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Abstract: *We show how pseudodifferential equations on the unit sphere of the 3-dimensional Euclidean space can be studied using the spherical harmonic Fourier series on the symmetry group of the sphere.*

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Suppose we are faced with a Dirichlet boundary value problem of an elliptic partial differential equation in a domain diffeomorphic to the unit ball of \mathbb{R}^3 . From the fundamental solution we obtain the Schwartz kernel of a singular integral operator on the 2-sphere \mathbb{S}^2 , and the corresponding integral equation needs to be solved. The integral operator turns out to be an elliptic *pseudodifferential operator*, which can be treated locally with Euclidean Fourier analysis. However, it turns out that one can directly deal with the spherical harmonics, which has computational advantages. An analogous case is the theory of so called periodic pseudodifferential operators, i.e. pseudodifferential theory exploiting the Fourier series on torus [1, 2, 7, 5].

Pseudodifferential calculus on the 2-sphere is a special case of pseudodifferential theory on a compact homogeneous space G/K based on Fourier analysis on a compact Lie G (see [6]); namely, the 2-sphere is diffeomorphic to a homogeneous space G/K , where $K \cong \text{SO}(2)$ is a subgroup of $G = \text{SO}(3)$. Basics of linear Lie groups can be found in many books, e.g. [8] is a fine reference. In [3] the special case of rotation-bi-invariant operators on the sphere was considered.

1 Sphere rotated

Let us endow the three-dimensional Euclidean space \mathbb{R}^3 with the usual inner product $(x, y) \mapsto \langle x, y \rangle_{\mathbb{R}^3} = x_1y_1 + x_2y_2 + x_3y_3$; the corresponding norm is $x \mapsto \|x\|_{\mathbb{R}^3} = (x_1^2 + x_2^2 + x_3^2)^{1/2}$. The unit sphere of \mathbb{R}^3 is the set

$$\mathbb{S}^2 = \{x = (x_j)_{j=1}^3 : \|x\|_{\mathbb{R}^3} = 1\}.$$

A rotation around the origin of \mathbb{R}^3 is a linear mapping preserving both the orientation and the distances. Such rotations form a non-commutative group, the so-called *special orthogonal group* of \mathbb{R}^3 , denoted by $\text{SO}(3)$. A rotation maps \mathbb{S}^2 bijectively onto \mathbb{S}^2 , so that $\text{SO}(3)$ can be regarded as the symmetry group of \mathbb{S}^2 .

Let $\{e_1, e_2, e_3\}$ be the standard orthonormal basis of \mathbb{R}^3 . A linear mapping $a : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ is of the form

$$x = (x_j)_{j=1}^3 \mapsto \left(\sum_{j=1}^3 a_{ij}x_j \right)_{i=1}^3,$$

where $a_{ij} = \langle e_j, ae_i \rangle_{\mathbb{R}^3}$. We can identify such a mapping with its matrix representation $(a_{ij})_{i,j=1}^3$. A rotation $g \in G = \text{SO}(3)$ can thus be identified with a real matrix $(g_{ij})_{i,j=1}^3$ having orthonormal column vectors and positive determinant (i.e. orientation is preserved). To put it otherwise,

$$G = \{g = (g_{ij})_{i,j=1}^3 : g_{ij} \in \mathbb{R}, g^t g = I, \det(g) = 1\},$$

where the transpose $g^t = (g_{ji})_{i,j=1}^3$ coincides with g^{-1} . The mapping

$$p : G \rightarrow \mathbb{S}^2, \quad (g_{ij})_{i,j=1}^3 \mapsto (g_{i3})_{i=1}^3$$

is C^∞ -smooth, and the inverse image of the north pole $e_3 \in \mathbb{S}^2$ is the subgroup

$$K := p^{-1}(\{e_3\}) = \{g \in G : p(g) = e_3\} = \{g \in G : ge_3 = e_3\}.$$

Thus \mathbb{S}^2 is diffeomorphic to the homogeneous space $G/K = \{gK : g \in G\}$, where $gK = \{gk : k \in K\}$. In the sequel $C^\infty(\mathbb{S}^2) \subset C^\infty(\text{SO}(3))$ means that we identify a function $f \in C^\infty(\mathbb{S}^2)$ with a function $f \in C^\infty(G)$ satisfying $f(g) = f(gk)$ for every $g \in G$ and $k \in K$.

