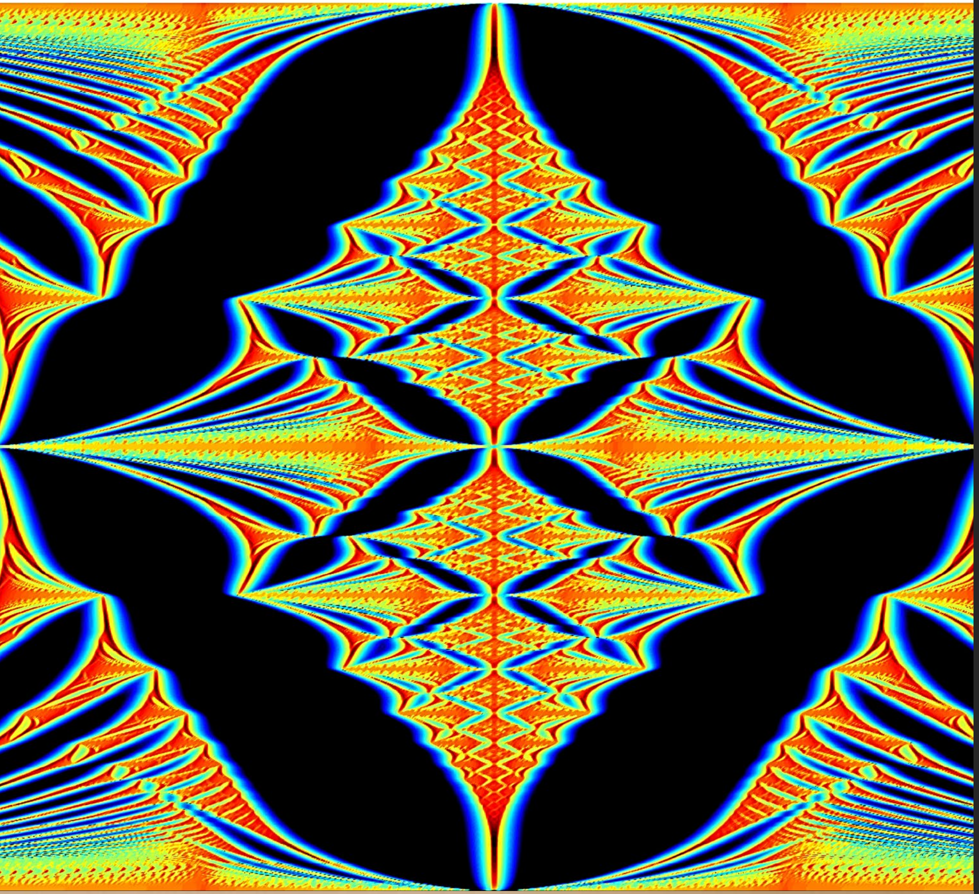

Fast Spectral Methods for Spectral Measures

Using spectral methods for computing spectral properties in infinite dimensions

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University of Cambridge

Spectral measures → diagonalisation

- **Fin.-dim.:** $B \in \mathbb{C}^{n\times n}$, $B^*B = BB^*$, o.n. basis of e-vectors $\{v_j\}_{j=1}^{n}$

$$v = \left[\sum_{j=1}^{n} v_j {v_j}^*\right] v, \qquad Bv = \left[\sum_{j=1}^{n} \lambda_j v_j {v_j}^*\right] v, \qquad \forall v \in \mathbb{C}^n$$

