How to diagonalize differential and integral operators

(with continuous spectrum)

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Computing with differential and integral operators

$$\mathcal{L} : \mathcal{D}(\mathcal{L}) \to \mathcal{H}$$ **Self-adjoint**

E.g., $$\mathcal{L} = a_K(x)\frac{d^K}{dx^K} + \cdots + a_1(x)\frac{d}{dx} + a_0(x) \qquad \mathcal{L}u(x) = a(x)u(x) + \int_{-1}^{1} k(x,y)u(y)\,dy$$

Matrix		Operator
$Ax = \hat{\lambda}x$	**Discretize** $\leftarrow$	$\mathcal{L}u = \lambda u$
Numerical linear algebra $\downarrow$		
$\hat{\lambda}_1, \ldots, \hat{\lambda}_m$ $\hat{x}_1, \ldots, \hat{x}_m$	$\rightarrow$ **Approximate**	$\lambda_1, \ldots, \lambda_m$ $u_1, \ldots, u_m$

Current paradigm

[Chatelin, 1983][Boyd, 1989][Reddy, 2006]

Spectral measures of operators

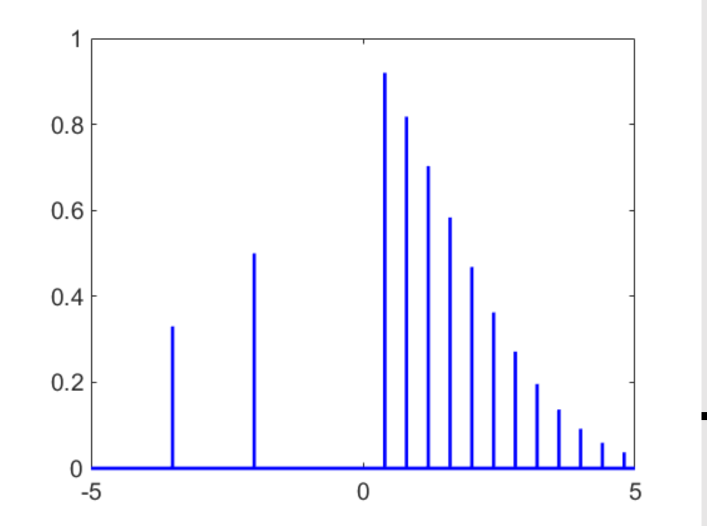
$$\mathcal{L} : \mathcal{D}(\mathcal{L}) \to \mathcal{H}$$ **Self-adjoint**

E.g., $$\mathcal{L} = a_K(x)\frac{d^K}{dx^K} + \cdots + a_1(x)\frac{d}{dx} + a_0(x) \qquad \mathcal{L}u(x) = a(x)u(x) + \int_{-1}^{1} k(x,y)u(y)\, dy$$

Matrix

$$d\mu_v(\lambda) = \sum_k c_k\, \delta(\lambda - \lambda_k)$$

$$c_k = \langle P_k v, v\rangle$$



Discretize

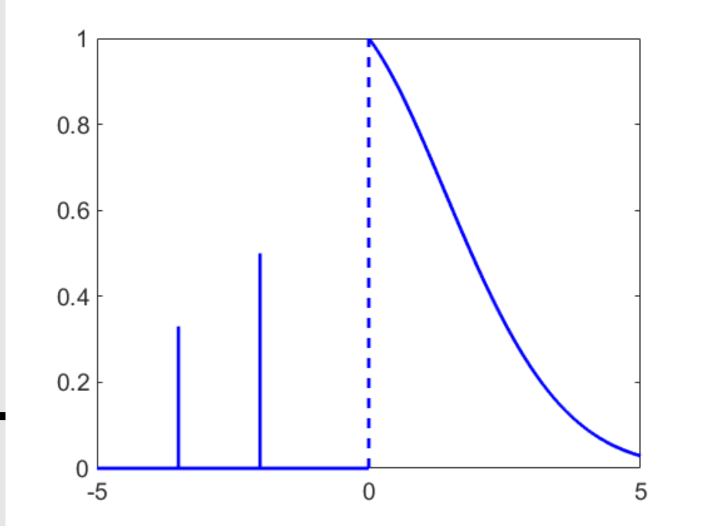
[Mayer et al, 1985]

Approximate

Operator

$$d\mu_f(\lambda) = \rho_f(\lambda) + \sum_k c_k\, \delta(\lambda - \lambda_k)$$

$$c_k = \langle \mathcal{P}_k f, f\rangle$$



Current paradigm?

Spectral measures of operators

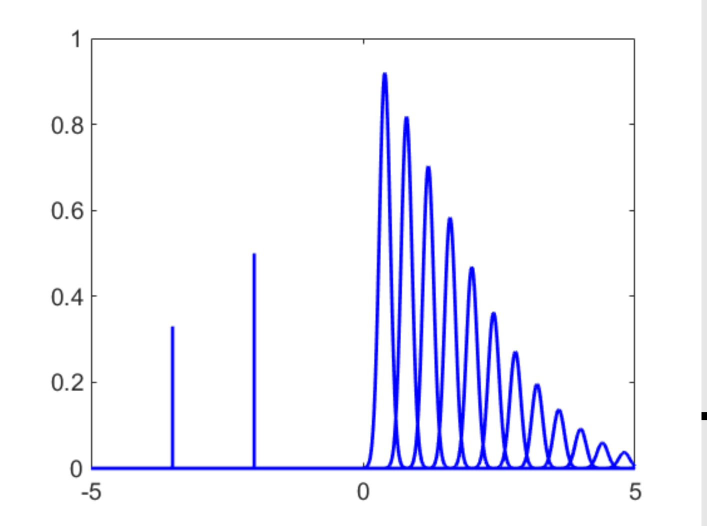
$$\mathcal{L} : \mathcal{D}(\mathcal{L}) \to \mathcal{H}$$ **Self-adjoint**

E.g., $$\mathcal{L} = a_K(x)\frac{d^K}{dx^K} + \cdots + a_1(x)\frac{d}{dx} + a_0(x) \qquad \mathcal{L}u(x) = a(x)u(x) + \int_{-1}^{1} k(x,y)u(y)\,dy$$

Matrix

$$d\mu_v^\epsilon(\lambda) = \sum_k c_k\, K_\epsilon(\lambda - \lambda_k)$$

$$c_k = \langle P_k v, v\rangle$$



Discretize

Smooth

[Haydock et al, 1972]

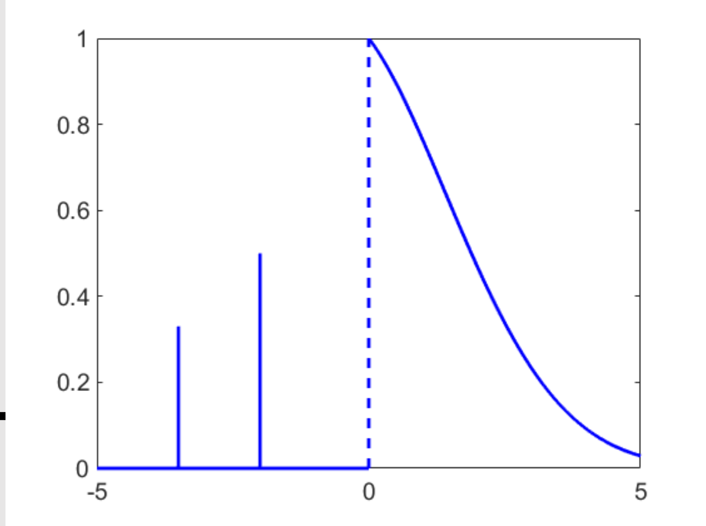
[Lin et al, 2016]

Approximate

Operator

$$d\mu_f(\lambda) = \rho_f(\lambda) + \sum_k c_k\, \delta(\lambda - \lambda_k)$$

$$c_k = \langle \mathcal{P}_k f, f\rangle$$



Current paradigm

Smoothed spectral measures

$$\mathcal{R}_{\mathcal{L}}(z) = (\mathcal{L} - z)^{-1}$$

Spectral identity for resolvent ⬇

$$\langle \mathcal{R}_{\mathcal{L}}(z) f, f \rangle = \int_{\mathbb{R}} \frac{d\mu_f(\lambda)}{\lambda - z}$$

$$\frac{1}{\pi} \overbrace{\left(\langle \mathcal{R}_{\mathcal{L}}(x + i\epsilon) f, f \rangle - \langle \mathcal{R}_{\mathcal{L}}(x - i\epsilon) f, f \rangle \right)}^{\mathrm{Im}\langle \mathcal{R}_{\mathcal{L}}(z) f, f \rangle} = \int_{\mathbb{R}} \overbrace{\frac{1}{\pi} \frac{\epsilon^2}{(\lambda - x)^2 + \epsilon^2}}^{\text{Poisson kernel (shifted and scaled)}} d\mu_f(\lambda)$$

$$= \sum_k \frac{1}{\pi} \frac{\epsilon^2 \langle \mathcal{P}_k f, f \rangle}{(\lambda_k - x)^2 + \epsilon^2} + \underbrace{\int_{\mathbb{R}} \frac{1}{\pi} \frac{\epsilon^2}{(\lambda - x)^2 + \epsilon^2} \rho_f(\lambda) d\lambda}_{\to \rho_f(x) \quad \text{(if continuous)}}$$