2 Exponential coordinates

A linear Lie group is a closed subgroup of the general linear group $\text{GL}(n)$ of invertible n -by- n matrices. The Lie algebra \mathfrak{g} of a linear Lie group G consists of those matrices X for which $\exp(tX) \in G$ for every $t \in \mathbb{R}$. This means that $e_X = (t \mapsto \exp(tX))$ is a group homomorphism $\mathbb{R} \rightarrow G$, so called *one-parameter subgroup*; notice that $X = e'_X(0)$. The tangent space at the neutral element $I \in G$ can be naturally identified with the Lie algebra \mathfrak{g} . In the case $G = \text{SO}(3)$, the Lie algebra $\mathfrak{g} = \mathfrak{o}(3)$ consists of real skew-symmetric (i.e. $X^t = -X$) 3-by-3 matrices. Hence $X \in \mathfrak{g}$ is of the form

$$X = X(x) = \begin{pmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{pmatrix},$$

where $x = (x_j)_{j=1}^3 \in \mathbb{R}^3$; we define the norm $\|X\|_{\mathfrak{g}}$ to be $\|x\|_{\mathbb{R}^3}$, so that $X^3 = -\|X\|_{\mathfrak{g}}^2 X$. When $\|X\|_{\mathfrak{g}} = 1$, we obtain the *Rodrigues' rotation formula* $\exp(tX) = I + X \sin t + X^2 (1 - \cos t)$, which equals to

$$\begin{pmatrix} 1 + (x_1^2 - 1)(1 - \cos t) & -x_3 \sin t + x_1 x_2 (1 - \cos t) & x_2 \sin t + x_1 x_3 (1 - \cos t) \\ x_3 \sin t + x_1 x_2 (1 - \cos t) & 1 + (x_2^2 - 1)(1 - \cos t) & -x_1 \sin t + x_2 x_3 (1 - \cos t) \\ -x_2 \sin t + x_1 x_3 (1 - \cos t) & x_1 \sin t + x_2 x_3 (1 - \cos t) & 1 + (x_3^2 - 1)(1 - \cos t) \end{pmatrix}.$$

From this one can prove that $(Y \mapsto \exp(Y)) : \{Y \in \mathfrak{g} : \|Y\|_{\mathfrak{g}} < \pi\} \rightarrow G$ is a smooth injection, and the reader may deduce expressions for the exponential coordinates $tx \in \mathbb{R}^3$ ($x \in \mathbb{S}^2$) in terms of the matrix $(g_{ij})_{i,j=1}^3 = \exp(tX(x)) \in G$.

When $0 < r < \pi$, exponential coordinates identify the ball $\{x \in \mathbb{R}^3 : \|x\|_{\mathbb{R}^3} < r\}$ with a neighbourhood of $I \in G = \text{SO}(3)$. For $\alpha \in \mathbb{N}^3$ and $g = \exp(X(x))$, $\|x\|_{\mathbb{R}^3} \leq r$, let us define a ‘‘monomial q_α in exponential coordinates’’ by

$$q_\alpha(g) := \frac{1}{\alpha!} x^\alpha = \frac{1}{\alpha_1! \alpha_2! \alpha_3!} x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3}.$$

For us the exact behaviour of q_α is relevant only in an arbitrary small neighbourhood of $I \in G$, and with an arbitrary smooth extension we may consider $q_\alpha \in C^\infty(G)$. Actually, we can first define q_γ when $|\gamma| = 1$, and then demand

that $\alpha! \beta! q_{\alpha+\beta} = (\alpha+\beta)! q_\alpha q_\beta$ for every $\alpha, \beta \in \mathbb{N}^3$. In an analogous manner, for $f \in C^\infty(G)$ and $g \in G$, we define

$$(\partial_g^\alpha f)(g) := \partial_{x_1}^{\alpha_1} \partial_{x_2}^{\alpha_2} \partial_{x_3}^{\alpha_3} f(\exp(X(x)) g)|_{x=0} = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \frac{\partial^{\alpha_2}}{\partial x_2^{\alpha_2}} \frac{\partial^{\alpha_3}}{\partial x_3^{\alpha_3}} f(\exp(X(x)) g)|_{x=0}.$$

Here we should warn that we have interpreted elements of \mathfrak{g} as *right-invariant* vector fields on G , not as *left-invariant* ones (which is more common in literature).