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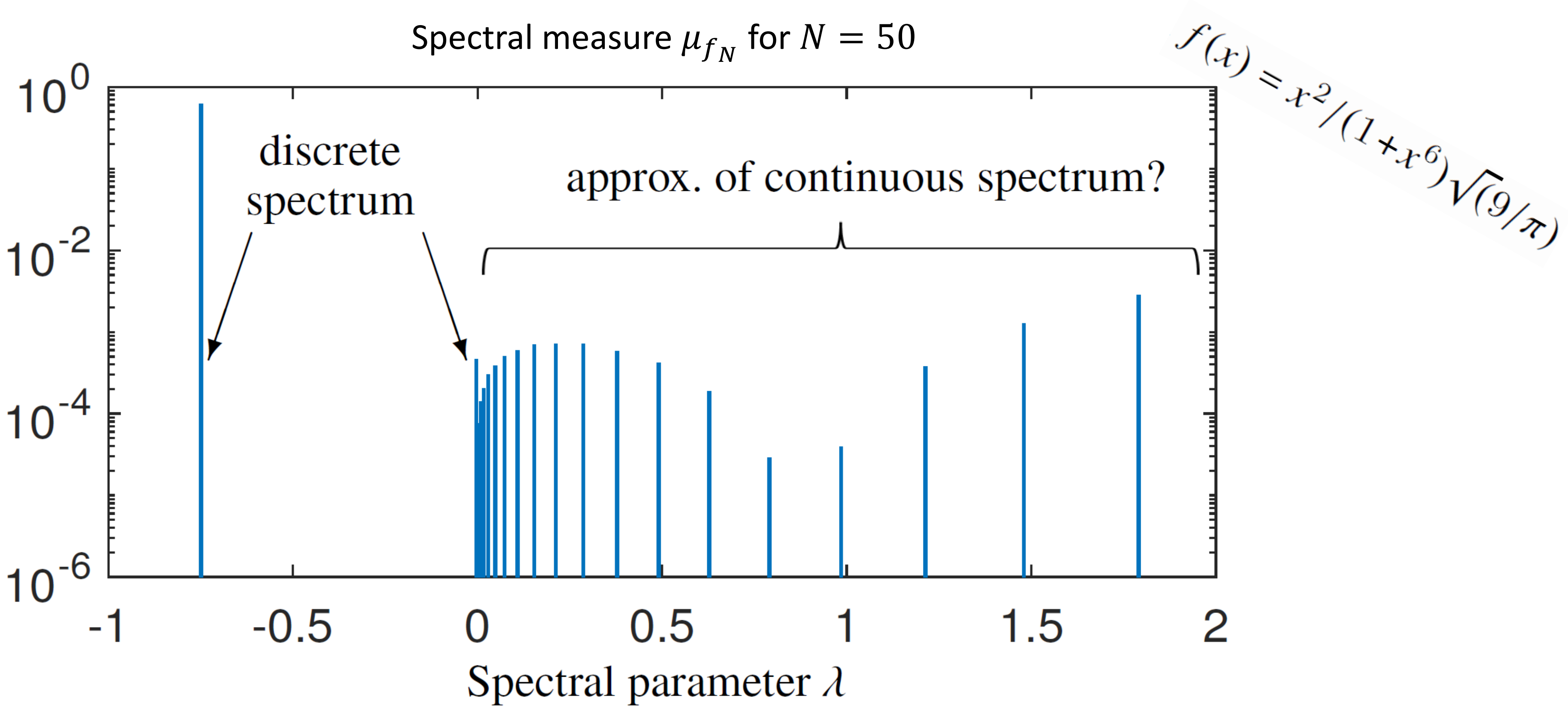
What about infinite dimensions?

Motivating Example on $\mathbb{R}$

- **Operator:** $[\mathcal{L}u](x) = -\frac{\partial^2 u}{\partial x^2}(x) - \frac{3/2}{1+x^2}u(x)$
- **Spectral method:** Mapped Fourier $x = 10i\frac{1-e^{i\theta}}{1+e^{i\theta}}$, basis $\{e^{-iN\theta}, \ldots, e^{iN\theta}\}$

Spectral measure μ_{f_N} for $N = 50$



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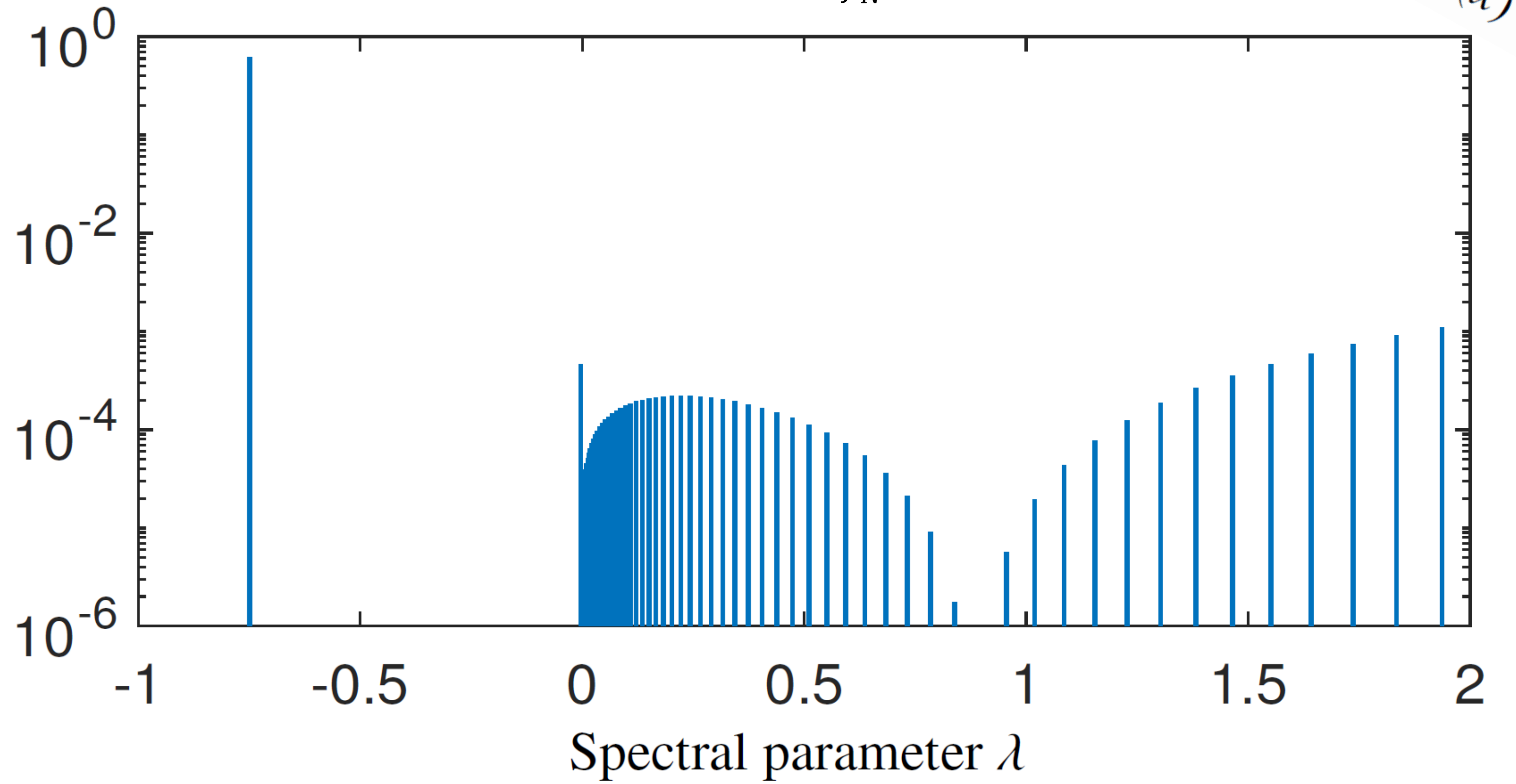