A simple framework

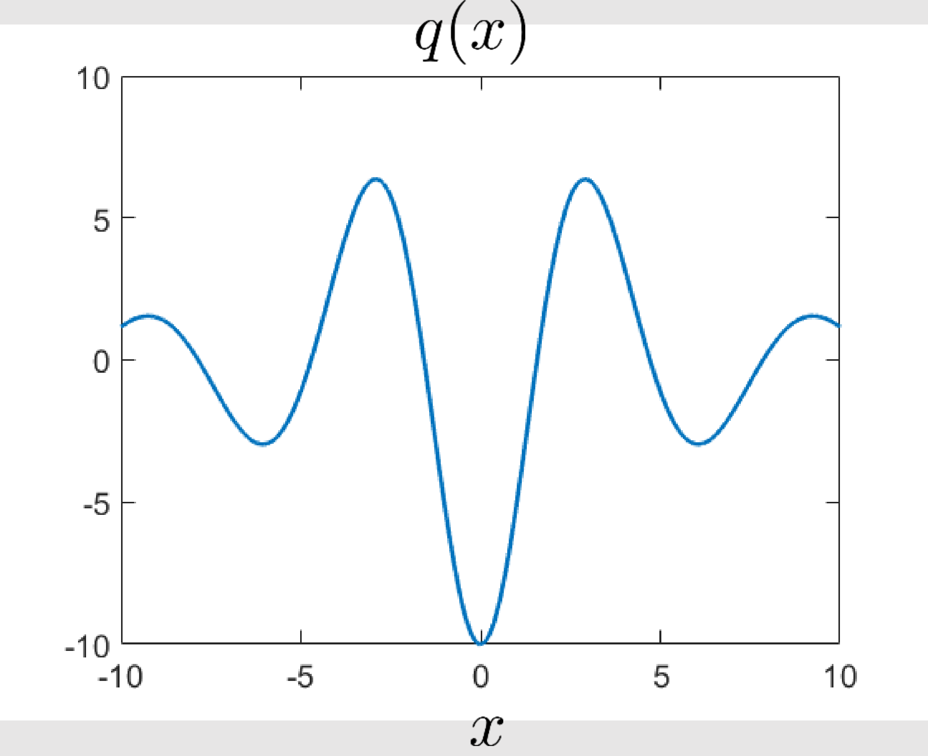
$$\mu_f^{\epsilon}(\lambda) = \frac{1}{\pi}\mathrm{Im}\langle \mathcal{R}(\lambda + i\epsilon, \mathcal{L})f, f\rangle$$

Given $\lambda_1, \ldots, \lambda_n \in \mathbb{R}$

$$\boxed{\begin{array}{l} \text{Fix } \epsilon > 0 \text{ and choose } f \in \mathcal{H} \\ \text{For } k = 1, \ldots, n \\ \qquad 1) \text{ Solve } (\mathcal{L} - (\lambda_k + i\epsilon)\mathcal{I})u_k = f \\ \qquad 2) \text{ Compute } \mu_f^{\epsilon}(\lambda_k) = \frac{1}{\pi}\mathrm{Im}\langle u_k, f\rangle \end{array}}$$

A simple framework

$$\mathcal{L}u = \frac{d^4 u}{dx^4} - q(x)u$$



1) Solve

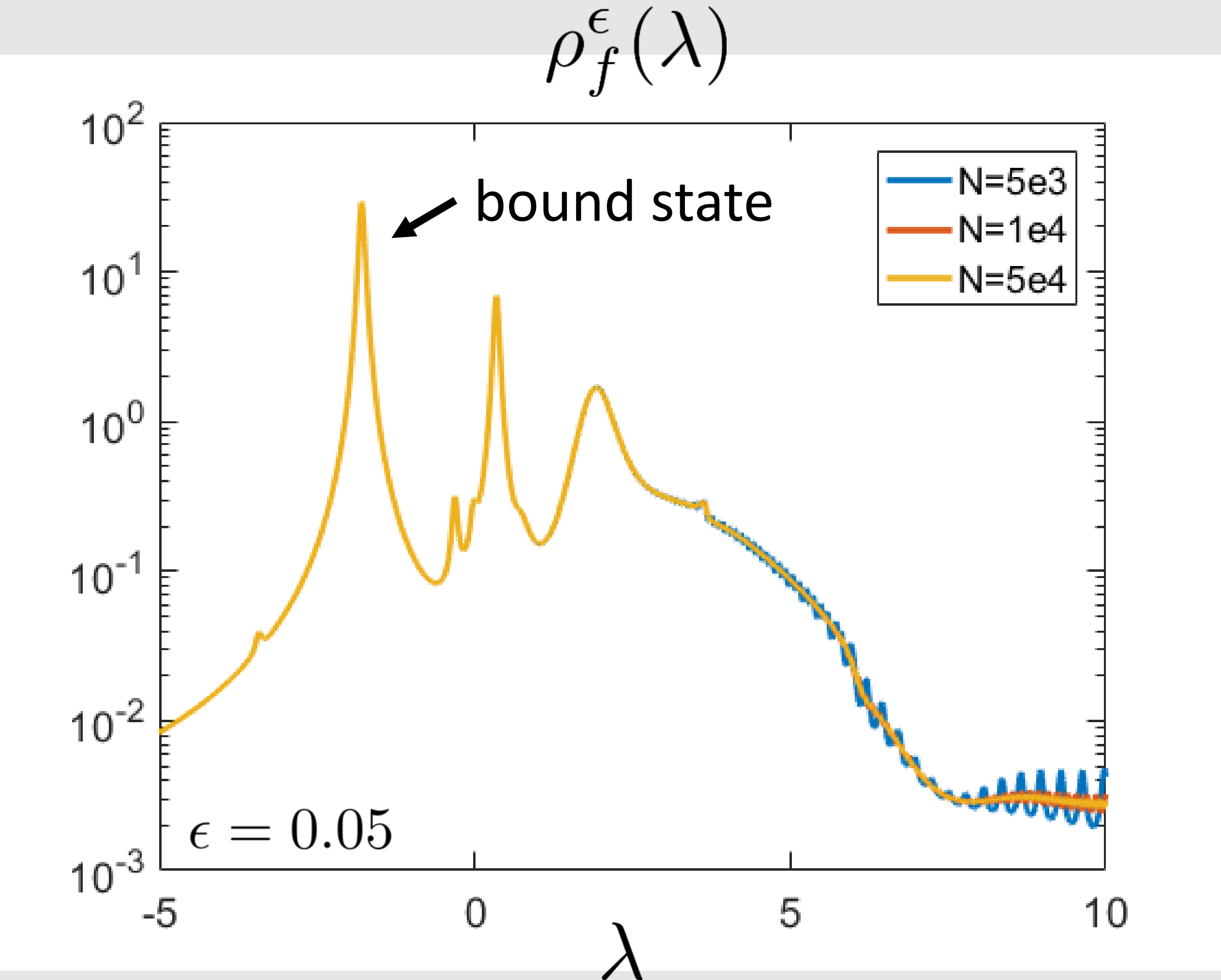
$$\frac{d^4 u}{dx^4} - (q(x) + \lambda + i\epsilon)u = f(x)$$

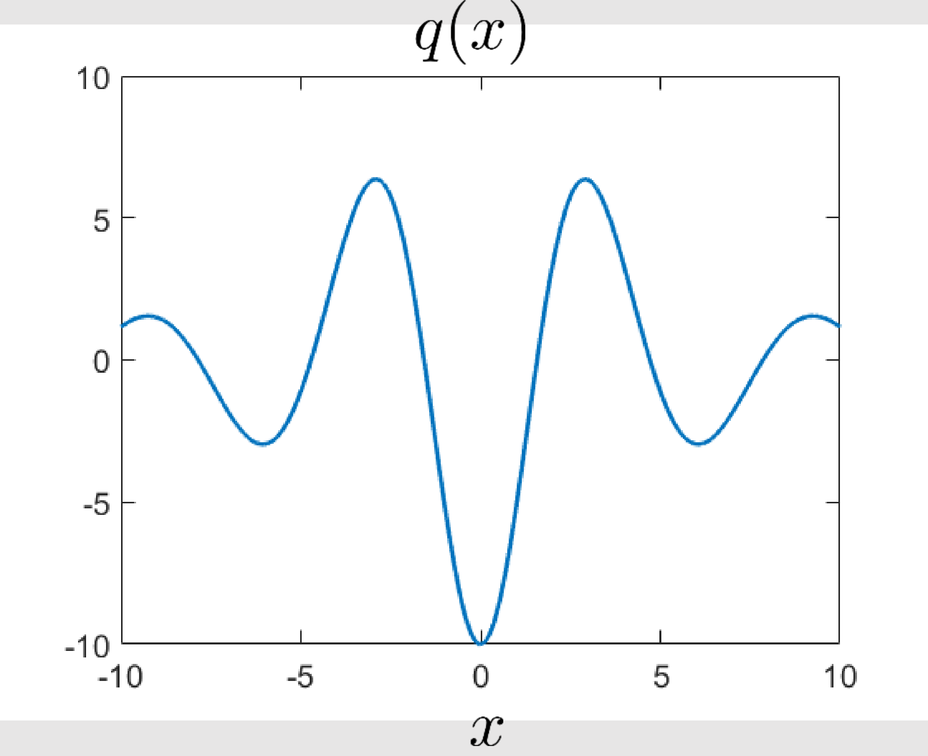
2) Compute

$$\mu_f^{\epsilon}(\lambda) = \frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{\infty} u(x)\overline{f(x)}dx$$

