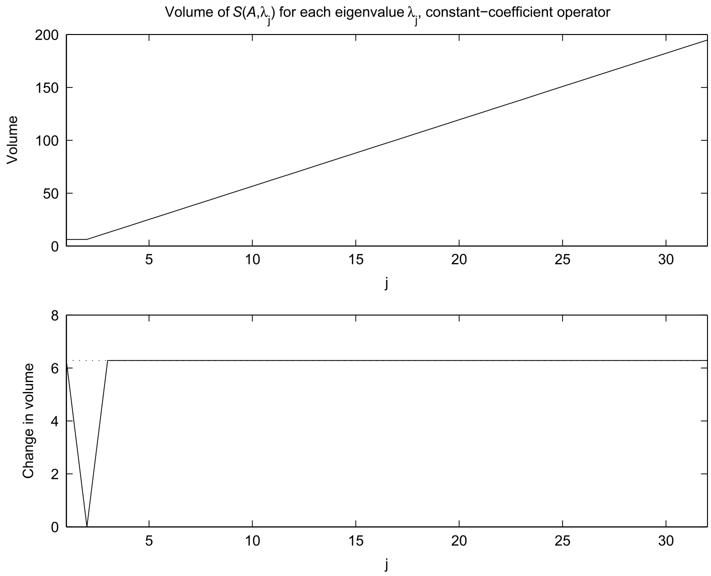

Fig. 2. The volume of the sets $S(A, K)$, as defined in (5), where $A(x, D) = -D^2 - 1$ and $K = \lambda_j(A)$ for $j = 1, \dots, 32$. The top figure plots the volume of $S(A, \lambda_j)$ as a function of j, and the bottom figure plots the change in volume between consecutive eigenvalues.

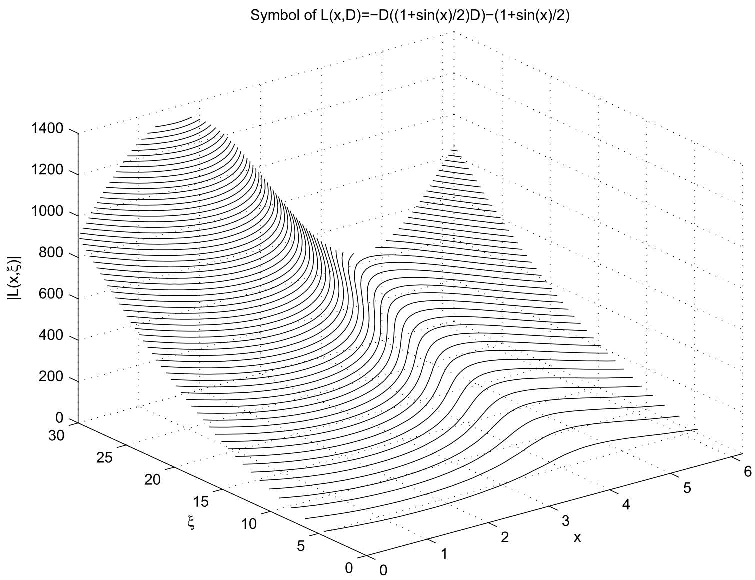

Fig. 3. Symbol of a variable-coefficient operator $A(x, D) = -D((1 + \frac{1}{2}\sin x)D) - \left(1 + \frac{1}{2}\sin x\right)$.

that is a discretization of $A(x, D)$ on an N-point uniform grid, with $N = 64$. For each α, $A_\alpha = \text{diag}(a_\alpha(x_0), \dots, a_\alpha(x_{N-1}))$ and D_h is a discretization of the differentiation operator. Note that in nearly all cases, the set differences

$$S(A, \lambda_j) - S(A, \lambda_{j-1}) = \{(x, \xi) | |\lambda_{j-1}| \le |A(x, \xi)| < |\lambda_j|\} \tag{7}$$

have the area 2π.

Now, consider a variable-coefficient operator $A(x, D)$, with a symbol $A(x, \xi)$ such as the one illustrated in Fig. 3. The *SAK* principle suggests that the eigenfunctions of $A(x, D)$ are concentrated in curved boxes of volume ≥ 1, where the geometry of these boxes is determined by the sets $S(A, K)$. Corresponding to Figs. 2 and 4 shows the volumes of the sets $S(A, \lambda_j)$ for the variable-coefficient operator $A(x, D)$ featured in Fig. 3. As in the constant-coefficient case, the set differences $S(A, \lambda_j) - S(A, \lambda_{j-1})$ have approximate area 2π. This ceases to be true for the largest eigenvalues, but those eigenvalues are not good approximations to the actual eigenvalues of $A(x, D)$ due to the limited resolution of the discretization.

These figures suggest that it is possible to construct a change of variable $\Phi : (y, \eta) \to (x, \xi)$ in phase space in order to "bend" $A(x, \xi)$ so that it more closely resembles the symbol of a constant-coefficient operator. If Φ preserves volume in phase space, then the volume of each set $S(A, K)$ is invariant under Φ, and therefore an operator with the symbol $A \circ \Phi$

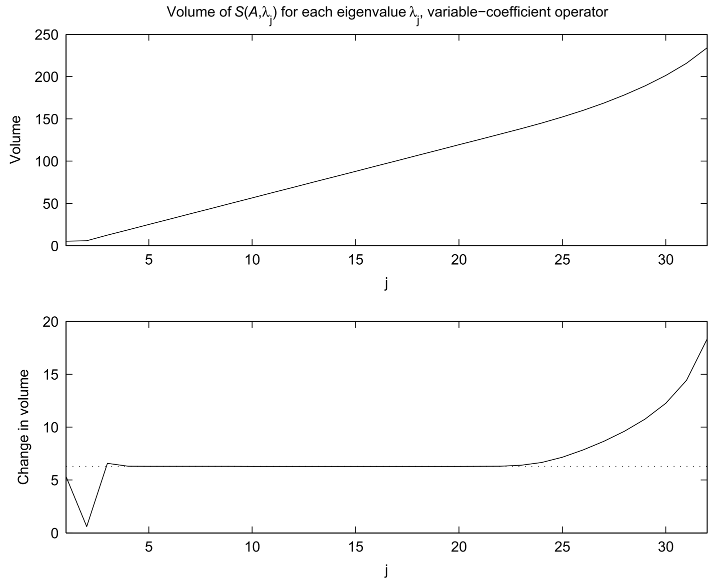

Fig. 4. Volume of the sets $S(A, K)$ where $A(x, D) = -D\left(\left(1 + \frac{1}{2}\sin x\right) D\right) - \left(1 + \frac{1}{2}\sin x\right)$ and $K = \lambda_j$ for $j = 1, \ldots, 32$. The top figure plots the volume of $S(A, \lambda_j)$ as a function of j, and the bottom figure plots the change in volume between consecutive eigenvalues.

should have approximately the same eigenvalues as $A(x, D)$. This leads us to ask whether such a transformation of the symbol $A(x, \xi)$ can induce a similarity transformation of the underlying operator $A(x, D)$.

The connection between the geometry of the symbol and the eigensystem of the underlying operator has been exploited before for numerical computation; see for instance recent work that uses symbol-based phase space decomposition to develop preconditioners for elliptic PDE or the Helmholtz equation using windowed Fourier frames [4] and wavelets [5], respectively. In this paper, by contrast, the focus is on bending symbols before cutting them.

3. Egorov's theorem

Egorov answered this question in the affirmative (see [6,3]), in the case where Φ is a *canonical transformation*, i.e. a change of variable in phase space that preserves Poisson brackets:

$$\{F, G\} \circ \Phi = \{F \circ \Phi, G \circ \Phi\}. \quad (8)$$

A consequence of this definition is that canonical transformations preserve volume in phase space.

We consider a block $\mathcal{B}^*$ in phase space that is the image under a canonical transformation Φ of a block $\mathcal{B}$ of size $M = \delta_y \times \delta_\eta$ centered at (y_0, η_0). Let i denote the natural change of scale $i : (y, \eta) \to ((y - y_0)/\delta_y, (\eta - \eta_0)/\delta_\eta)$ that carries $\mathcal{B}$ to the unit cube. Φ is said to satisfy "natural estimates" if $i\Phi i^{-1} \in C^\infty$, with derivatives of all orders bounded independent of M. Furthermore, we say that a symbol $A(x, \xi)$ belongs to S^m if

$$|\partial_x^\alpha \partial_\xi^\beta A| \le C_{\alpha\beta}(1 + |\xi|)^{m-|\beta|}, \quad \alpha, \beta \ge 0, \quad (9)$$

where the constants $C_{\alpha\beta}$ are independent of x and ξ. A symbol $A(x, \xi) \in S^m$ is related to an underlying *pseudodifferential operator* (or $\psi d0$) [7–10] $A(x, D)$ of order m by the Fourier inversion formula

$$A(x, D)u(x) = \int e^{i\xi x} A(x, \xi)\hat{u}(\xi)\, d\xi,$$

which is a differential operator if $A(x, \xi)$ is a polynomial in ξ with coefficients that are functions of x.