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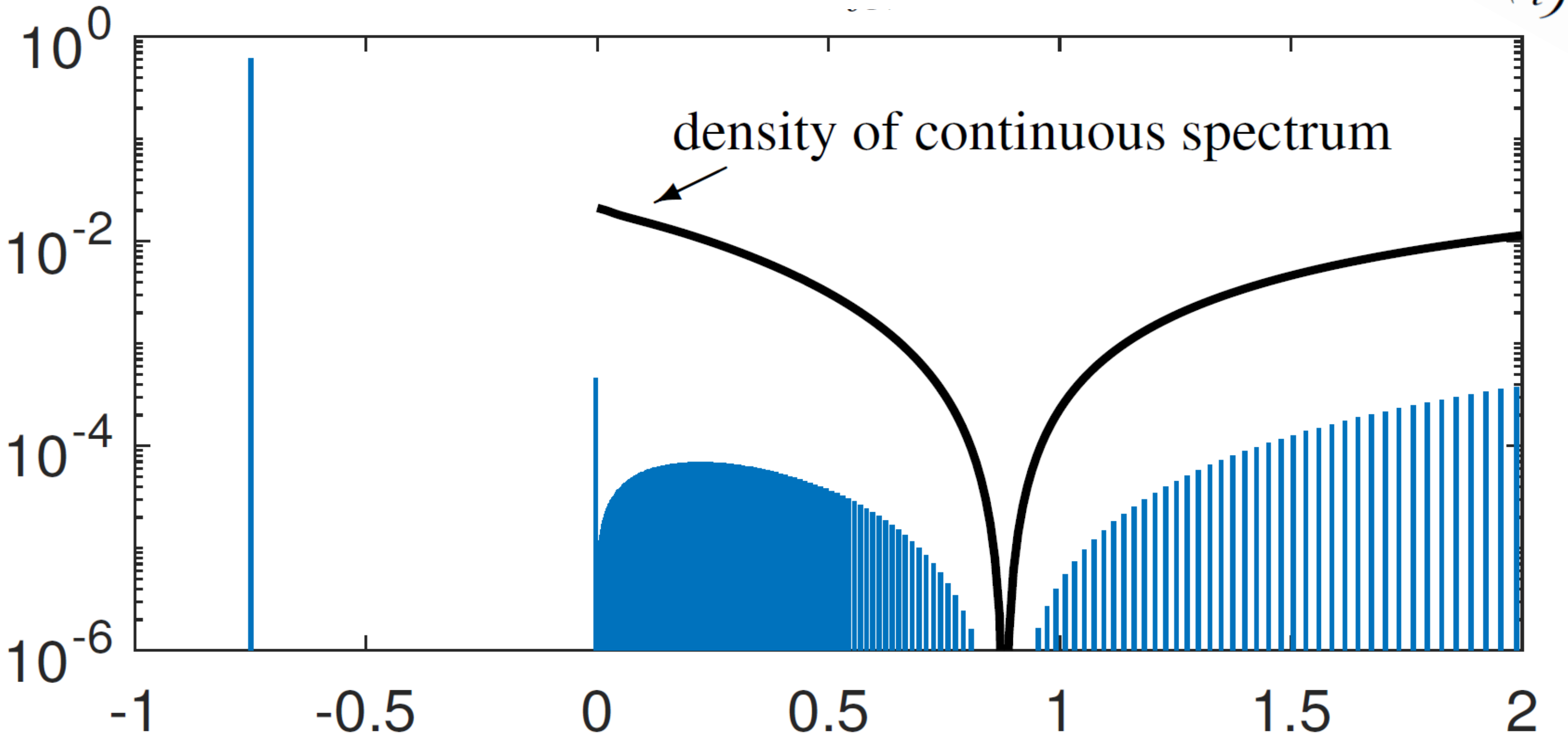

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- **Inf.-dim.:** Operator $\mathcal{L}: \mathcal{D}(\mathcal{L}) \to \mathcal{H}$. Typically, no basis of e-vectors!
  Spectral theorem: (projection-valued) spectral measure E