A simple framework

$$\mathcal{L}u = \frac{d^4u}{dx^4} - q(x)u$$





1) Solve

Fourier spectral method + Conformal map

- Adaptive discretization
- Well-conditioned
- Fast (if coefficients are smooth)

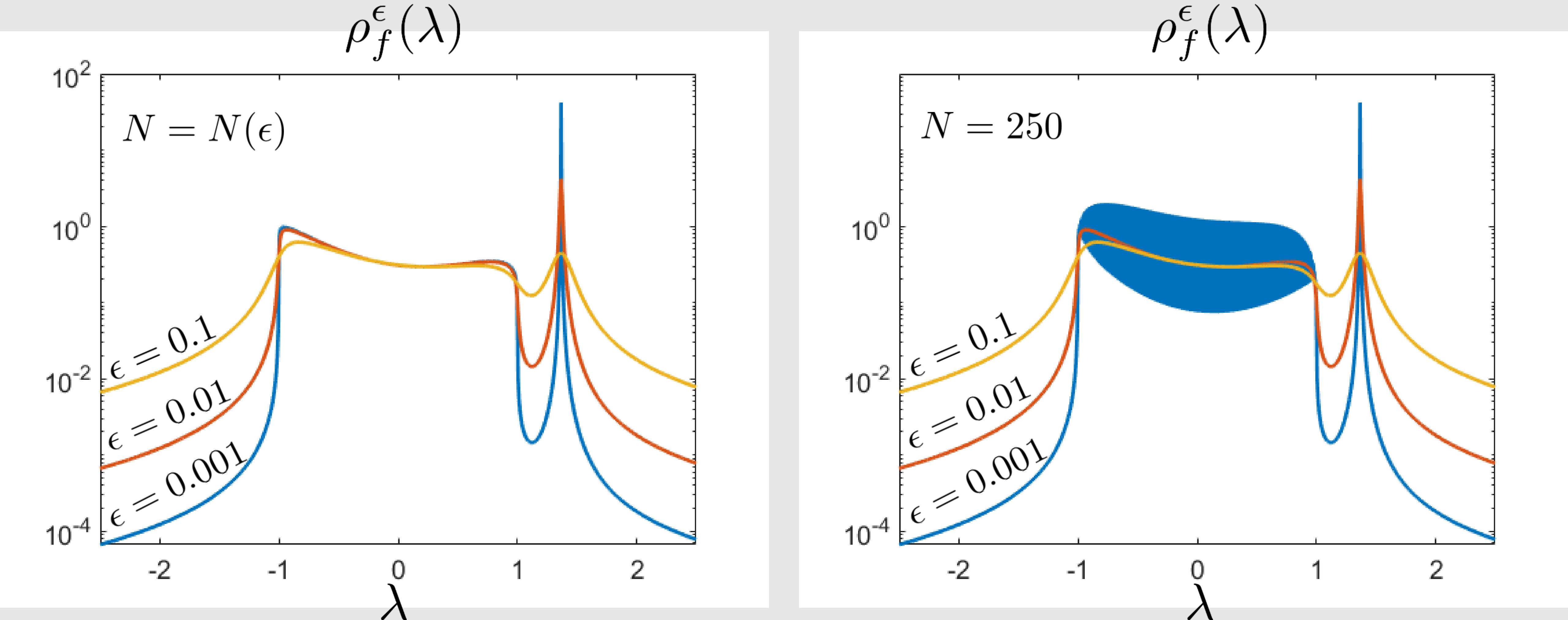
2) Compute

Trapezoid rule + Conformal map

[Trefethen and Weideman, 2014] [Boyd, 1986]

Refining N and epsilon

$$\mathcal{L}u(x) = x\,u(x) + \int_{-1}^{1} e^{-(x^2+y^2)}\,u(y)\,dy$$

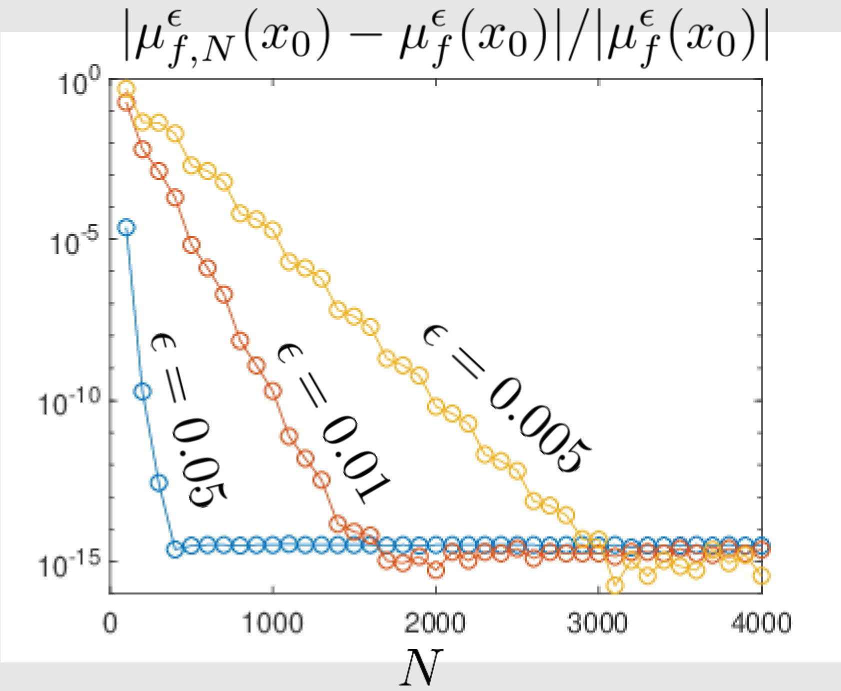


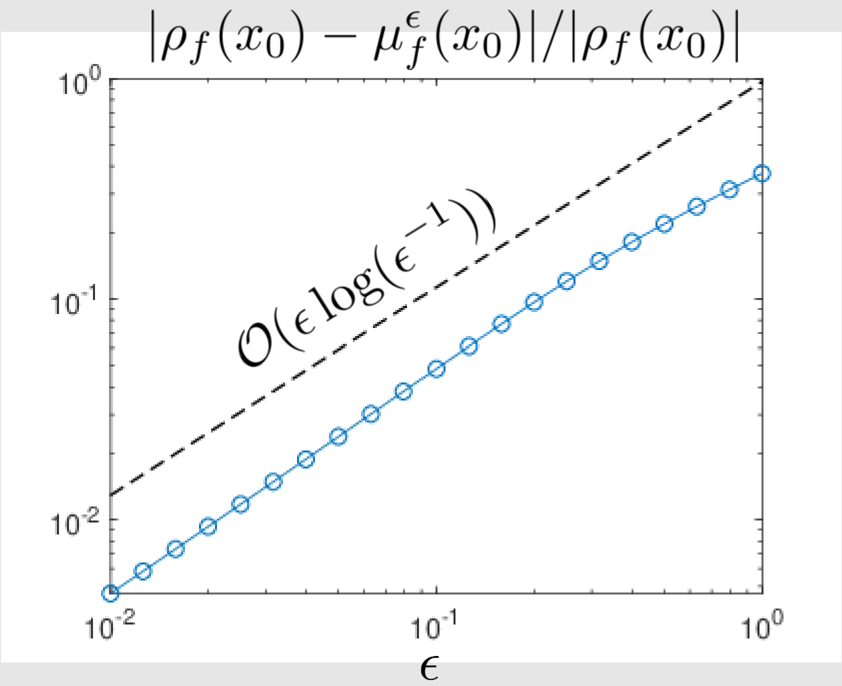
Convergence of smoothed measures

Theorem

If μ_f is absolutely continuous in $I = (x-\delta, x+\delta)$ with Radon-Nikodym derivative $\rho_f \in C^\alpha$, where $0 < \alpha < 1$, then