3 Euler angles

Rotations by angle $\phi \in \mathbb{R}$ around the x_1 -, x_2 - and x_3 -axis, respectively, are expressed by the matrices $\omega_1(\phi)$, $\omega_2(\phi)$, $\omega_3(\phi)$ given by

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos(\phi) & -\sin(\phi) \\ 0 & \sin(\phi) & \cos(\phi) \end{pmatrix}, \quad \begin{pmatrix} \cos(\phi) & 0 & \sin(\phi) \\ 0 & 1 & 0 \\ -\sin(\phi) & 0 & \cos(\phi) \end{pmatrix}, \quad \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

We represent rotations by *Euler angles* $\phi, \theta, \psi \in \mathbb{R}$. Any $g \in G = \text{SO}(3)$ has a form

$$g = \omega(\phi, \theta, \psi) := \omega_3(\phi) \omega_2(\theta) \omega_3(\psi),$$

where $0 \leq \phi, \psi < 2\pi$ and $0 \leq \theta \leq \pi$. If $0 < \theta_1, \theta_2 < \pi$ then $\omega(\phi_1, \theta_1, \psi_1) = \omega(\phi_2, \theta_2, \psi_2)$ if and only if $\theta_1 = \theta_2$ and $\phi_1 \equiv \phi_2 \pmod{2\pi}$ and $\psi_1 \equiv \psi_2 \pmod{2\pi}$; thus we conclude that the Euler angles provide local coordinates for the manifold G nearby a point $\omega(\phi, \theta, \psi)$ whenever $\theta \not\equiv 0 \pmod{\pi}$.

The group G acts transitively on the space \mathbb{S}^2 . Since $\omega(\phi, \theta, \psi) \in G$ equals to

$$\begin{pmatrix} \cos \phi \cos \theta \cos \psi - \sin \phi \sin \psi & -\cos \phi \cos \theta \sin \psi - \sin \phi \cos \psi & \cos \phi \sin \theta \\ \sin \phi \cos \theta \cos \psi + \cos \phi \sin \psi & -\sin \phi \cos \theta \sin \psi + \cos \phi \cos \psi & \sin \phi \sin \theta \\ -\sin \theta \cos \psi & \sin \theta \sin \psi & \cos \theta \end{pmatrix},$$

it moves the north pole $e_3 \in \mathbb{S}^2$ to the point $\omega(\phi, \theta, \psi)e_3 = \begin{pmatrix} \cos \phi \sin \theta \\ \sin \phi \sin \theta \\ \cos \theta \end{pmatrix}$.

4 Invariant integration

On a compact group G there exists a unique translation-invariant regular Borel probability measure, called the *Haar measure* μ_G ; customarily $L^2(G)$ refers to $L^2(G, \mu_G)$. Using the Euler angle coordinates on $G = \text{SO}(3)$, we define an orthogonal projection $P_{\mathbb{S}^2} \in \mathcal{L}(L^2(G))$ by

$$(P_{\mathbb{S}^2} f)(\omega(\phi, \theta, \psi)) = \frac{1}{2\pi} \int_0^{2\pi} f(\omega(\phi, \theta, \tilde{\psi})) d\tilde{\psi}$$

for almost all $g = \omega(\phi, \theta, \psi)$. With the natural interpretation $P_{\mathbb{S}^2} f \in L^2(\mathbb{S}^2)$, and if $f \in C^\infty(G)$ then $P_{\mathbb{S}^2} f \in C^\infty(\mathbb{S}^2)$. Thereby $\int_G f \, d\mu_G = \int_{\mathbb{S}^2} P_{\mathbb{S}^2} f$, where the measure on the sphere is the normalized angular part of the Lebesgue measure of \mathbb{R}^3 . This yields the *Haar integral*

$$f \mapsto \int_G f \, d\mu_G = \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^\pi \int_0^{2\pi} f(\omega(\phi, \theta, \psi)) \sin(\theta) \, d\phi \, d\theta \, d\psi.$$