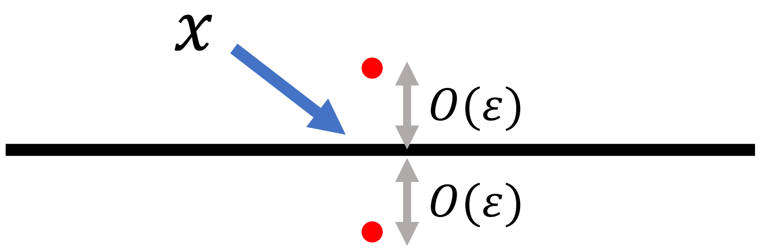
$$f = \left[\int_{\mathrm{Spec}(\mathcal{L})} 1\, \mathrm{d}E(\lambda)\right] f, \qquad \mathcal{L}f = \left[\int_{\mathrm{Spec}(\mathcal{L})} \lambda\, \mathrm{d}E(\lambda)\right] f, \qquad \forall f \in \mathcal{H}$$

- **Spectral measures:** $\mu_f(U) = \langle E(U)f, f\rangle$ ($\|f\| = 1$) prob. Measure on $\mathbb{R}$.

Stone's formula

Smoothed spectral measure:

$$\mu_f^\varepsilon(x) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{\varepsilon\, \mathrm{d}\mu_f(\lambda)}{(x-\lambda)^2+\varepsilon^2} = \frac{\langle [(\mathcal{L}-[x+i\varepsilon])^{-1}-(\mathcal{L}-[x-i\varepsilon])^{-1}]f, f\rangle}{2\pi i}$$



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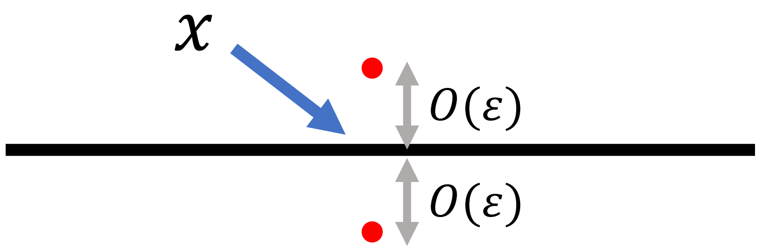
- Smaller ε needs larger N ($N = N(\varepsilon)$ crucial!)
- Very slow convergence: $\mathcal{O}(\varepsilon \log(1/\varepsilon))$



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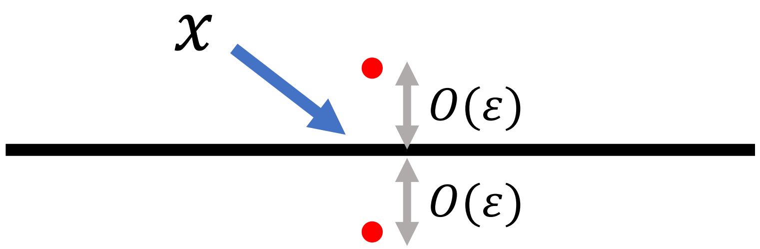


$\varepsilon =$ "smoothing parameter"

Can we do better?

High-order Stone's formula

mth order rational "smoothing" kernels:

$$K(x) = \frac{1}{2\pi i}\sum_{j=1}^{m} \frac{\alpha_j}{x - a_j} - \frac{\bar{\alpha}_j}{x - \bar{a}_j}, \qquad K_\varepsilon(x) = K(x/\varepsilon)/\varepsilon$$

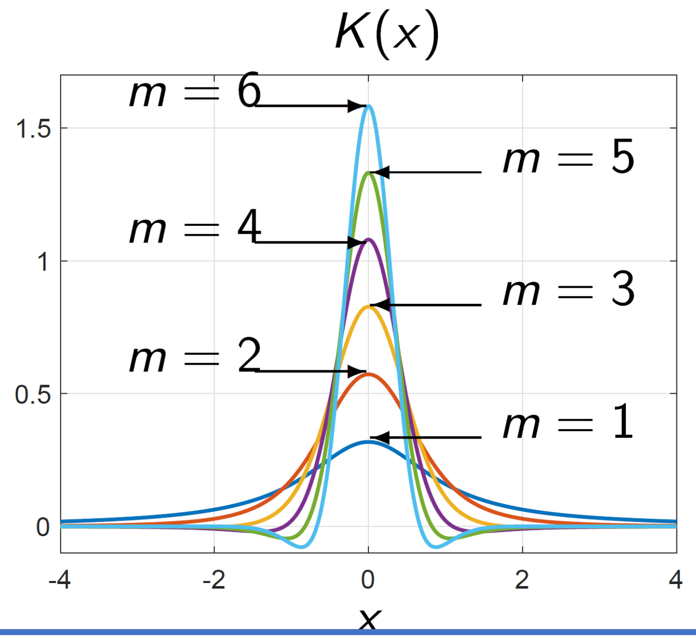
$$[K_\varepsilon * \mu_f](x) = \frac{-1}{2\pi i}\sum_{j=1}^{m}\langle [\alpha_j(\mathcal{L} - [x - \varepsilon a_j])^{-1} - \bar{\alpha}_j(\mathcal{L} - [x - \varepsilon \bar{a}_j])^{-1}]f, f\rangle$$

$\Longrightarrow \mathcal{O}(\varepsilon^m \log(1/\varepsilon))$ **convergence**

$\Longrightarrow$ **smaller** $N(\varepsilon)$ **for a given accuracy**

Two steps:

- Solve linear systems $(\mathcal{L} - z)^{-1}$
- Compute inner products



- C., Horning, Townsend *"Computing spectral measures of self-adjoint operators,"* **SIAM Rev.**, 2021.