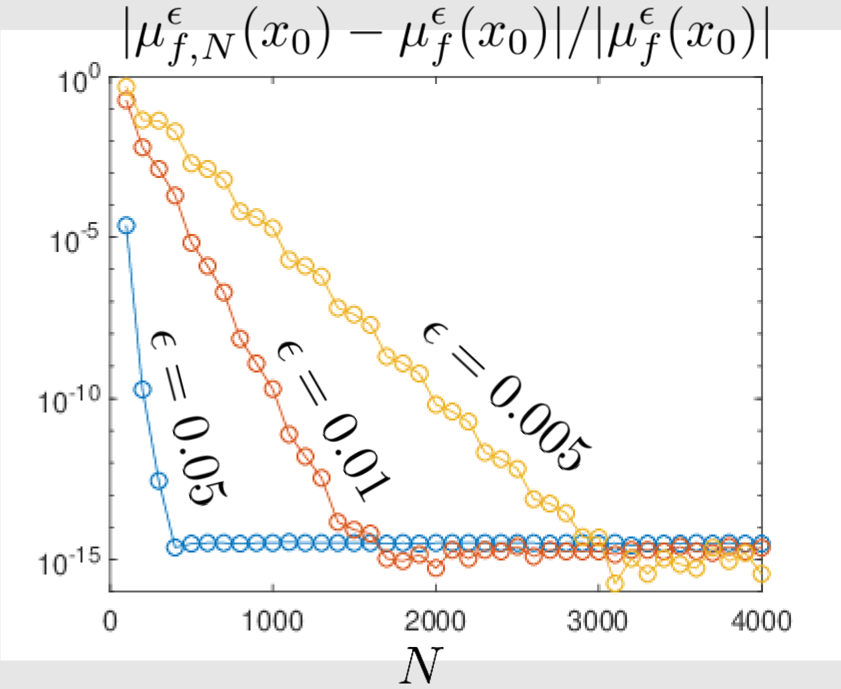
$$|\rho_f(x) - \mu_f^\epsilon(x)| = \mathcal{O}(\epsilon^\alpha) \qquad \text{as} \qquad \epsilon \downarrow 0.$$



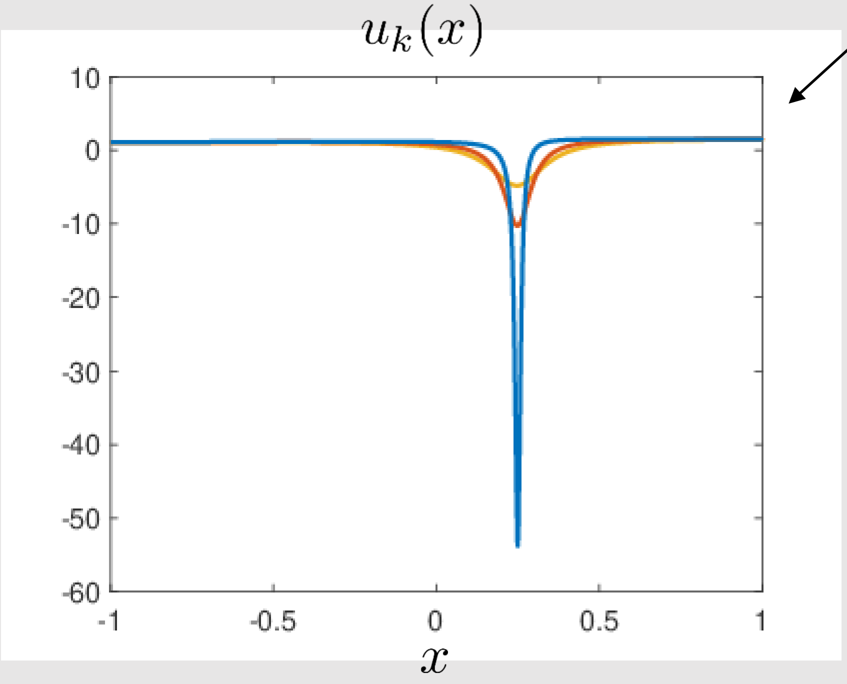


Convergence of smoothed measures

$$1)\ \text{Solve}\ \underbrace{(\mathcal{L} - (\lambda_k + i\epsilon)\mathcal{I})}_{\text{singular in the limit } \epsilon \to 0} u_k = f$$



Integral operator



Convergence of smoothed measures

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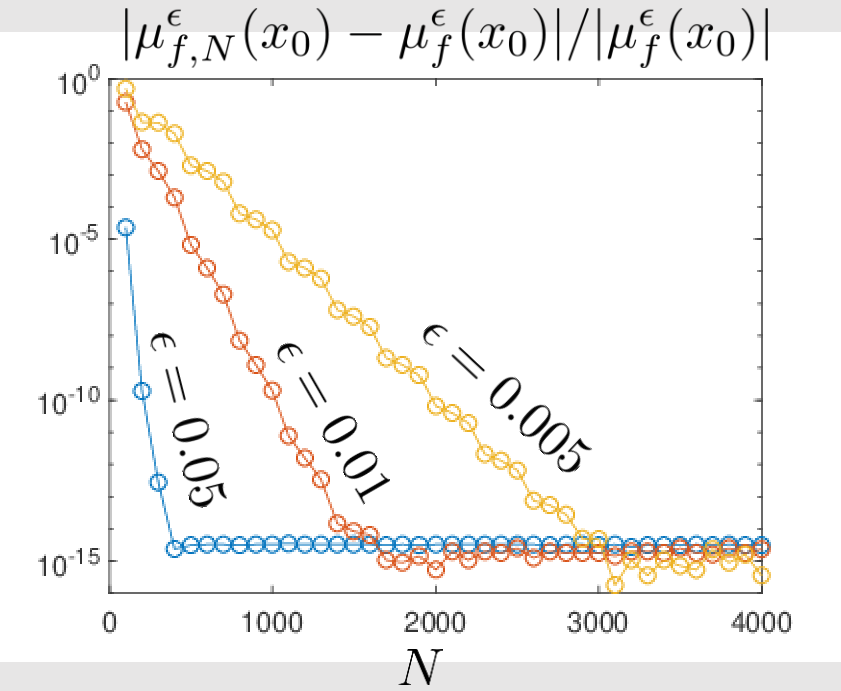
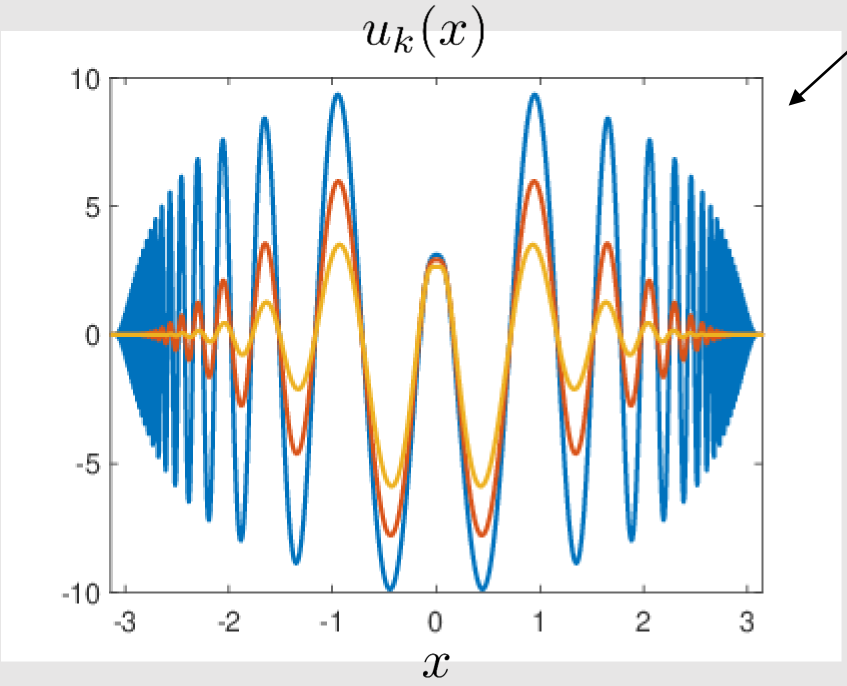