Theorem 3.1 (*Egorov*). *Let Φ be a canonical transformation satisfying natural estimates and carrying $\mathcal{B}$ into its double $\mathcal{B}^*$. Let $A(x, \xi) \in S^m$ be a symbol supported in $\Phi(\mathcal{B})$ and define $\tilde{A}(y, \eta) = A \circ \Phi(y, \eta)$. Then the operators $A(x, D)$ and $\tilde{A}(y, D)$ are related by*

$$\tilde{A}(y, D) = UA(x, D)U^{-1} + \text{lower-order terms} \quad (10)$$

for a suitable unitary transformation U.

The error

$$A(y, D) - UA(x, D)U^{-1}$$

is an operator whose symbol belongs to S^{m-1}; recent improvements to the theorem show that this error can be reduced to order $m - 2$ by a careful choice of U [11].

For "most" Φ (see [6,3]), the operator U is given explicitly as a Fourier integral operator [12,13,10]

$$Uf(y) = \int e(y, \xi) e^{iS(y,\xi)} \hat{f}(\xi)\, d\xi, \quad e \in S^0, S \in S^1, \tag{11}$$

where the function S is related to Φ by

$$\Phi(y, \eta) = (x, \xi) \iff \eta_k = \frac{\partial S}{\partial y_k}, \qquad x_k = \frac{\partial S}{\partial \xi_k}. \tag{12}$$

This choice of S is based on the need to guarantee a valid canonical transformation between the two sets of variables, meaning that the form of the Hamiltonian is preserved. By Liouville's Theorem, this condition implies the preservation of volume in phase space [14].

The function $S(y, \xi)$ is called a *generating function* for the transformation Φ. In the case of a canonical transformation induced by a change of variable $y = \phi(x)$, $S(y, \xi) = \xi \cdot \phi^{-1}(y)$ and the factor $e(y, \xi) = |\det D\phi^{-1}(y)|^{-1/2}$ is added to make U unitary, and therefore $Uf(y) = |\det D\phi^{-1}(y)|^{-1/2}(f \circ \phi^{-1})(y)$.

It should be noted that while Egorov's theorem applies to operators supported in a curved box in phase space, it applies to general differential operators when the canonical transformation Φ arises from a change of variable $y = \phi(x)$, provided that Φ satisfies the natural estimates required by the theorem.

Our goal is to construct unitary similarity transformations that will have the effect of smoothing the coefficients of a variable-coefficient $\psi d0 A(x, D)$. In the spirit of Egorov's theorem, we will construct such transformations by acting on the symbol $A(x, \xi)$.

4. Symbolic calculus and anti-differential operators

We will rely on the rules of *symbolic calculus* to work with pseudodifferential operators, or $\psi d0$, more easily and thus perform similarity transformations of such operators with much less computational effort than would be required if we were to apply transformations that acted on matrices representing discretizations of these operators.

4.1. Basic rules of symbolic calculus

We will be constructing and applying unitary similarity transformations of the form

$$\tilde{L}(x, D) = U^* L(x, D) U \tag{13}$$

where U is a $\psi d0$. In such cases, it is necessary to be able to compute the adjoint of a $\psi d0$, as well as the product of $\psi d0$.

To that end, given an mth-order differential operator $A(x, D)$ whose symbol $A(x, \xi)$ belongs to S^m, the symbol of the adjoint $A^*(x, D)$ is given by Fefferman [3]

$$A^*(x, \xi) = \sum_\alpha \frac{(-i)^\alpha}{\alpha!} \frac{\partial^\alpha}{\partial x^\alpha} \frac{\partial^\alpha}{\partial \xi^\alpha} \overline{A(x, \xi)}. \tag{14}$$

Similarly, if the nth-order differential operator $B(x, D)$ has symbol $B(x, \xi) \in S^n$, the symbol of the product $A(x, D)B(x, D)$, denoted by $AB(x, \xi)$, is given by

$$AB(x, \xi) = \sum_\alpha \frac{(-i)^\alpha}{\alpha!} \frac{\partial^\alpha A}{\partial \xi^\alpha} \frac{\partial^\alpha B}{\partial^\alpha x}. \tag{15}$$

The terms of these series are symbols of lower order ($m - \alpha$ in (14) and $m + n - \alpha$ in (15)), thus the sums are formally asymptotic.

These rules are direct consequences of the product rule for differentiation. Without loss of generality, we assume

$$A(x, D) = a(x) D^j, \qquad B(x, D) = b(x) D^k$$

where the coefficients $a(x)$ and $b(x)$ are real. Then

$$\begin{aligned} A^*(x, \xi) &= e^{-i\xi x} A^*(x, D) e^{i\xi x} \\ &= e^{-i\xi x} (-1)^j D^j [a(x) e^{i\xi x}] \\ &= e^{-i\xi x} i^{-j} \frac{d^j}{dx^j} [a(x) e^{i\xi x}] \\ &= i^{-j} \sum_{\ell=0}^{j} \binom{j}{\ell} \frac{d^\ell a(x)}{dx^\ell} (i\xi)^{j-\ell} \end{aligned}$$

$$
\begin{aligned}
&= \sum_{\ell=0}^{j} \frac{1}{\ell!}\frac{d^\ell}{dx^\ell}\left[\frac{j!}{(j-\ell)!} i^{-\ell} a(x)(\xi)^{j-\ell}\right] \\
&= \sum_{\ell=0}^{j} \frac{(-i)^\ell}{\ell!}\frac{d^\ell}{d\xi^\ell}\frac{d^\ell}{dx^\ell}\left[a(x)(\xi)^j\right] \\
&= \sum_{\ell} \frac{(-i)^\ell}{\ell!}\frac{\partial^\ell}{\partial\xi^\ell}\frac{\partial^\ell}{\partial x^\ell}\overline{A(x,\xi)}.
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
AB(x,\xi) &= e^{-i\xi x}A(x,D)B(x,D)e^{i\xi x} \\
&= \xi^k e^{-i\xi x} a(x) D^j [b(x)e^{i\xi x}] \\
&= \xi^k a(x) i^{-j} \sum_{\ell=0}^{j} \frac{j!}{\ell!(j-\ell)!}\frac{d^\ell b(x)}{dx^\ell}(i\xi)^{j-\ell} \\
&= \sum_{\ell=0}^{j} \frac{(-i)^\ell}{\ell!} a(x) \frac{j!}{(j-\ell)!}\xi^{j-\ell}\frac{\partial^\ell B(x,\xi)}{\partial x^\ell} \\
&= \sum_{\ell=0}^{j} \frac{(-i)^\ell}{\ell!}\frac{\partial^\ell A(x,\xi)}{\partial\xi^\ell}\frac{\partial^\ell B(x,\xi)}{\partial x^\ell}.
\end{aligned}
$$

4.2. The pseudo-inverse of the differentiation operator

For general $\psi d0$, the rules (14), (15) do not always apply, but they do yield an approximation. However, it will be necessary for us to work with $\psi d0$ of negative order, so we must identify a class of negative-order $\psi d0$ for which these rules do apply, as closely as possible. It makes sense to consider describing operators of negative order using anti-differentiation, as differentiation operators are of positive order, but as they are also singular, it is necessary to specify a particular antiderivative.