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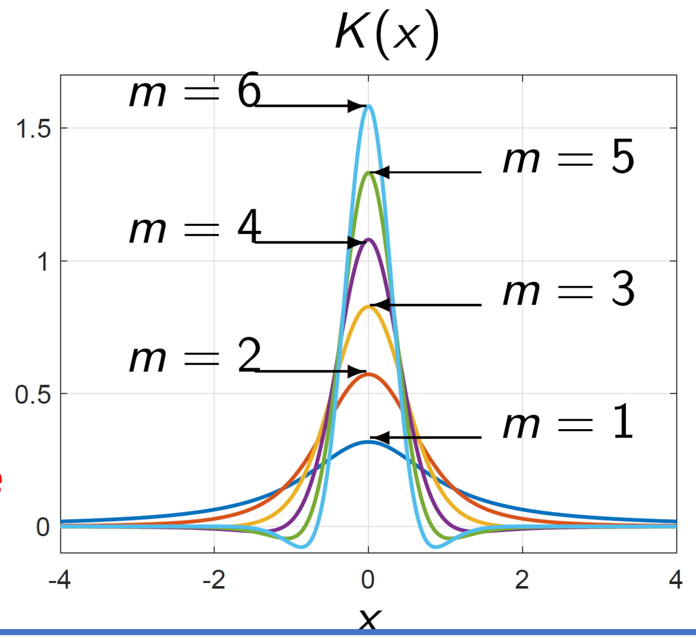

Two steps:

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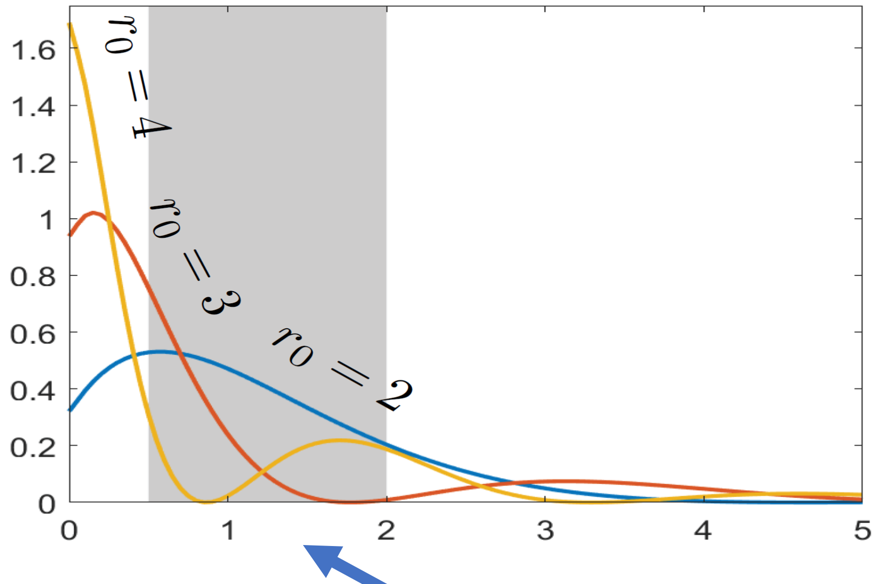
Use whatever you want here, as long as truncation size can be chosen adaptively. We use fast spectral methods!

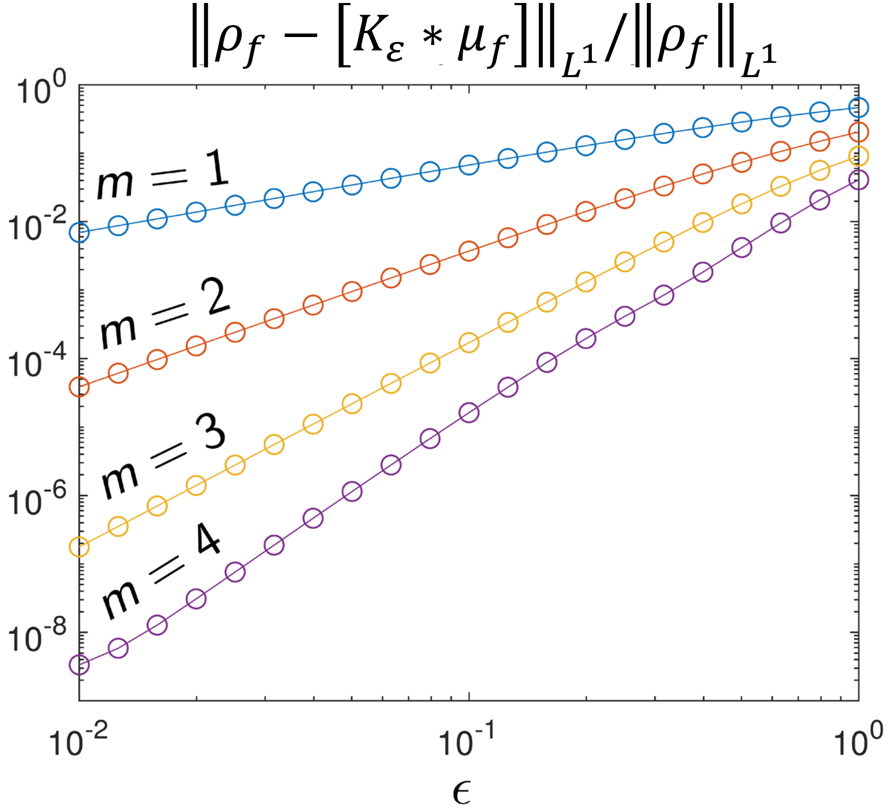
- C., Horning, Townsend "*Computing spectral measures of self-adjoint operators,*" **SIAM Rev.**, 2021.