5 Fourier series on $\text{SO}(3)$ and \mathbb{S}^2

Let $G = \text{SO}(3)$. For each $l \in \mathbb{N}$ there exists a group homomorphism $t^l : G \rightarrow \text{GL}(2l+1)$, where $t^l(g)$ is a unitary matrix for every $g \in G$. Actually, any unitary representation of G is equivalent to a direct sum of such unitary matrix representations. The matrix elements of $t^l(g) = (t_{mn}^l(g))_{m,n=-l}^l$ can be factorized with respect to the Euler angles:

$$t_{mn}^l(\omega(\phi, \theta, \psi)) = e^{-i(m\phi+n\psi)} P_{mn}^l(\cos(\theta));$$

the exact expression for P_{mn}^l can be found in [8]. Now $\{\sqrt{2l+1} \overline{t_{mn}^l} : l \in \mathbb{N}, m, n \in \mathbb{Z}, -l \leq m, n \leq l\}$ is an orthonormal basis for $L^2(G)$, and thus $f \in C^\infty(G)$ has a Fourier series representation

$$f = \sum_{l=0}^{\infty} (2l+1) \sum_{m=-l}^l \sum_{n=-l}^l \widehat{f}(l)_{mn} \overline{t_{mn}^l},$$

where the Fourier coefficients are computed by

$$\widehat{f}(l)_{mn} := \langle f, \overline{t_{mn}^l} \rangle_{L^2(G)} = \int_G f(g) t_{mn}^l(g) \, d\mu_G(g).$$

Notice that $\overline{t_{mn}^l(g)} = (t^l(g)^*)_{nm} = t_{nm}^l(g^{-1})$. Evidently, the values of $f \in C^\infty(\mathbb{S}^2) \subset C^\infty(G)$ do not depend on the Euler angle ψ , so that in this case $\widehat{f}(l)_{mn} = 0$ whenever $n \neq 0$.

Let M be a smooth compact manifold without a boundary, i.e. a smooth closed manifold. In the sequel, $\mathcal{D}(M)$ denotes the space $C^\infty(M)$ endowed with the usual Fréchet space structure of test functions. The convolution $f_1 * f_2 \in \mathcal{D}(G)$ of $f_1, f_2 \in \mathcal{D}(G)$ is defined by

$$(f_1 * f_2)(g) := \int_G f_1(gh^{-1}) f_2(h) \, d\mu_G(h).$$

Since t^l is a group homomorphism, we get

$$\widehat{f_1 * f_2}(l) = \widehat{f_1}(l) \widehat{f_2}(l), \quad \text{i.e.} \quad \widehat{f_1 * f_2}(l)_{mn} = \sum_{k=-l}^l \widehat{f_1}(l)_{mk} \widehat{f_2}(l)_{kn}.$$

The Fourier transform of distributions $f_1, f_2 \in \mathcal{D}'(G)$ is defined by duality.

Let A be a continuous linear operator $\mathcal{D}(G) \rightarrow \mathcal{D}(G)$. Then for each $l \in \mathbb{N}$ there is a unique matrix-valued function $g \mapsto \sigma_A(g, l) = (\sigma_A(g, l)_{mn})_{m,n=-l}^l$ such that

$$\begin{aligned} (Af)(g) &= \sum_{l=0}^{\infty} (2l+1) \operatorname{Tr} \left(\sigma_A(g, l) \widehat{f}(l) t^l(g)^* \right) \\ &= \sum_{l=0}^{\infty} (2l+1) \sum_{m=-l}^l \sum_{n=-l}^l \left(\sum_{k=-l}^l \sigma_A(g, l)_{mk} \widehat{f}(l)_{kn} \right) \overline{t_{mn}^l(g)} \end{aligned}$$

for every $f \in \mathcal{D}(G)$ and $g \in G$; actually,

$$\sigma_A(g, l) = t^l(g) (A(t^{l*}))(g), \quad \text{i.e.} \quad \sigma_A(g, l)_{mk} = \sum_{j=-l}^l t_{mj}^l(g) (\overline{At_{kj}^l})(g).$$