Differential operator



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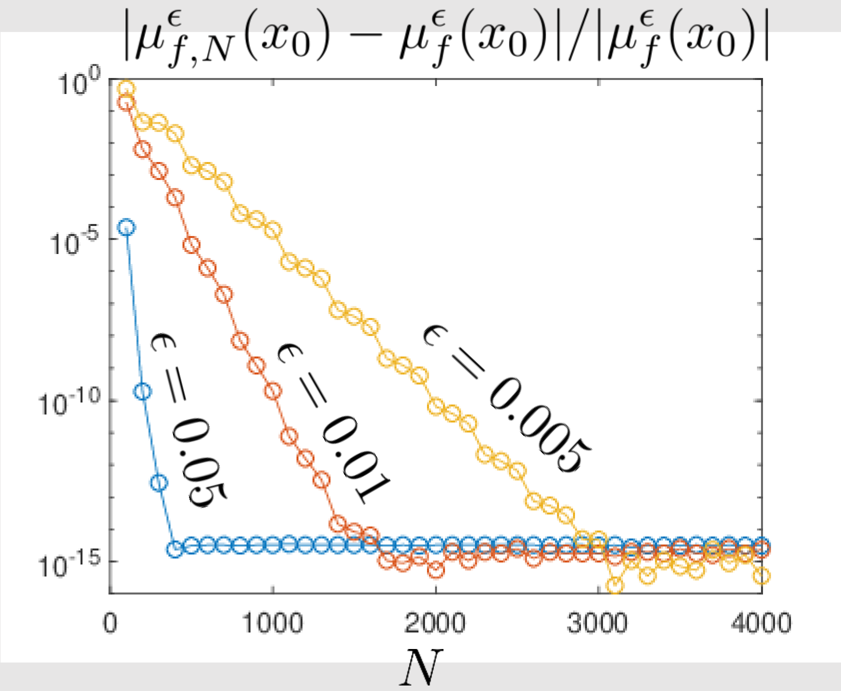
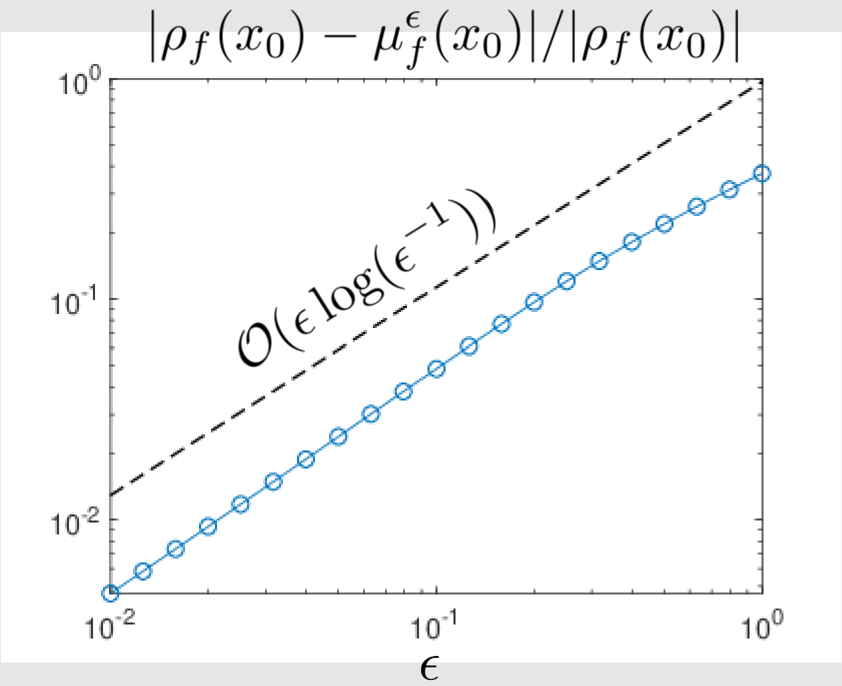
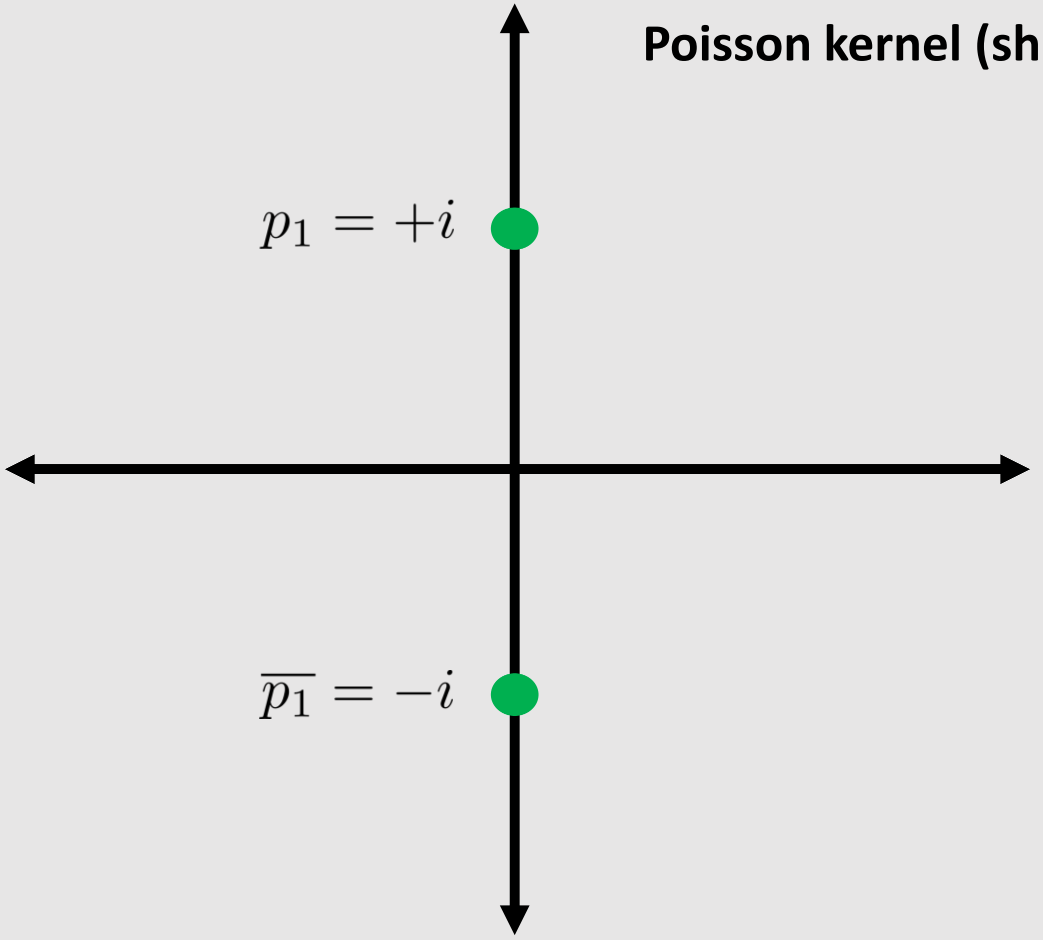




Can we exploit additional smoothness in the density?

Rational kernels

$$\frac{1}{\pi}\mathrm{Im}\langle \mathcal{R}(x+i\epsilon,\mathcal{L})f,f\rangle = \int_{\mathbb{R}} \underbrace{\frac{1}{\pi}\frac{\epsilon^2}{(\lambda-x)^2+\epsilon^2}}_{\text{Poisson kernel (shifted and scaled)}} d\mu_f(\lambda)$$



$$K^{(m)}(x) = \overbrace{\frac{1}{2\pi i}\sum_{k=1}^{m}\frac{r_k}{x-p_k} - \frac{\overline{r_k}}{x-\overline{p_k}}}^{\text{Need } \|K^{(m)}\|_{L^1(\mathbb{R})}=1}$$

scale

$$K_\epsilon^{(m)}(x) = \epsilon^{-1}K^{(m)}(x/\epsilon)$$

resolvent link

$$[K_\epsilon^{(m)} * \mu_f](x) = \frac{1}{\pi}\sum_{k=1}^{m}\mathrm{Im}\left(r_k\langle \mathcal{R}(x+\epsilon p_k),\mathcal{L})f,f\rangle\right)$$