Example 2: Radial Schrödinger

- **Operator:** $[\mathcal{L}u](r) = -\frac{d^2u}{dr^2}(r) + \left(\frac{\ell(\ell+1)}{r^2} + \frac{1}{r}(e^{-r}-1)\right)u(r), \qquad r > 0.$
- **Spectral method(+):** Mapped ultraspherical (sparse spectral method)



Wavefunction $\propto e^{-(r-r_0)^2}$



(+) Olver, Townsend, *"A fast and well-conditioned spectral method,"* **SIAM Rev.**, 2013.

Self-adjoint pencils

$$\mathcal{A} - \lambda\mathcal{B} \;\rightarrow\; \mathcal{L} = \mathcal{B}^{-1}\mathcal{A}, \qquad \mathcal{H}_{\mathcal{B}} = \mathcal{D}\left(\mathcal{B}^{1/2}\right), \qquad \langle f, g\rangle_{\mathcal{B}} = \left\langle \mathcal{B}^{1/2} f, \mathcal{B}^{1/2} g\right\rangle$$

Algorithm A computational framework for evaluating an approximate spectral measure of an operator $\mathcal{L}$ corresponding to the pencil $\mathcal{A} - \lambda\mathcal{B}$ at $x_0 \in \mathbb{R}$ with respect to a vector $f \in \mathcal{D}(\mathcal{B})$.

Input: $\mathcal{A}$, $\mathcal{B}$, $f \in \mathcal{D}(\mathcal{B})$, $x_0 \in \mathbb{R}$, $a_1, \ldots, a_m \in \{z \in \mathbb{C} : \mathrm{Im}(z) > 0\}$, and $\epsilon > 0$.

1: Compute $g = \mathcal{B} f$.

2: Solve the Vandermonde system (6) for the residues $\alpha_1, \ldots, \alpha_m \in \mathbb{C}$.

3: Solve $(\mathcal{A} - (x_0 - \epsilon a_j)\mathcal{B})u_j^{\epsilon} = g$ for $1 \leq j \leq m$.

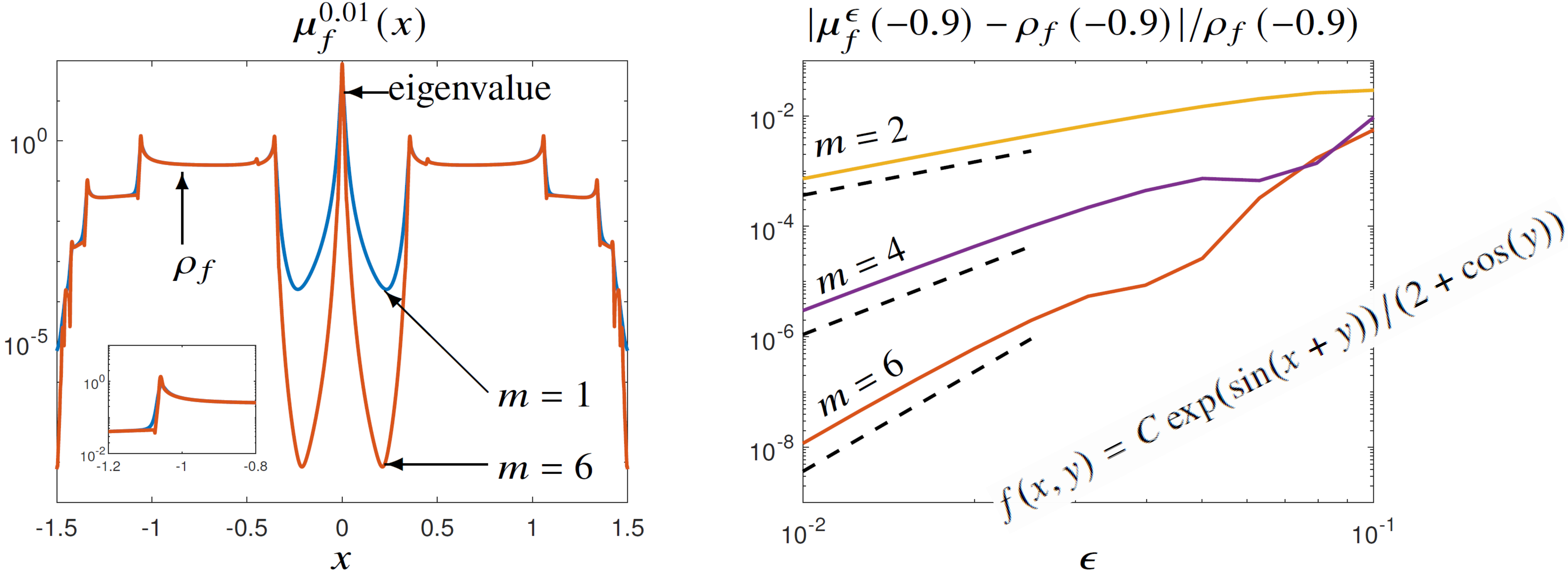
4: Compute $\mu_f^{\epsilon}(x_0) = \frac{-1}{\pi}\mathrm{Im}\left(\sum_{j=1}^{m} \alpha_j \langle u_j^{\epsilon}, g\rangle\right)$.