Let A be an $m \times n$ matrix of rank r, and let $A = U\Sigma V^T$ be the singular value decomposition of A, where $U^TU = I_m$, $V^TV = I_n$, and $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_r, 0, \ldots, 0)$. Then, the *pseudo-inverse* (see [15]) of A is defined as

$$A^+ = V\Sigma^+U^T, \tag{16}$$

where the $n \times m$ diagonal matrix Σ^+ is given by

$$\Sigma^+ = \begin{bmatrix} \sigma_1^{-1} & & & & & \\ & \ddots & & & & \\ & & \sigma_r^{-1} & & & \\ & & & 0 & & \\ & & & & \ddots & \\ & & & & & 0 \end{bmatrix}. \tag{17}$$

We can generalize this concept to define the pseudo-inverse of the differentiation operator D on the space of 2π-periodic functions by

$$D^+u(x) = \frac{i}{\sqrt{2\pi}}\sum_{\omega=-\infty}^{\infty} e^{i\omega x}\omega^+\hat{u}(\omega), \tag{18}$$

where

$$\omega^+ = \begin{cases} \omega^{-1} & \omega \neq 0 \\ 0 & \omega = 0. \end{cases} \tag{19}$$

The effect of this operator on a function $u(x)$ is to compute the antiderivative of each Fourier component of $u(x)$, with a constant of integration of zero, except for the component corresponding to $\omega = 0$. Equivalently,

$$D^+u(x) = i\int_{+0}[u(s) - \text{Avg}\, u]\, dx,$$

where the subscript of $+0$ of the integral sign indicates that *indefinite* integration is performed, but a constant of integration of zero is assumed to ensure uniqueness. It is also interesting to note that

$$DD^+u(x) = D^+Du(x) = \frac{i}{\sqrt{2\pi}} \sum_{\omega=-\infty,\omega\neq 0}^{\infty} e^{i\omega x}\hat{u}(\omega) = u(x) - \operatorname{Avg} u.$$

The rules (14) and (15) can be used for pseudodifferential operators defined using D^+, at least up to a symbol of lower order.

Lemma 4.1. *Let $A(x, D)$ be the anti-differential operator defined by*

$$A(x, D)u = D^+[a(x)u], \tag{20}$$

where $a(x) \in C_p^n[0, 2\pi]$. Then

$$A(x, \xi) = \sum_{\alpha=0}^{n-1} i^\alpha \frac{d^\alpha a_\xi(x)}{dx^\alpha}(\xi^+)^{\alpha+1} + (i\xi^+)^n e^{-i\xi x} D^+[a_\xi^{(n)}(x)e^{i\xi x}], \tag{21}$$

where

$$a_\xi(x) = a(x) - \frac{1}{\sqrt{2\pi}}\hat{a}(-\xi)e^{-i\xi x}. \tag{22}$$

Proof. Using the definition of $A(x, \xi)$ and integration by parts, we obtain, for $\xi \neq 0$,

$$\begin{aligned}
A(x, \xi) &= e^{-i\xi x}A(x, D)e^{i\xi x} \\
&= e^{-i\xi x}D^+[a(x)e^{i\xi x}] \\
&= e^{-i\xi x} i \int_{+0} \left[a(x)e^{i\xi x} - \operatorname{Avg} a(x)e^{i\xi x}\right] dx \\
&= e^{-i\xi x} i \int_{+0} \left[a(x)e^{i\xi x} - \frac{1}{2\pi}\int_0^{2\pi} a(y)e^{i\xi y}\, dy\right] dx \\
&= e^{-i\xi x} i \int_{+0} \left[a(x)e^{i\xi x} - \frac{1}{\sqrt{2\pi}}\hat{a}(-\xi)\right] dx \\
&= e^{-i\xi x} i \int_{+0} \left[a(x) - \frac{1}{\sqrt{2\pi}}\hat{a}(-\xi)e^{-i\xi x}\right] e^{i\xi x}\, dx \\
&= e^{-i\xi x} i \int_{+0} a_\xi(x)e^{i\xi x}\, dx \\
&= e^{-i\xi x} i \left[\frac{1}{i\xi}a_\xi(x)e^{i\xi x} - \frac{1}{i\xi}\int_{+0} a_\xi'(x)e^{i\xi x}\, dx\right] \\
&= a_\xi(x)\xi^+ + i\xi^+ e^{-i\xi x}D^+[a_\xi'(x)e^{i\xi x}].
\end{aligned}$$

Applying repeatedly yields (21). □

It follows that (15) applies to the product of D^+ and $a(x)$, but only approximately. However, the error

$$\begin{aligned}
\mathcal{E}(x, \xi) &= e^{-i\xi x} i \int_{+0} \frac{1}{\sqrt{2\pi}}\hat{a}(-\xi)e^{-i\xi x}e^{i\xi x}\, dx \\
&= \frac{i}{\sqrt{2\pi}}\hat{a}(-\xi)xe^{-i\xi x}\, dx,
\end{aligned}$$

which is a symbol of order $-(n + 1)$, due to the smoothness of $a(x)$ that determines the rate of decay of its Fourier coefficients [16]. We now consider adjoints and products involving both anti-differential and differential operators.

Proposition 4.2. *The rules (14) and (15) approximately hold for anti-differential operators of the form*

$$A(x, D) = a(x)(D^+)^k, \quad k > 0 \tag{23}$$

that belong to S^{-k}, and differential operators $L(x, D)$ of the form (1). That is, if the coefficient $a(x)$ belongs to $C_p^\infty[0, 2\pi]$, as do the coefficients of $L(x, D)$, then for $\xi \neq 0$,

$$A^*(x,\xi) = \sum_\alpha \frac{(-i)^\alpha}{\alpha!}\frac{\partial^\alpha}{\partial x^\alpha}\frac{\partial^\alpha}{\partial \xi^\alpha}\overline{A(x,\xi)} + \mathcal{E}_1(x,\xi), \tag{24}$$

$$AL(x,\xi) = \sum_\alpha \frac{(-i)^\alpha}{\alpha!}\frac{\partial^\alpha A}{\partial \xi^\alpha}\frac{\partial^\alpha B}{\partial^\alpha x} + \mathcal{E}_2(x,\xi), \tag{25}$$

and

$$LA(x,\xi) = \sum_\alpha \frac{(-i)^\alpha}{\alpha!}\frac{\partial^\alpha A}{\partial \xi^\alpha}\frac{\partial^\alpha B}{\partial^\alpha x}, \tag{26}$$

where $\mathcal{E}_1(x,\xi)$, $\mathcal{E}_2(x,\xi)$ are symbols of arbitrarily large negative order.

Proof. Without loss of generality, we will assume $L(x, D) = b(x)D^j$ where $j \geq 0$. Then, by repeated application of Lemma 4.1, we have

$$\begin{aligned}
A^*(x,\xi) &= e^{-i\xi x}(D^+)^k[\overline{a(x)}e^{i\xi x}] \\
&\approx \left[\sum_{\alpha=0}^\infty i^\alpha \binom{\alpha+k-1}{\alpha}\frac{d^\alpha \overline{a_\xi(x)}}{dx^\alpha}(\xi^+)^{\alpha+k}\right] \\
&\approx \sum_{\alpha=0}^\infty \frac{i^\alpha}{\alpha!}(-1)^\alpha \frac{(\alpha+k-1)!}{(k-1)!}\frac{d^\alpha \overline{a_\xi(x)}}{dx^\alpha}(\xi^+)^{\alpha+k} \\
&\approx \sum_{\alpha=0}^\infty \frac{(-i)^\alpha}{\alpha!}\frac{d^\alpha}{d\xi^\alpha}(\xi^+)^k\frac{d^\alpha \overline{a_\xi(x)}}{dx^\alpha} \\
&\approx \sum_{\alpha=0}^\infty \frac{(-i)^\alpha}{\alpha!}\frac{\partial^\alpha}{\partial x^\alpha}\frac{\partial^\alpha}{\partial \xi^\alpha}\overline{A(x,\xi)}
\end{aligned}$$

which is (14). The error in the approximation arises from the first application of D^+ to $\overline{a(x)}e^{i\xi x}$, as described in Lemma 4.1. The resulting error in $A^*(x,\xi)$ is of the form $\mathcal{E}_1(x,\xi) = p_k(x)\hat{a}(-\xi)e^{-i\xi x}$, where $p_k(x)$ is a polynomial of degree k, and therefore $\mathcal{E}_1(x,\xi)$ is a symbol of arbitrarily large negative order, due to the decay rate of the Fourier coefficients of $a(x) \in C_p^\infty[0, 2\pi]$.