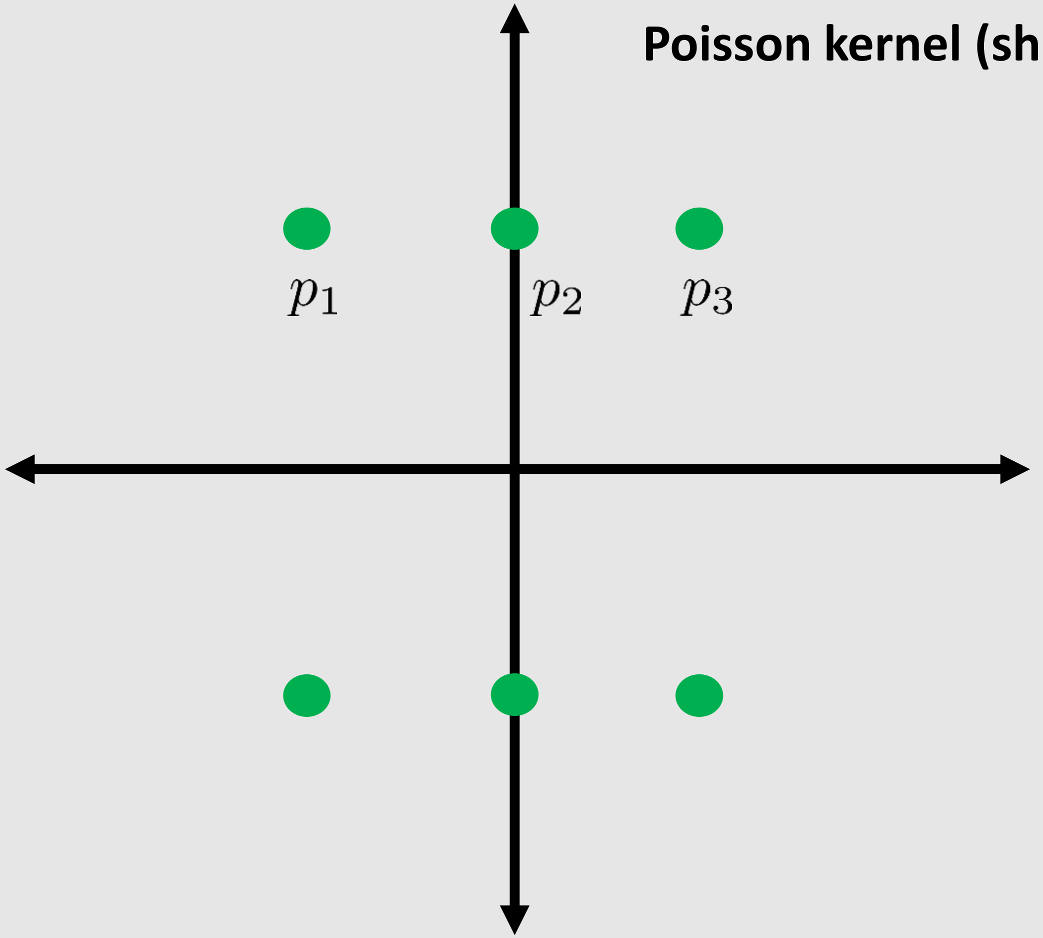
convergence

For $\mathcal{O}(\epsilon^m)$ convergence, key requirement is

$$\int_{\mathbb{R}} K^{(m)}(x)x^j\,dx = 0, \quad j=1,\dots,m-1$$

Rational kernels

$$\frac{1}{\pi}\mathrm{Im}\langle\mathcal{R}(x+i\epsilon,\mathcal{L})f,f\rangle=\int_{\mathbb{R}}\underbrace{\frac{1}{\pi}\frac{\epsilon^2}{(\lambda-x)^2+\epsilon^2}}_{\text{Poisson kernel (shifted and scaled)}}\,d\mu_f(\lambda)$$



Need $\|K^{(m)}\|_{L^1(\mathbb{R})}=1$

$$K^{(m)}(x)=\frac{1}{2\pi i}\sum_{k=1}^{m}\frac{r_k}{x-p_k}-\frac{\overline{r_k}}{x-\overline{p_k}}$$

scale

$$K_\epsilon^{(m)}(x)=\epsilon^{-1}K^{(m)}(x/\epsilon)$$

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convergence

For $\mathcal{O}(\epsilon^m)$ convergence, key requirement is

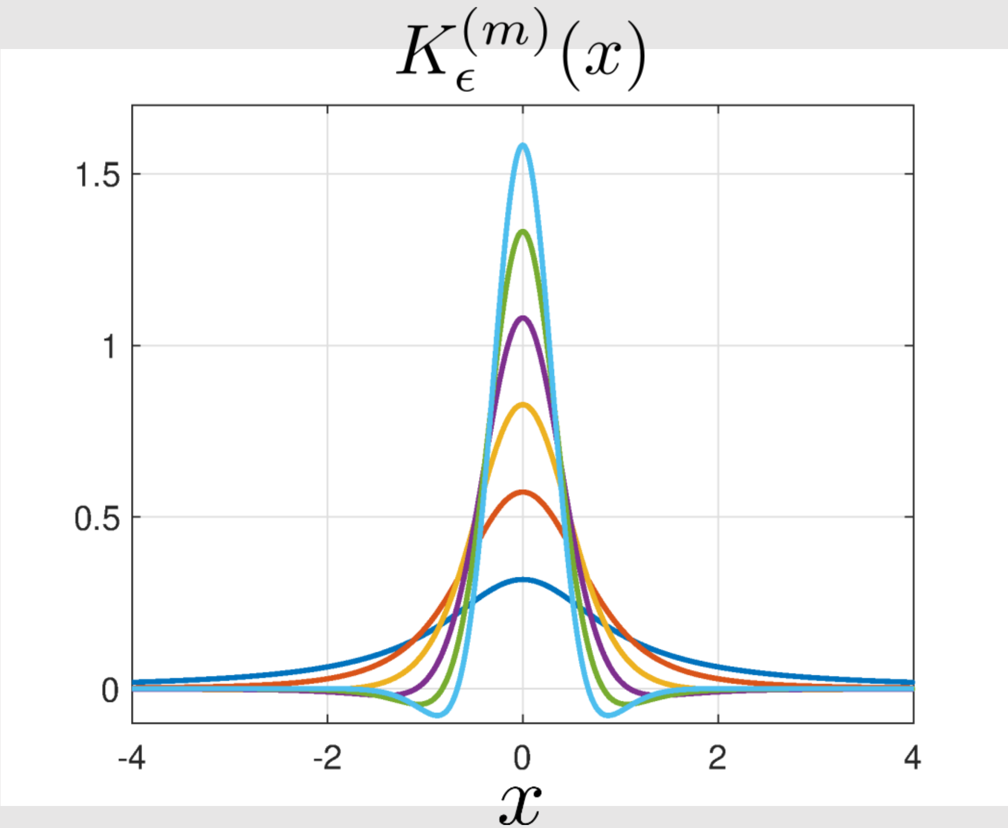
$$\int_{\mathbb{R}}K^{(m)}(x)x^j\,dx=0,\quad j=1,\dots,m-1$$

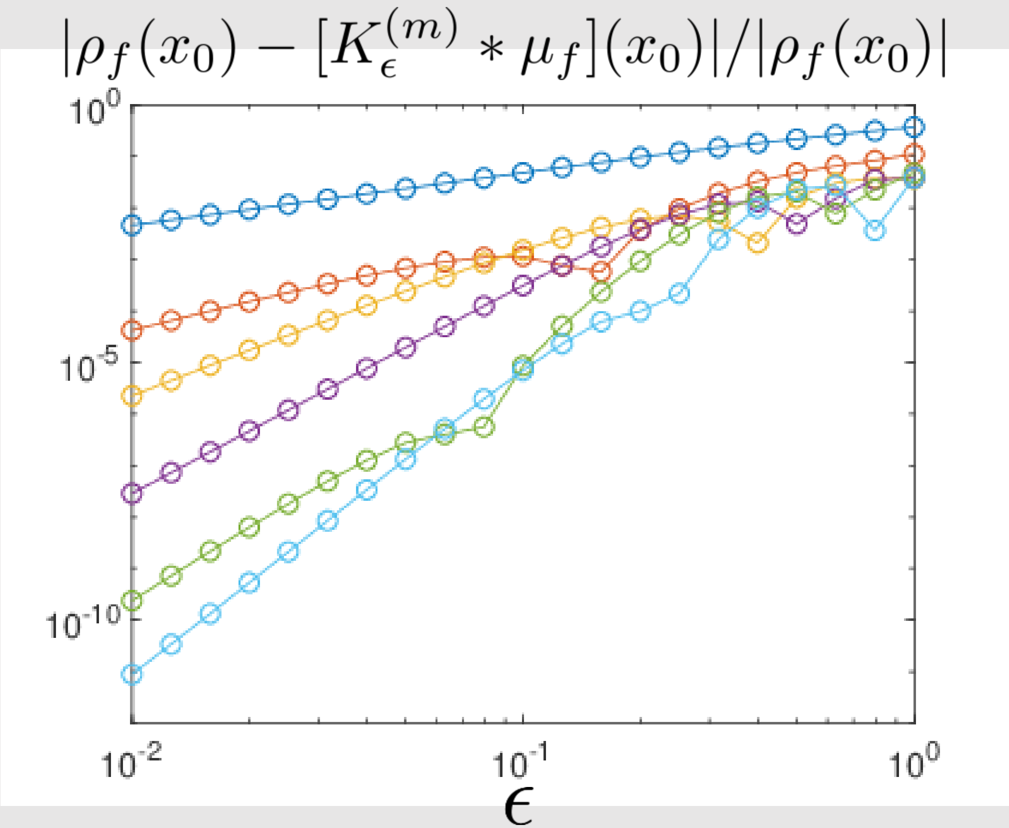
Rational kernels

Theorem [Colbrook, H., and Townsend, 2020]

If μ_f is absolutely continuous in $I = [x-\delta, x+\delta]$ with Radon-Nikodym derivative $\rho_f \in C^{k,\alpha}$, then