Output: The approximate spectral measure $\mu_f^{\epsilon}(x_0)$.

- C., Horning "*SpecSolve: Spectral methods for spectral measures,*" **ICOSAHOM.**, 2021.

Example 3: Pseudo-differential operators

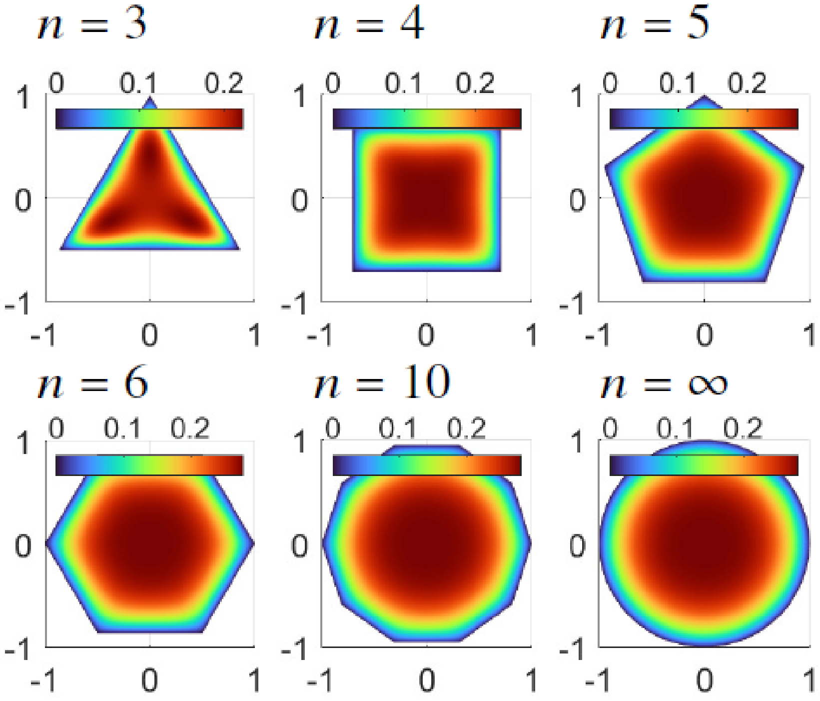
- **Operator:** $\mathcal{A} = -i(1 + \cos(x)/2)\partial_y, \quad \mathcal{B} = (1 - \partial_y^2)^{1/2}, \quad x, y \in [-\pi, \pi]_{\text{per}}$
- **Spectral method:** Tensorised Fourier



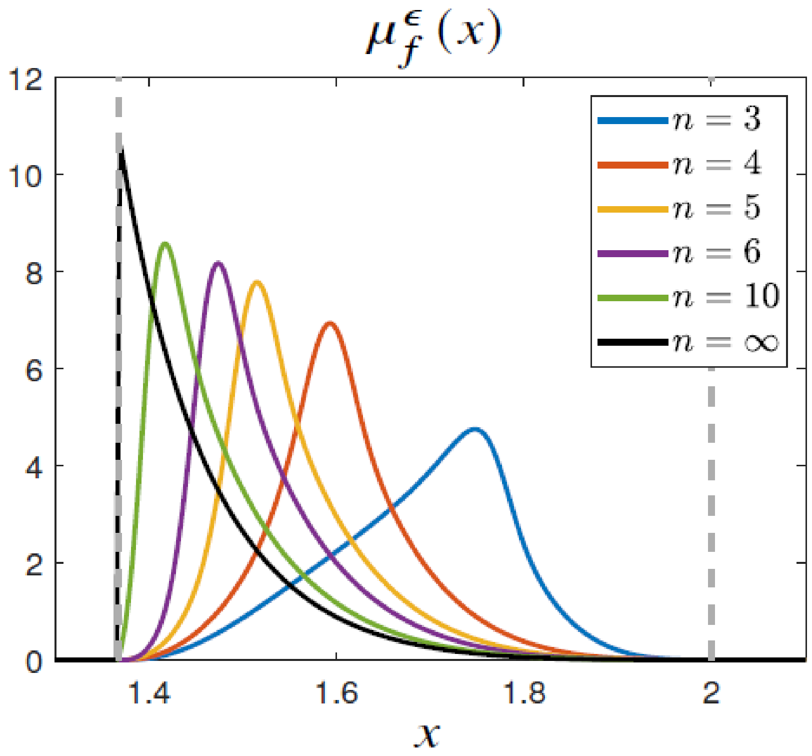
- De Verdiere, Saint-Raymond, *"Attractors for Two-Dimensional Waves with Homogeneous Hamiltonians of Degree 0,"* **CPAM**, 2020.