Next, we have

$$\begin{aligned}
AL(x,\xi) &= e^{-i\xi x}a(x)(D^+)^k[b(x)D^j e^{i\xi x}] \\
&\approx e^{-i\xi x}\xi^j a(x)(D^+)^k[b(x)e^{i\xi x}] \\
&\approx \xi^j a(x)\sum_{\alpha=0}^\infty i^\alpha \binom{\alpha+k-1}{\alpha}\frac{d^\alpha b(x)}{dx^\alpha}(\xi^+)^{\alpha+k} \\
&= \sum_{\alpha=0}^\infty \frac{i^\alpha}{\alpha!}a(x)(-1)^k\frac{(\alpha+k-1)!}{(k-1)!}\frac{\partial^\alpha L}{\partial x^\alpha} \\
&= \sum_{\alpha=0}^\infty \frac{(-i)^\alpha}{\alpha!}\frac{\partial^\alpha A}{\partial \xi^\alpha}\frac{\partial^\alpha L}{\partial x^\alpha}
\end{aligned}$$

which is (15). The error in the approximation arises from the first application of D^+ to $b(x)e^{i\xi x}$, as described in Lemma 4.1. The resulting error in $AL(x,\xi)$ is of the form $\mathcal{E}_2(x,\xi) = a(x)q_k(x)\hat{b}(-\xi)e^{-i\xi x}(\xi)^j$, where $q_k(x)$ is a polynomial of degree k, and therefore $\mathcal{E}_2(x,\xi)$ is a symbol of arbitrarily large negative order, due to the decay rate of the Fourier coefficients of $b(x) \in C_p^\infty[0, 2\pi]$.

Finally, we consider

$$\begin{aligned}
LA(x,\xi) &= e^{-ixix}b(x)D^j a(x)(D^+)^k e^{i\xi x} \\
&= (-i)^j b(x)\sum_{\alpha=0}^j \binom{j}{\alpha}\frac{d^j a(x)}{dx^j}(i\xi)^{j-\alpha}i^k(\xi^+)^k \\
&= \sum_{\alpha=0}^j \frac{(-i)^\alpha}{\alpha!}\frac{\partial^\alpha L}{\partial \xi^\alpha}\frac{\partial^\alpha A}{\partial x^\alpha},
\end{aligned}$$

which is (15). □

This result allows us to use symbolic calculus to develop heuristics that aid in the construction of unitary similarity transformations based on $\psi d0$ of the form

$$U(x, D) = \sum_{\alpha=0}^{\infty} a_\alpha(x)(D^+)^{-\alpha}. \tag{27}$$

Such transformations will be considered in Section 6.

5. Local preconditioning

A special case that is useful for practical computation is where Φ arises from a simple change of variable $y = \phi(x)$, where $\phi(x)$ is a differentiable function and

$$\phi'(x) > 0, \qquad \frac{1}{2\pi}\int_0^{2\pi} \phi'(s)\, ds = 1. \tag{28}$$

The transformation Φ has the form

$$\Phi(y, \eta) \to (x, \xi), \quad x = \phi^{-1}(y), \xi = \phi'(x)\eta. \tag{29}$$

In this case, we set $e(y, \xi) = |\det D\phi^{-1}(y)|^{1/2}$ and $S(y, \xi) = \phi^{-1}(y)\xi$, and the Fourier inversion formula yields $Uf(y) = |\det D\phi^{-1}(y)|^{1/2} f \circ \phi^{-1}(y)$.

Suppose that $L(x, D)$ is an mth order differential operator such that the leading coefficient $a_m(x)$ does not change sign. Using this simple canonical transformation, we can precondition a differential operator $L(x, D)$ as follows: Choose $\phi(x)$ and construct a canonical transformation $\Phi(y, \eta)$ by (29) so that the transformed symbol

$$\tilde{L}(y, \eta) = L(x, \xi) \circ \Phi(y, \eta) = L(\phi^{-1}(y), \phi'(\phi^{-1}(y))\eta) \tag{30}$$

resembles a constant-coefficient symbol as closely as possible for a *fixed* frequency η_0 in transformed phase space. This will yield a symbol $\tilde{L}(y, \eta)$ that is smooth in a region of phase space concentrated around $\eta = \eta_0$. Then, we can select another value for η_0 and repeat, until our symbol is sufficiently smooth in the region of phase space $\{(y, \eta) | |\eta| < N/2\}$.

Since we are using a canonical transformation based on a change of spatial variable $y = \phi(x)$, we can conclude by Egorov's theorem that there exists a unitary Fourier integral operator U such that if $A = U^{-1}LU$, then the symbol of A agrees with $\tilde{L}$ modulo lower-order errors. Using the chain rule and symbolic calculus, it is a simple matter to construct this new operator $A(y, D)$.

We will now illustrate the process for a second-order self-adjoint operator

$$L(x, D) = a_2(x)D^2 + a_2'(x)D + a_0(x), \tag{31}$$

with symbol

$$L(x, \xi) = a_2(x)\xi^2 - a_2'(x)i\xi + a_0(x). \tag{32}$$

We will attempt to smooth out this symbol in a region of phase space concentrated around the line $\eta = \eta_0$. Our goal is to choose $\phi(x)$ so that the canonical transformation (29) yields a symbol $\tilde{L}(y, \eta)$ satisfying $\tilde{L}(y, \eta_0)$ is independent of y. In this case, the expression $L(\phi^{-1}(y), \phi'(\phi^{-1}(y))\eta_0)$ would also be independent of y, and therefore we can reduce the problem to that of choosing ϕ so that $L(x, \phi'(x)\eta_0)$ is independent of x.

The result is, for each x, a polynomial equation in $\phi'(x)$,

$$a_2(x)\phi'(x)^2\eta_0^2 - ia_2'(x)\phi'(x)\eta_0 + a_0(x) = L_{\eta_0}, \tag{33}$$

where the constant L_{η_0} is independent of x. This equation cannot be solved exactly for a real-valued $\phi'(x)$, but we can try to solve it approximately in some sense. For example, we can choose a real constant L_{η_0}, perhaps as the average value of $L(x, \eta_0)$ over the interval $[0, 2\pi]$, and then choose $\phi(x)$ in order to satisfy

$$a_2(x)\phi'(x)^2\eta_0^2 + a_0(x) = L_{\eta_0} \tag{34}$$

at each gridpoint, which yields

$$\phi'(x) = c_{\eta_0}\sqrt{\frac{\operatorname{Avg} a_2}{a_2(x)} + \frac{\operatorname{Avg} a_0 - a_0(x)}{a_2(x)\eta_0^2}}, \tag{35}$$

where the constant c_{η_0} is added to ensure that $\operatorname{Avg}\phi' = 1$. Figs. 5 and 6 illustrate the effect of this technique of local preconditioning on the symbol of the operator

$$L(x, D) = -D\left(\left(1 + \frac{1}{2}\sin x\right)D\right) - \left(1 - \frac{1}{2}\cos 2x\right), \tag{36}$$

first on regions of phase space corresponding to lower frequencies, and then regions corresponding to higher frequencies. We make the following observations:

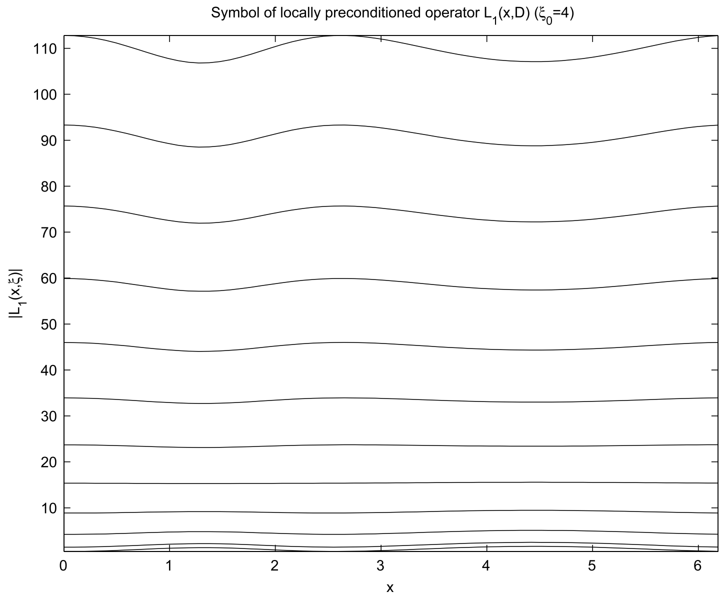

Fig. 5. Local preconditioning applied to operator $L(x, D)$ with $\eta_0 = 4$ to obtain new operator $L(y, D)$.