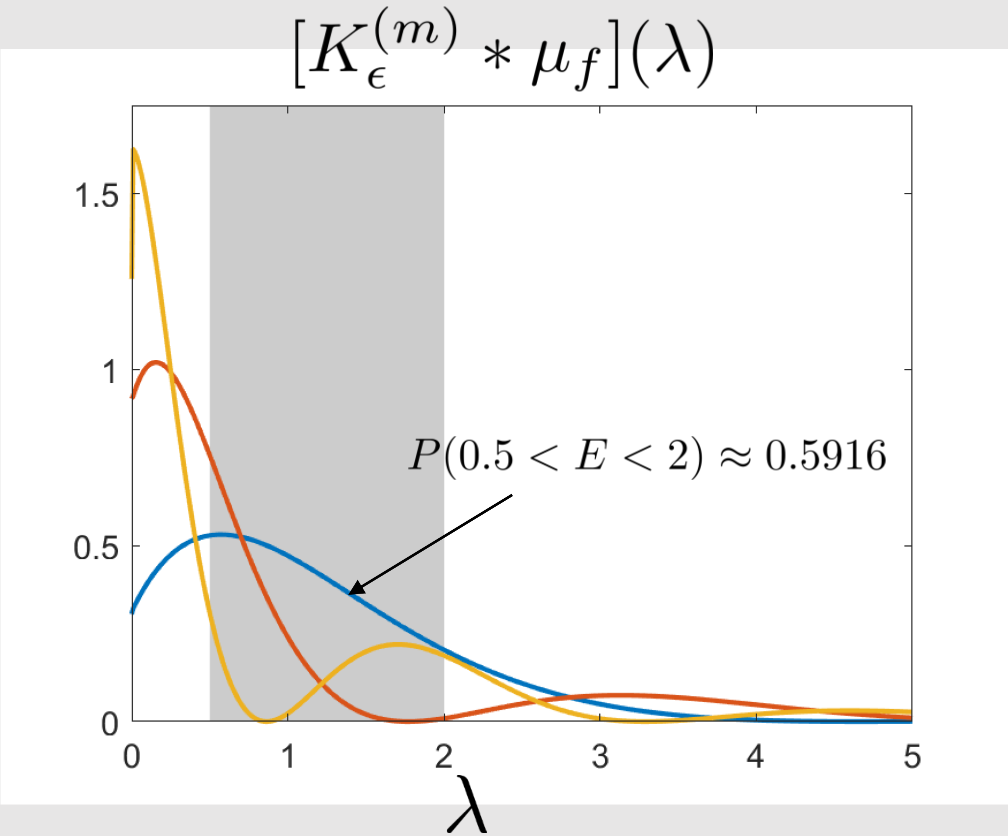
$$|\rho_f(x) - [K_\epsilon^{(m)} * \mu_f](x)| = \mathcal{O}(\epsilon^{k+\alpha}) + \mathcal{O}(\epsilon^m \log(1/\epsilon)) \qquad \text{as} \qquad \epsilon \downarrow 0.$$





Rational kernels

$$\mathcal{L}u = -\frac{d^2u}{dr^2} + \Bigg(\underbrace{\frac{\ell(\ell+1)}{r^2}}_{\textbf{centrifugal term}} + \overbrace{\frac{1}{r}\left(e^{-r}-1\right)}^{\textbf{Hellman potential}} \Bigg) u$$



$$f_{r_0}(r) = C_{r_0} e^{-(r-r_0)^2}$$

$$r_0 = 2 \quad (yellow)$$

$$r_0 = 3 \quad (red)$$

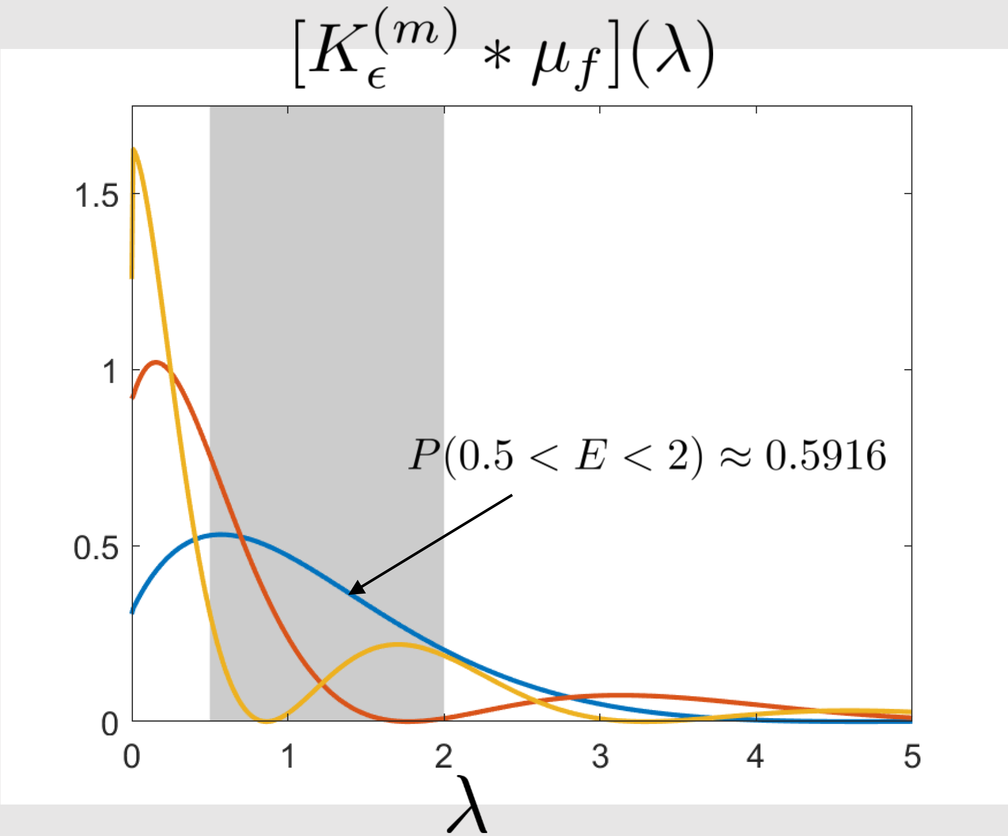
$$r_0 = 4 \quad (blue)$$

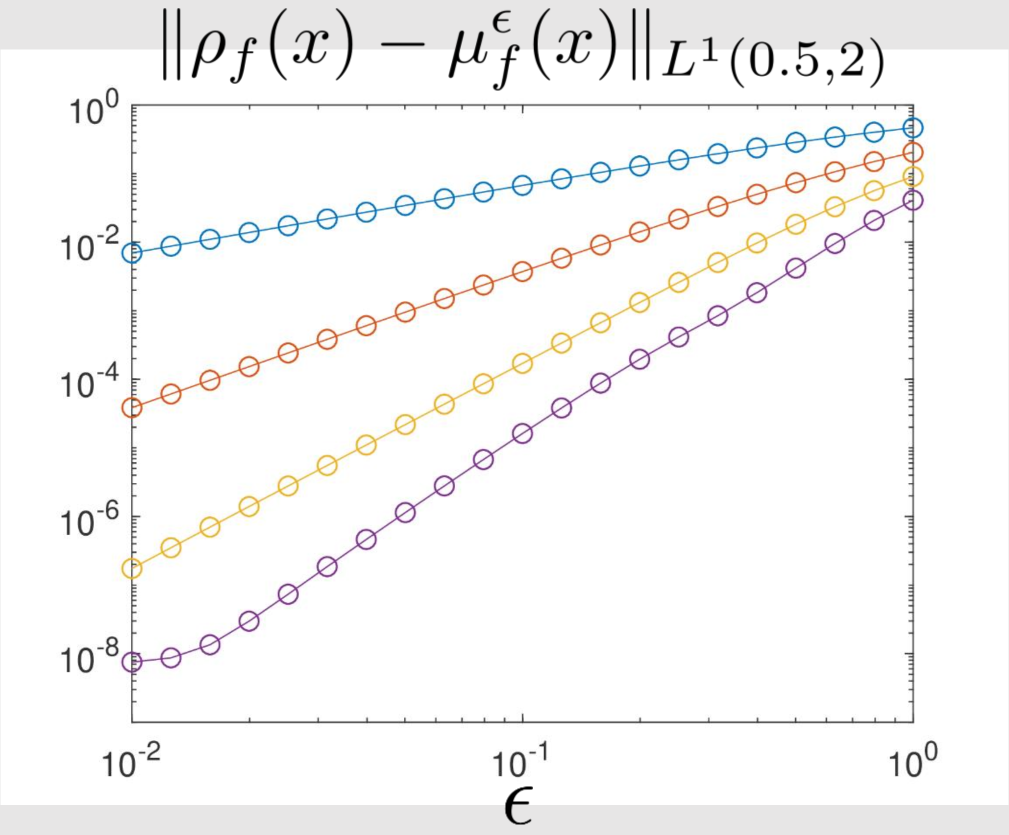
Rational kernels

Theorem [Colbrook, H., and Townsend, 2020]

If μ_f is absolutely continuous in $I = [a-\delta, b+\delta]$ with Radon-Nikodym derivative $\rho_f \in W^{m,p}(I)$, then

$$\|\rho_f(x) - [K_\epsilon^{(m)} * \mu_f](x)\|_{L^p(a,b)} = \mathcal{O}(\epsilon^m \log(1/\epsilon)) \qquad \text{as} \qquad \epsilon \downarrow 0.$$