Example 4: Preconditioners for PDEs

- **Operator:** Bounded Lip. domain, $\mathcal{A}u = -\nabla \cdot [(1 + \exp(-x^2 - y^2))\nabla u], \quad \mathcal{B}u = -\nabla^2 u$
- **Spectral method**(+)**:** (hp-adap. and sparse) ultraspherical spectral element method



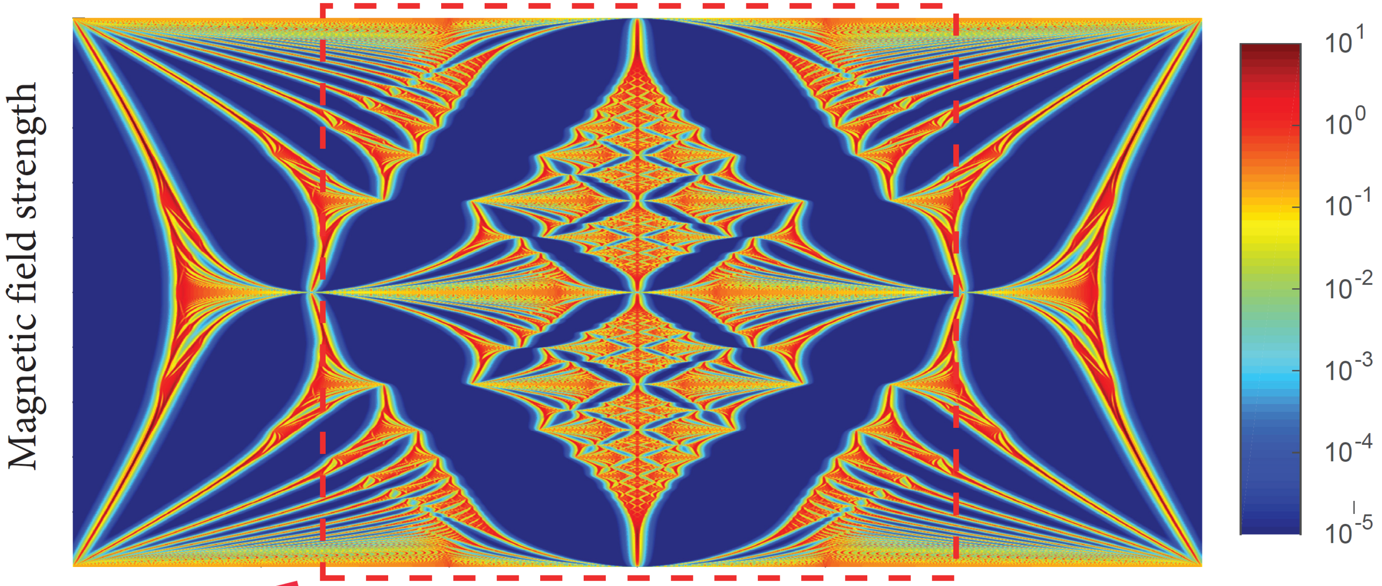
$f = C(\Omega)\mathcal{B}^{-1}g$, where $g(x, y) = x^2 + y^2$



- Gergelits, Mardal, Nielsen, Strakos, *"Laplacian preconditioning of elliptic PDEs: Localization of the eigenvalues of the discretized operator,"* **SINUM**, 2019.

(+) Fortunato, Hale, Townsend, *"The ultraspherical spectral element method." **J. Comput. Phys**, 2021.*

Spectral measures of self-adjoint operators



Horizontal slice = spectral measure at constant magnetic field strength.

Software package

`SpecSolve` available at https://github.com/SpecSolve

Capabilities: ODEs, PDEs, integral operators, discrete operators.

- C., Horning, Townsend "*Computing spectral measures of self-adjoint operators,*" **SIAM Rev.**, 2021.

Wider programme

Foundations of computation ↔ **Practical computation**

- **Solvability Complexity Index Hierarchy**: classify difficulty of comp. problems.
- Prove algorithms are optimal.
- Figure out assumptions + methods needed for computational goal.

- Infinite-dimensional numerical analysis.
- "**Solve-then-discretize**": avoid the woes of discretization!
- Compute quantities rigorously.

- Horning, Townsend, *"FEAST for Differential Eigenvalue Problems,"* **SIAM J. Numer. Anal.,** 2020.
- Colbrook, *"Computing semigroups with error control,"* **SIAM J. Numer. Anal.**, 2022.
- Colbrook, *"On the computation of geometric features of spectra of linear operators on Hilbert spaces,"* **Found. Comput. Math.**, 2022.
- Colbrook, Antun, Hansen, "*The difficulty of computing stable and accurate neural networks: On the barriers of deep learning and Smale's 18th problem,*" **PNAS**, 2022.
- Ben-Artzi, Colbrook, Hansen, Nevanlinna, Seidel, *"On the solvability complexity index hierarchy and towers of algorithms,"* arXiv, 2020.