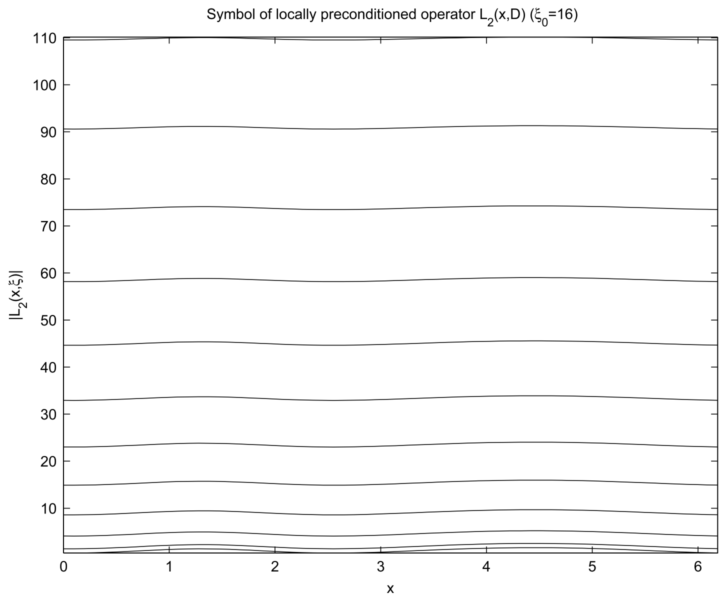

Fig. 6. Local preconditioning applied to operator $L(y, D)$ from Fig. 5, with $\eta_0 = 16$.

- It is not necessary to apply local preconditioning to every frequency, because transformations applied to lower frequencies have far-reaching effects on the symbol, thus requiring less work to be done at higher frequencies. These far-reaching effects are due to the smoothing of the leading coefficient.
- As $\eta_0 \to \infty$, $\phi'(x) \to C[a_2(x)]^{-1/2}$, where C is chosen so that Avg $\phi' = 1$. It follows from (33) that the leading coefficient of the transformed symbol $\tilde{L}(y, \eta)$ (and, by Egorov's Theorem, the leading coefficient of the transformed operator $\tilde{L}(y, D)$) is a constant, and from (35), this convergence is linear in η_0^{-1}. A variation of this transformation was used by Guidotti, the author, and Sølna in [17] to obtain approximate high-frequency eigenfunctions of a second-order operator.
- The above mentioned convergence of $\phi'(x)$ can be observed by comparing Figs. 5 and 6. In Fig. 6, with a larger value of η_0, the variation in the symbol with respect to x does not significantly increase with η; that is, it is more like the zero-order variation exhibited by a self-adjoint operator with a constant leading coefficient. On the other hand, in Fig. 5, the variation in the symbol with respect to x increases with η.

6. Global preconditioning

It is natural to ask whether it is possible to construct a unitary transformation U that smoothes $L(x, D)$ globally, i.e. yield the decomposition

$$U^*L(x, D)U = \tilde{L}(\eta). \tag{37}$$

In this section, we will attempt to answer this question. We begin by examining a simple eigenvalue problem, and then attempt to generalize the solution technique employed.

Consider a first-order differential operator of the form

$$L(x, D) = a_1 D + a_0(x), \tag{38}$$

where $a_0(x)$ is a 2π-periodic function. We will solve the eigenvalue problem

$$L(x, D)u(x) = \lambda u(x), \quad 0 < x < 2\pi, \tag{39}$$

with periodic boundary conditions

$$u(x) = u(x + 2\pi), \quad -\infty < x < \infty. \tag{40}$$

This eigenvalue problem is a first-order linear differential equation

$$a_1 u'(x) + a_0(x)u(x) = \lambda u(x). \tag{41}$$

Because the coefficients are periodic, we can apply Floquet's Theorem [18] to conclude that the fundamental solution $u_\lambda(x)$ satisfies

$$u_\lambda(x + 2\pi) = u_\lambda(x)[u_\lambda(0)]^{-1}u_\lambda(2\pi),$$

where

$$u_\lambda(x) = \exp\left[\int_0^x \frac{\lambda - a_0(s)}{a_1}\, ds\right].$$

The periodic boundary conditions can be used to determine the eigenvalues of $L(x, D)$. Specifically, $u_\lambda(x)$ must satisfy $u_\lambda(0) = u_\lambda(2\pi)$, which yields the condition

$$\int_0^{2\pi} \frac{\lambda - a_0(s)}{a_1}\, ds = i2\pi k, \tag{42}$$

for some integer k. If we denote by Avg a_0 the average value of $a_0(x)$ on the interval $[0, 2\pi]$,

$$\operatorname{Avg} a_0 = \frac{1}{2\pi}\int_0^{2\pi} a_0(s)\, ds, \tag{43}$$

then the periodicity of $u_\lambda(x)$ yields the discrete spectrum of $L(x, D)$,

$$\lambda_k = \operatorname{Avg} a_0 + ia_1 k, \tag{44}$$

for all integers k, with corresponding eigenfunctions

$$u_k(x) = \exp\left[\int_0^x \frac{\operatorname{Avg} a_0 - a_0(s)}{a_1}\, ds + ikx\right]. \tag{45}$$

Let

$$v(x) = \exp\left[\int_0^x \frac{\operatorname{Avg} a_0 - a_0(s)}{a_1}\, ds\right]. \tag{46}$$

Then $u_k(x) = v(x)e^{ikx}$ and

$$[v(x)]^{-1}L(x, D)v(x)e^{ikx} = \lambda_k e^{ikx}. \tag{47}$$

We have succeeded in diagonalizing $L(x, D)$ by using the zeroth-order symbol $v(x)$ to perform a similarity transformation of $L(x, D)$ into a constant-coefficient operator

$$\tilde{L}(x, D) = [v(x)]^{-1}L(x, D)v(x) = a_1 D + \operatorname{Avg} a_0. \tag{48}$$

The same technique can be used to transform an mth-order differential operator of the form

$$L(x, D) = a_m D^m + \sum_{\alpha=0}^{m-1} a_\alpha(x)D^\alpha, \tag{49}$$

so that the constant coefficient a_m is unchanged and the coefficient $a_{m-1}(x)$ is transformed into a constant equal to $\tilde{a}_{m-1} = \text{Avg}\, a_{m-1}$. This is accomplished by computing $\tilde{L}(x, D) = [v_m(x)]^{-1} L(x, D) v_m(x)$ where

$$v_m(x) = \exp\left[\int_0^x \frac{\text{Avg}\, a_{m-1} - a_{m-1}(s)}{m a_m}\, ds\right]. \tag{50}$$

Note that if $m = 1$, then we have $v_1(x) = v(x)$, where $v(x)$ is defined in (46).

We now seek to generalize this technique in order to eliminate lower-order variable coefficients. The basic idea is to construct a transformation U_α such that

1. U_α is unitary;
2. The transformation $\tilde{L}(x, D) = U_\alpha^* L(x, D) U_\alpha$ yields an operator $\tilde{L}(x, D) = \sum_{\beta=-\infty}^{m} b_\beta(x) \left(\frac{\partial}{\partial x}\right)^\beta$ such that $a_\alpha(x)$ is constant; and
3. The coefficients $a_\beta(x)$ of $L(x, D)$, where $\beta > \alpha$, are invariant under the similarity transformation $\tilde{L} = U_\alpha^* L(x, D) U_\alpha$.

It turns out that such an operator is not difficult to construct. First, we note that if $\phi(x, D)$ is a skew-symmetric pseudodifferential operator, then $U(x, D) = \exp[\phi(x, D)]$ is a unitary operator, since

$$\begin{aligned} U(x, D)^* U(x, D) &= (\exp[\phi(x, D)])^* \exp[\phi(x, D)] \\ &= \exp[-\phi(x, D)] \exp[\phi(x, D)] \\ &= I. \end{aligned}$$

We consider an example to illustrate how one can determine a operator $\phi(x, D)$ so that $U(x, D) = \exp[\phi(x, D)]$ satisfies the second and third conditions given above. Given a second-order self-adjoint operator of the form (31), we know that we can use a canonical transformation to make the leading-order coefficient constant, and since the corresponding Fourier integral operator is unitary, symmetry is preserved, and therefore our transformed operator has the form

$$L(x, D) = a_2 D^2 + a_0(x). \tag{51}$$

In an effort to transform L so that the zeroth-order coefficient is constant, we apply the similarity transformation $\tilde{L} = U^* L U$, which yields an operator of the form

$$\begin{aligned} \tilde{L} &= e^{-\phi} L e^{\phi} \\ &= e^{-\text{ad}(\phi)} L \\ &= L + [L, \phi] + \frac{1}{2}[[L, \phi], \phi] + \cdots \end{aligned} \tag{52}$$

where $\text{ad}(X)Y = [X, Y]$ [19].