We call the mapping $(g, l) \mapsto \sigma_A(g, l)$ (where $g \in G, l \in \mathbb{N}$) the *matrix symbol* of A . Let $s_A : G \rightarrow \mathcal{D}'(G)$ satisfy $\widehat{s_A(g)}(l) = \sigma_A(g, l)$, and let $\sigma_A(g)$ denote the convolution operator $f \mapsto s_A(g) * f$. Then $(Af)(g) = (\sigma_A(g)f)(g)$, and if K_A is the Schwartz kernel of A then $K_A(g, h) = s_A(g)(gh^{-1})$ in the sense of distributions. One can say that the symbol σ_A presents a linear operator A as a G -parametrized family of convolution operators.

Operator $A \in \mathcal{L}(\mathcal{D}(G))$ belongs to $\mathcal{L}(\mathcal{D}(\mathbb{S}^2))$ if and only if it maps $C^\infty(\mathbb{S}^2)$ into $C^\infty(\mathbb{S}^2)$, or equivalently if and only if $g \mapsto \sigma_A(g, l)$ belongs to $C^\infty(\mathbb{S}^2)$ for every $l \in \mathbb{N}$.

The Sobolev space $H^s(G)$ of order $s \in \mathbb{R}$ consists of distributions f on G having a finite norm

$$\|f\|_{H^s} := \left(\sum_{l=0}^{\infty} (2l+1)^{2s+1} \sum_{m=-l}^l \sum_{n=-l}^l |\widehat{f}(l)_{mn}|^2 \right)^{1/2}.$$

For any $r \in \mathbb{R}$, $\widehat{\Xi^r f}(l) := (2l+1)^r \widehat{f}(l)$ defines a linear Sobolev space isomorphism $\Xi^r : H^s(G) \rightarrow H^{s-r}(G)$. It is noteworthy that Ξ^r commutes with any convolution operator. Hence, to characterize Sobolev boundedness of convolution operators, it is enough to characterize L^2 -boundedness (after all, $L^2(G) = H^0(G)$): the norm $\|\sigma_A(g_0)\|_{\mathcal{L}(L^2(G))}$ of a convolution operator $\sigma_A(g_0)$ is

$$\sup_{l \in \mathbb{N}} \|\sigma_A(g_0, l)\|_{\mathcal{L}(C^{2l+1})} := \sup_{l \in \mathbb{N}} \sup_{x: \|x\|_{C^{2l+1}} \leq 1} \|\sigma_A(g_0, l)x\|_{C^{2l+1}}$$

where $x \mapsto \|x\|_{C^{2l+1}} = (|x_1|^2 + \dots + |x_{2l+1}|^2)^{1/2}$.

6 Pseudodifferential calculus

Let $\mathcal{S}(\mathbb{R}^n)$ be the Schwartz test function space (i.e. rapidly decreasing smooth functions with the natural Fréchet space structure) on \mathbb{R}^n ; the Fourier transform $\widehat{f} \in \mathcal{S}(\mathbb{R}^n)$ of $f \in \mathcal{S}(\mathbb{R}^n)$ is given by

$$\widehat{f}(\xi) = \int_{\mathbb{R}^n} f(x) e^{-i2\pi x \cdot \xi} dx.$$

A linear operator $A : \mathcal{S}(\mathbb{R}^n) \rightarrow \mathcal{S}(\mathbb{R}^n)$ of the form

$$(Af)(x) = \int_{\mathbb{R}^n} \sigma_A(x, \xi) \widehat{f}(\xi) e^{i2\pi x \cdot \xi} d\xi$$

is called a *pseudodifferential operator of order $m \in \mathbb{R}$* , denoted by $A \in \Psi^m(\mathbb{R}^n)$, if its *symbol* $\sigma_A \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$ satisfies the inequalities

$$|\partial_\xi^\alpha \partial_x^\beta \sigma_A(x, \xi)| \leq C_{Am\alpha\beta} (1 + |\xi|)^{m-|\alpha|}$$

uniformly in $x \in \mathbb{R}^n$, for every $\alpha, \beta \in \mathbb{N}^n$; $C_{Am\alpha\beta}$ is a constant depending on A, m, α, β .