Since we want the first and second-order coefficients of L to remain unchanged, the perturbation E of L in $\tilde{L} = L + E$ must not have order greater than zero. If we require that ϕ has negative order $-k$, then the highest-order term in E is $[L, \phi] = L\phi - \phi L$, which has order $1 - k$, so in order to affect the zero-order coefficient of L we must have ϕ be of order -1.

By symbolic calculus, it is easy to determine that the highest-order coefficient of $L\phi - \phi L$ is $2a_2 b'_{-1}(x)$ where $b_{-1}(x)$ is the leading coefficient of ϕ. Therefore, in order to satisfy

$$a_0(x) + 2a_2 b'_{-1}(x) = \text{constant}, \tag{53}$$

we must have $b'_{-1}(x) = -(a_0(x) - \text{Avg}\, a_0)/2a_2$. In other words,

$$b_{-1}(x) = -\frac{1}{2a_2} D^+(a_0(x)), \tag{54}$$

where D^+ is the pseudo-inverse of the differentiation operator D introduced in Section 4. Therefore, for our operator $\phi(x, D)$, we can use

$$\begin{aligned} \phi(x, D) &= \frac{1}{2}[b_{-1}(x) D^+ - (b_{-1}(x) D^+)^*] \\ &= b_{-1}(x) D^+ + \text{lower-order terms}. \end{aligned} \tag{55}$$

Using symbolic calculus, it can be shown that the coefficient of order -1 in $\tilde{L}$ is zero. To see this, we first note that with ϕ being of order -1, in the previously described expansion

$$\tilde{L} = L + [L, \phi] + \frac{1}{2}[[L, \phi], \phi] + \cdots,$$

the third term is of order -2, due to the terms corresponding to $\alpha = 0$ in (15) being canceled in the commutator, so this term (and subsequent terms, which are of still lower order) need not be examined.

Next, we note that

$$[L, \phi]^* = (L\phi - \phi L)^* = \phi^* L^* - L^*\phi^* = -\phi L + L\phi = [L, \phi].$$

Furthermore, we have

$$L + [L, \phi] = a_2 D^2 + (\text{Avg}\, a_0) - ia_{-1}(x)D^+ + \text{lower-order terms}.$$

However, the leading-order portion $a_2D^2 + (\text{Avg}\, a_0)$ is self-adjoint, which implies that the remainder $-ia_{-1}(x)D^+ +$ lower-order terms is also self-adjoint. By (14), the leading-order term of the adjoint is $ia_{-1}(x)D^+$, and therefore we must have $a_{-1}(x) \equiv 0$.

More generally, suppose that $L(x, D)$ is an mth-order operator of the form (49) whose leading-order variable coefficient $a_{m-1}(x)$ has also been homogenized by a transformation of the form $\bar{L}(x, D) = [v_m(x)]^{-1}L(x, D)v_m(x)$ where $v_m(x)$ is defined by (50), to yield an operator of the form

$$\bar{L}(x, D) = a_m D^m + \overline{a_{m-1}}D^{m-1} + \sum_{\alpha=0}^{m-2} \overline{a_\alpha}(x)D^\alpha.$$

In order to transform $\bar{L}(x, D)$ so that $\overline{a_{m-2}}(x)$ is also made constant, we use a similarity transformation of the form $\tilde{L}(x, E) = U(x, D)^*\bar{L}U(x, D)$, where $U(x, D) = \exp[\phi(x, D)]$ and $\phi(x, D)$ is an anti-self-adjoint operator; that is, $\phi^*(x, D) = -\phi(x, D)$.

As in the preceding example involving a second-order operator, we examine the leading-order term of the deviation of $\tilde{L} = U^*\bar{L}U$ from $\bar{L}$, which is given by $\bar{L}\phi - \phi\bar{L}$. By requiring that ϕ is of order -1, we ensure that this term is of order $m - 2$, in view of (15), if we stipulate that

$$\phi(x, D) = \frac{1}{2}[\varphi(x, D) - \varphi^*(x, D)], \quad \varphi(x, D) = b_{-1}(x)D^+,$$

which, by (14), yields

$$\phi(x, D) = b_{-1}(x)D^+ + \text{lower-order terms}.$$

We then have

$$\bar{L}\phi - \phi\bar{L} = ma_m b'_{-1}(x)D^{m-2} + \text{lower-order terms}.$$

Therefore, in order to ensure that the term of order $m - 2$ in the transformed operator has a constant coefficient, we set

$$b_{-1}(x) = -\frac{1}{ma_m}D + (\bar{a}_{m-2}(x)),$$

by analogy with (54). If L is also self-adjoint (for m even) or skew-self-adjoint (for m odd), then $\overline{a_{m-1}} = 0$ and after homogenizing $\bar{a}_{m-2}(x)$, the coefficient of order $m - 3$ in the transformed operator $\tilde{L}$ is zero, just as the coefficient of order -1 in the transformed second-order operator $\tilde{L}$ is zero.

We can use similar transformations to make lower-order coefficients constant as well. In doing so, the following result is helpful:

Proposition 6.1. *Let $L(x, D)$ be an mth order self-adjoint pseudodifferential operator of the form*

$$L(x, D) = \sum_{-\infty}^{m} a_\alpha(x) i^\alpha D^\alpha, \tag{56}$$

where we define $D^{-k} = (D^+)^k$ for $k > 0$ and the coefficients $\{a_\alpha(x)\}$ are all real. For any odd integer α_0, if $a_\alpha(x)$ is constant for all $\alpha > \alpha_0$, then $a_{\alpha_0}(x) \equiv 0$.

Proof. Because the leading-order portion of $L(x, D)$,

$$L_m(x, D) = \sum_{\alpha=\alpha_0+1}^{m} a_\alpha i^\alpha D^\alpha$$

is constant-coefficient, and must itself be self-adjoint, the reminder

$$L_0(x, D) = \sum_{\alpha=-\infty}^{\alpha_0} a_\alpha(x) i^\alpha D^\alpha$$

must also be self-adjoint. We then have, by (14),

$$L_0^*(x, \xi) = \overline{L_0(x, \xi)} + \text{lower-order terms} = -i^{\alpha_0} a_{\alpha_0}(x)\xi^{\alpha_0} + \text{lower-order terms}. \tag{57}$$

Because α_0 is odd, this implies that $a_{\alpha_0}(x) = -a_{\alpha_0}(x)$, from which the result follows. □

Example. Let $L(x, D) = D^2 + \sin x$. Let

$$b_{-1}(x) = \frac{1}{2}\cos x \tag{58}$$

and

$$\begin{aligned}\phi(x, D) &= \frac{1}{4}[\cos xD^+ - (\cos xD^+)^*] \\ &= \frac{1}{2}(\cos x)D^+ + \text{lower-order terms.}\end{aligned} \tag{59}$$

Then, since Avg $\sin x = 0$, it follows that

$$\begin{aligned}\tilde{L}(x, D) &= U_\alpha^* L(x, D) U_\alpha \\ &= \exp[-\phi(x, D)]L(x, D)\exp[\phi(x, D)] \\ &= D^2 + E(x, D),\end{aligned}$$

where $E(x, D)$ is of order -2. □

6.1. Non-normal operators

If the operator $L(x, D)$ is not normal, then it is not unitarily diagonalizable, and therefore cannot be approximately diagonalized using unitary transformations. Instead, we can use similarity transformations of the form

$$\tilde{L}(x, D) = \exp[-\phi(x, D)]L(x, D)\exp[\phi(x, D)], \tag{60}$$

where $\phi(x)$ is obtained in the same way as for self-adjoint operators, except that we do not take its skew-symmetric part. For example, if $L(x, D) = a_2 D^2 + a_1 D + a_0(x)$, then we can make the zeroth-order coefficient of $\tilde{L}(x, D)$ constant by setting

$$\phi(x) = b_{-1}(x)D^+ = -\frac{1}{2a_2}D^+(a_0(x))D^+. \tag{61}$$

In this case, the variable-coefficient remainder is of order -1, rather than -2 as in the self-adjoint case.

6.2. Operators in higher spatial dimensions

Consider the operator $L(\mathbf{x}, D) = a_2\Delta + a_0(\mathbf{x})$, defined on the n-dimensional cube $[0, 2\pi]^n$. Using symbolic calculus, by analogy with (54), it can be shown that the zero-order coefficient $a_0(x)$ can be homogenized through the similarity transformation U^*LU, where

$$U(x, D) = \exp[(\phi(\mathbf{x}, D) - \phi^*(\mathbf{x}, D))/2], \tag{62}$$

$$\phi(\mathbf{x}, \xi) = -\frac{1}{(2\pi)^{n/2}}\sum_{\omega\in\mathbb{Z}^n, \omega\neq\mathbf{0}} \phi_\omega(\mathbf{x}, \xi, \omega), \quad \xi \neq \mathbf{0}, \tag{63}$$

where

$$\phi_\omega(\mathbf{x}, \xi, \omega) = \begin{cases} \dfrac{\hat{a}_0(\omega)e^{i\omega\cdot\mathbf{x}}}{2ia_2(\omega\cdot\xi)} & \omega\cdot\xi \neq 0 \\ \dfrac{\hat{a}_0(\omega)(\xi\cdot\mathbf{x})e^{i\omega\cdot\mathbf{x}}}{2ia_2(\xi\cdot\xi)} & \omega\cdot\xi = 0 \end{cases}. \tag{64}$$

This can be seen by equating the zeroth-order term of (52) to a constant $\overline{a_0}$, using a higher-dimensional analogue of (15), and then solving for $\phi(x, \xi)$. That is,

$$\begin{aligned}a_0 &= a_0(\mathbf{x}) + i\sum_{j=1}^n \frac{\partial L(x, \xi)}{\partial \xi_j}\frac{\partial \phi(x, \xi)}{\partial x_j} \\ &= a_0(\mathbf{x}) + 2ia_2\sum_{j=1}^n \xi_j \frac{\partial \phi(x, \xi)}{\partial x_j}\end{aligned}$$

which yields

$$\nabla_x \phi(\mathbf{x}, \vec{\xi}) \cdot \vec{\xi} = \frac{\text{Avg}\, a_0 - a_0(\mathbf{x})}{2ia_2}.$$

Expressing $a_0(\mathbf{x})$ in terms of its discrete Fourier series and solving this equation leads to (64). Future work will explore the efficient implementation of such transformations using discrete symbol calculus [20].

7. Implementation

The rules for symbolic calculus introduced in Section 4 can easily be implemented and provide a foundation for algorithms to perform unitary similarity transformations on pseudodifferential operators. In this section we will develop practical implementations of the local and global preconditioning techniques discussed in Sections 5 and 6.

7.1. Simple canonical transformations

First, we will show how to efficiently transform a differential operator $L(x, D)$ into a new differential operator $\tilde{L}(y, D) = U^*L(x, D)U$ where U is a Fourier integral operator related to a canonical transformation $\Phi(y, \eta) = (x, \xi)$ by Egorov's Theorem. For clarity we will assume that $L(x, D)$ is a second-order operator, but the resulting algorithm can easily be applied to operators of arbitrary order.

Algorithm 7.1. Given a self-adjoint differential operator $L(x, D)$ and a function $\phi'(x)$ satisfying $\phi'(x) > 0$ and $\int_0^{2\pi} \phi'(x)\,dx = 1$, the following algorithm computes the differential operator $\tilde{L} = U^*LU$ where $Uf(x) = \sqrt{\phi'(x)}f(\phi(x))$.

$\phi = \int_0^x \phi'(s)\,ds$
$L = \phi^{-1/2}L\phi^{1/2}$
$C_1 = 1$
$\tilde{L} = 0$
for $j = 0, \ldots, m$,
  for $k = j + 1, \ldots, 2$,
    $C_k = C_k' + C_{k-1}\phi'$
  end
  $L_j = 0$
  for $k = 0, \ldots, j$,
    $L_j = L_j + ((a_jC_{k+1}) \circ \phi^{-1})D^k$
  end
  $\tilde{L} = \tilde{L} + L_j$
end

This algorithm requires $O(N \log N)$ floating-point operations, assuming that each function is discretized on an N-point grid and that the fast Fourier transform is used for differentiation.

7.2. Eliminating variable coefficients

Suppose we wish to transform an mth-order self-adjoint differential operator $L(x, D)$ into $\tilde{L}(x, D) = Q^*(x, D)L(x, D)Q(x, D)$ where coefficients of order J and above are constant. After we apply Algorithm 7.1 to make $a_m(x)$ constant, we can proceed as follows:

$j = m - 2$
$k = 1$
while $j >= J$
  Let $a_j(x)$ be the coefficient of order j in $L(x, D)$
  $\phi_j = D^+(a_j(x)/2a_m(x))$
  Let $E(x, D) = \phi_j(x)(D^+)^k$
  Let $Q(x, D) = \exp[(E(x, D) - E^*(x, D))/2]$
  $L(x, D) = Q^*(x, D)L(x, D)Q(x, D)$
  $j = j - 2$
  $k = k + 2$
end

Since $L(x, D)$ is self-adjoint, this algorithm is able to take advantage of Proposition 6.1 to avoid examining odd-order coefficients.

In a practical implementation, one should be careful in computing Q^*LQ. Using symbolic calculus, there is much cancellation among the coefficients. However, it is helpful to note that from (52),

$$\exp[-A(x, D)]L(x, D)\exp[A(x, D)] = \sum_{\ell=0}^{\infty} \frac{1}{\ell!}C_\ell(x, D), \tag{65}$$

where the operators $\{C_\ell(x, D)\}$ satisfy the recurrence relation

$$C_0 = L,$$
$$C_\ell = C_{\ell-1}A - AC_{\ell-1}, \quad \ell > 0,$$

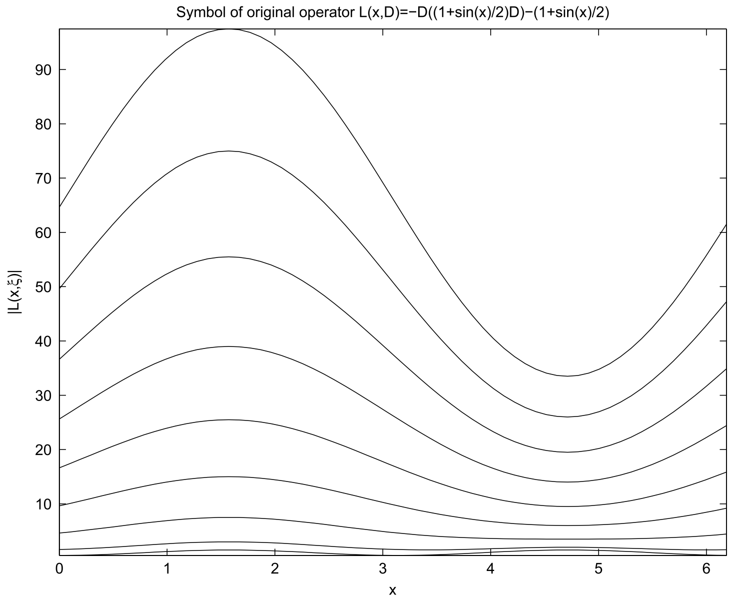

Fig. 7. Symbol of original variable-coefficient operator $P(x, D)$ defined in (66).

and each $C_\ell(x, D)$ is of order $m + \ell(k - 1)$, where $k < 0$ is the order of $A(x, D)$. Expressions of the form $A(x, D)B(x, D) - B(x, D)A(x, D)$ can be computed without evaluating the first term in (15) for each of the two products, since it is clear that it will be cancelled.

The operator $Q(x, D)$ must be represented using a truncated series. In order to ensure that all coefficients of $L(x, D)$ of order J or higher are correct, it is necessary to compute terms of order $J - m$ or higher. With this truncated series representation of $Q(x, D)$ in each iteration, the algorithm requires $O(N \log N)$ floating-point operations when an N-point discretization of the coefficients is used and the fast Fourier transform is used for differentiation. It should be noted, however, that the number of terms in the transformed operator $L(x, D)$ can be quite large, depending on the choice of J.

7.3. Using multiple transformations

When applying multiple similarity transformations such as those implemented in this section, it is recommended that a variable-grid implementation be used in order to represent transformed coefficients as accurately as possible. In applying these transformations, errors are introduced by pointwise multiplication of coefficients and computing composition of functions using interpolation, and these errors can accumulate very rapidly when applying several transformations.