Corresponding pseudodifferential operator classes $\Psi^m(M)$ on a smooth closed manifold M can be defined via chart neighbourhood localizations, since the class $\Psi^m(\mathbb{R}^n)$ is diffeomorphism invariant. In [6] there is a Fourier series characterization of pseudodifferential operators on compact Lie groups and certain homogeneous spaces. In [4] and [6] the symbolic calculus formulae are presented in general form, but here it is best to express them explicitly for \mathbb{S}^2 and $\text{SO}(3)$.

Let $G = \text{SO}(3)$. Recall the functions $q_\alpha \in C^\infty(G)$, “monomials in exponential coordinates”. Recall that if $s \in \mathcal{S}(\mathbb{R}^n)$ then $x \mapsto x^\alpha s(x)$ has the Fourier transform $\xi \mapsto (\partial_\xi^\alpha \widehat{s})(\xi)$; this motivates the definition of a “quasi-difference operator” Q^α acting on symbols of linear operators $A \in \mathcal{L}(\mathcal{D}(G))$:

$$Q^\alpha \sigma_A(g, l) := \widehat{q_\alpha s_A}(g)(l).$$

The idea is roughly that Q^α resembles a “differentiation of order $\alpha \in \mathbb{N}$ ” with respect to the variable l . For instance, if $A, B \in \Psi^m(G)$ then an asymptotic expansion for the symbol of the composite AB is

$$\sigma_{AB}(g, l) \sim \sum_{\alpha \geq 0} (Q^\alpha \sigma_A(g, l)) \partial_g^\alpha \sigma_B(g, l);$$

that is, in one just replaces the convolution operators $\sigma_A(x)$ and $\sigma_B(x)$ of [6] by matrices $\sigma_A(g, l)$ and $\sigma_B(g, l)$, and so on. In [6] one finds analogous asymptotic expansions for “amplitude operators”, adjoints and parametrices, so that we are not going to state them again.

From [6] it follows that if $A \in \Psi^m(G)$ maps $\mathcal{D}(\mathbb{S}^2)$ into $\mathcal{D}(\mathbb{S}^2)$ then $A|_{\mathcal{D}(\mathbb{S}^2)} \in \Psi^m(\mathbb{S}^2)$. Conversely, if $B \in \Psi^m(\mathbb{S}^2)$ then there exists $A \in \Psi^m(G)$ such that $A|_{\mathcal{D}(\mathbb{S}^2)} = B$. Moreover, operations Q^α and ∂_g^β respect the K -right-invariance in the sense that if $\sigma_A(gk, l) = \sigma_A(g, l)$ for $k \in K$ then $Q^\alpha \sigma_A(gk, l) = Q^\alpha \sigma_A(g, l)$ and $\partial_g^\beta \sigma_A(gk, l) = \partial_g^\beta \sigma_A(g, l)$. This means that the asymptotic expansion formulae for $G = \text{SO}(3)$ hold also for \mathbb{S}^2 ! The main point is that if $A \in \Psi^m(G)$ is elliptic and maps $\mathcal{D}(\mathbb{S}^2)$ into $\mathcal{D}(\mathbb{S}^2)$ then we can compute an asymptotic expansion for the parametrix of $A|_{\mathcal{D}(\mathbb{S}^2)} \in \Psi^m(\mathbb{S}^2)$ using the symbolic calculus described above.

7 Future prospects

Much remains to be studied in pseudodifferential calculus on the sphere \mathbb{S}^2 . For instance, for $B \in \Psi^m(\mathbb{S}^2)$ there always exists $A \in \Psi^m(G)$ such that $A|_{\mathcal{D}(\mathbb{S}^2)} = B$, but sometimes A necessarily fails to be elliptic even if B is elliptic [6].

Finally, numerical Fourier analysis on \mathbb{S}^2 needs to be refined: not only would it be important to have stable FFT-like algorithms, but also estimate convergence rates for sequences of Sobolev space interpolation projections. Applications would be widespread, concerning not just pseudodifferential calculus.

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