8. Numerical results

In this section we will illustrate the effects of preconditioning on differential operators. We will use the operator that was first introduced in (36) to illustrate local preconditioning,

$$P(x, D) = -D\left(\left(1 + \frac{1}{2}\sin x\right)D\right) - \left(1 - \frac{1}{2}\cos 2x\right). \qquad (66)$$

8.1. Preconditioning

Fig. 7 shows the symbol $P(x, \xi)$ before preconditioning is applied. Fig. 8 shows the symbol of $A = U^*PU$ where U is a Fourier integral operator induced by a canonical transformation that makes the leading coefficient constant. Finally, Fig. 9 shows the symbol of $B = Q^*AQ$ where Q is designed to make the zero-order coefficient of A constant, using the technique described in Section 6. The transformation U smooths the symbol of $P(x, D)$ so that the curvature in the surface defined by $|A(x, \xi)|$ has uniform curvature with respect to ξ. The transformation Q yields a symbol that closely resembles that of a constant-coefficient operator except at the lowest frequencies.

8.2. Approximating eigenfunctions

By applying the preconditioning transformations to Fourier waves $e^{i\omega x}$, excellent approximations to eigenvalues and eigenfunctions can be obtained. This follows from the fact that if the operator $Q^*L(x, D)Q$ is close to a constant-

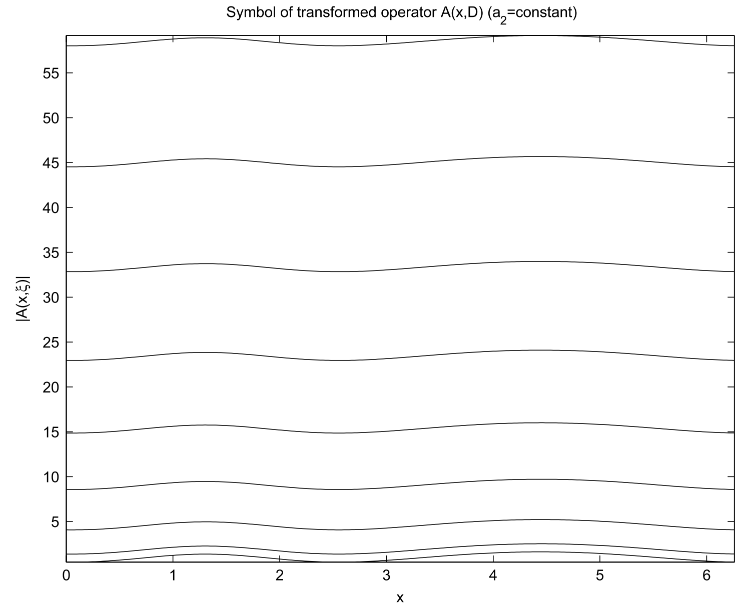

Fig. 8. Symbol of transformed operator $A(x, D) = U^*P(x, D)U$ where $P(x, D)$ is defined in (66) and U is chosen to make the leading coefficient of $A(x, D)$ constant.

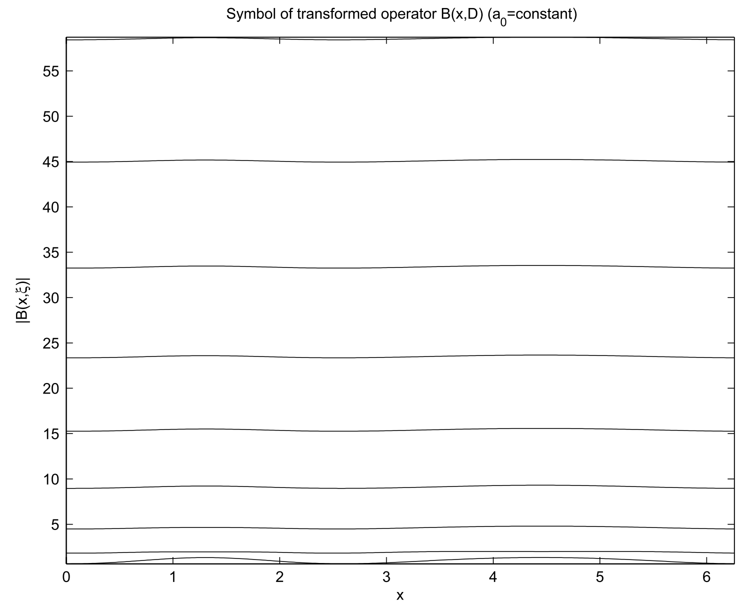

Fig. 9. Symbol of transformed operator $B(x, D) = Q^*U^*L(x, D)UQ$ where $P(x, D)$ is defined in (66) and the unitary similarity transformations Q and U make $B(x, D)$ a constant-coefficient operator modulo terms of negative order.

coefficient operator, then $e^{i\omega x}$ is an approximate eigenfunction of $Q^*L(x, D)Q$, and therefore $Qe^{i\omega x}$ should be an approximate eigenfunction of $L(x, D)$.

Let $L(x, D) = P(x, D)$ from (66). Fig. 10 displays the relative error, measured using the L_2 norm, in eigenfunctions corresponding to the lowest 40 eigenvalues of $P(x, D)$. In the first experiment, the transformation Q makes the second-order and zeroth-order coefficients constant, using the techniques presented in Sections 5 and 6. In the second experiment, an additional transformation is used to make the coefficient of order -2 constant. We observe that the accuracy of the approximate eigenfunctions increases rapidly with the frequency, and this improvement is much more dramatic when a second transformation is used.

It should be noted that this strategy does not work well for low frequencies. However, it does largely orthogonalize eigenfunctions corresponding to low frequencies against high-frequency waves, which allows computation of accurate eigenfunctions by restricting to a much coarser grid. In the results shown in Fig. 10, this approach is used for $|\omega| \leq 4$

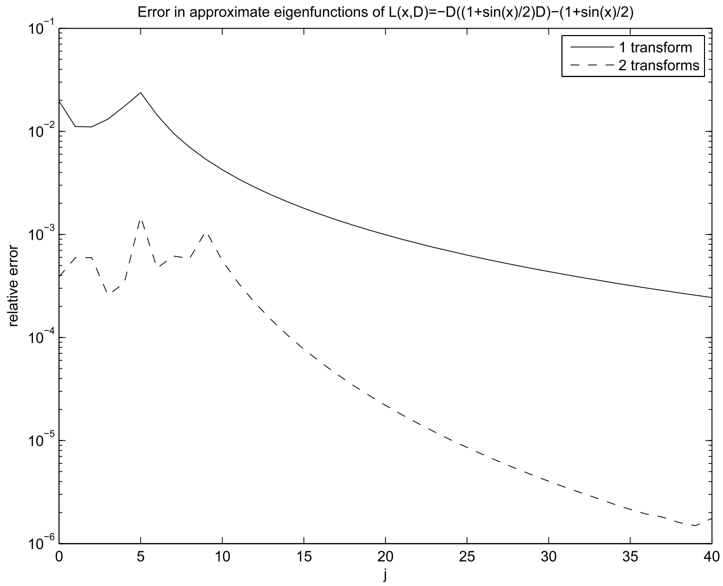

Fig. 10. Relative error, measured using the L_2 norm, in approximate eigenfunctions of $P(x, D)$ from (66) generated by diagonalizing discretization matrix and by preconditioning to make second-order and zeroth-order coefficients constant (solid curve) and coefficient of order −2 constant as well (dashed curve).

for the case of one transformation, and $|\omega| \leq 8$ for two transformations; the higher threshold is chosen in this case to match the higher accuracy achieved at higher frequencies.

9. Summary

We have succeeded in constructing unitary similarity transformations that smooth the coefficients of a self-adjoint differential operator locally in phase space so that the symbol of the transformed operator more closely resembles that of a constant-coefficient operator. In addition, we have shown how unitary similarity transformations can be used to eliminate variable coefficients of arbitrary order, at the expense of introducing lower-order variable coefficients.

In [1] it was demonstrated that these techniques for smoothing coefficients improve the accuracy of the Krylov subspace spectral (KSS) methods developed in [1,2]. Furthermore, it has been seen that these transformations can yield accurate approximations of eigenvalues and eigenfunctions of self-adjoint differential operators.

In addition, we have managed to apply the ideas of Fefferman and Egorov to develop practical similarity transformations of differential operators to obtain new operators with smoother coefficients, along with good approximations of eigenvalues and eigenfunctions of these operators.

With future research along the directions established in this paper, it is hopeful that more efficient solution methods for variable-coefficient PDE, as well as a deeper understanding of the eigensystems of variable-coefficient differential operators, can be realized.

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