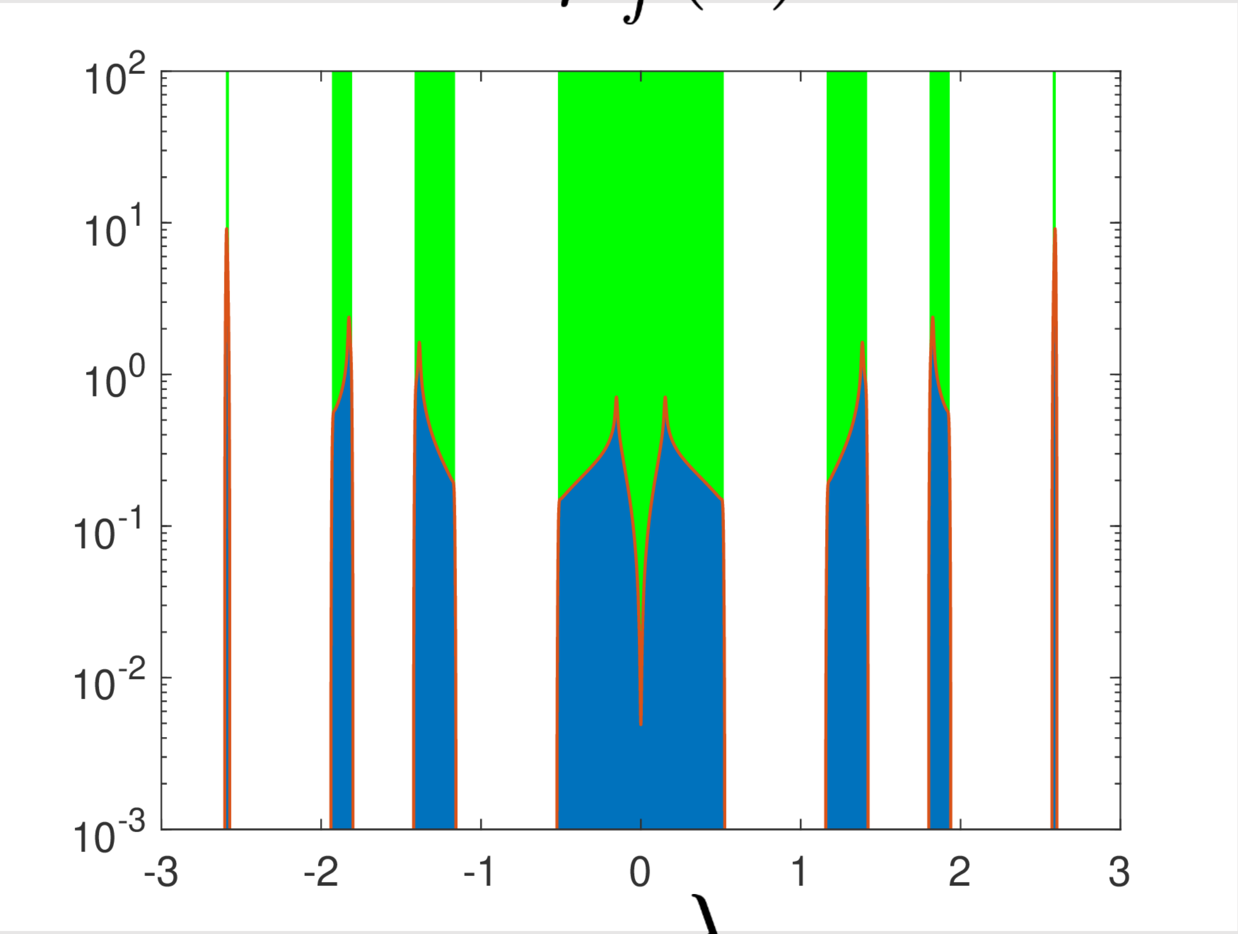




No spectral pollution

Discrete Schrodinger operator on a graphene lattice

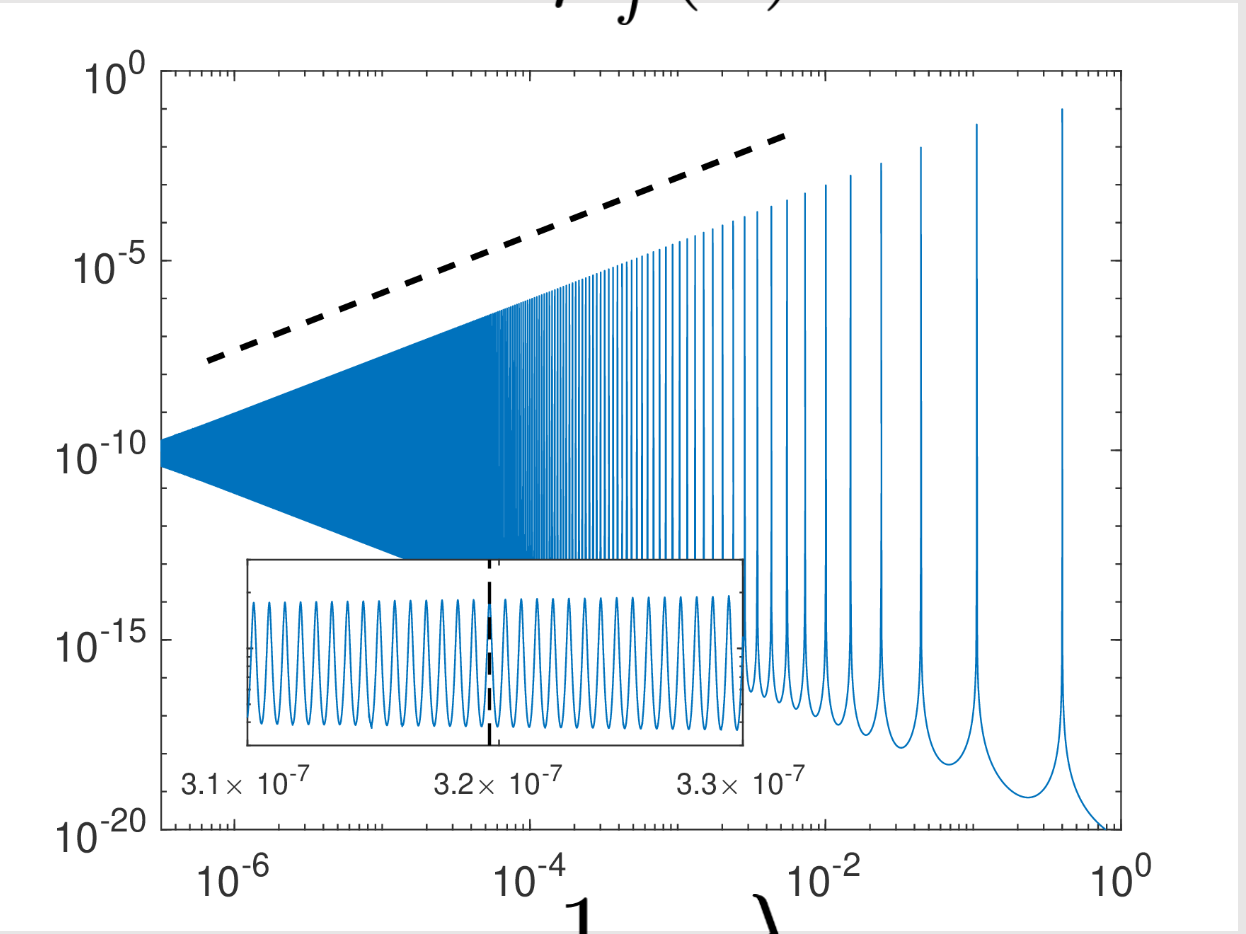
$$\mu_f^\epsilon(\lambda)$$



$$\lambda$$

Radially symmetric Dirac operator with a Coulomb potential

$$\epsilon\mu_f^\epsilon(\lambda)$$



$$1-\lambda$$

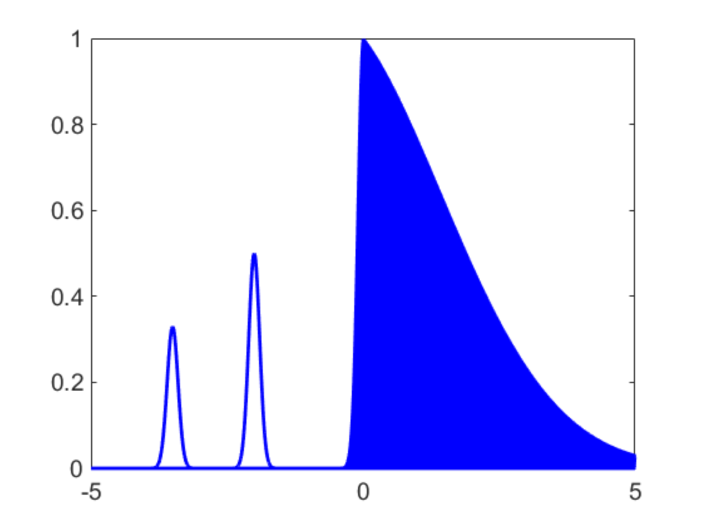
Spectral measures of operators

$$\mathcal{L} : \mathcal{D}(\mathcal{L}) \to \mathcal{H}$$

E.g., $$\mathcal{L} = a_K(x)\frac{d^K}{dx^K} + \cdots + a_1(x)\frac{d}{dx} + a_0(x) \qquad \mathcal{L}u(x) = a(x)u(x) + \int_{-1}^{1} k(x,y)u(y)\,dy$$

Resolvent

$$d\mu_f^{\epsilon}(\lambda) = \sum_k \mathrm{Im}(w_k \langle \mathcal{R}(z_k, \mathcal{L})f, f\rangle)$$



Smooth

Discretize

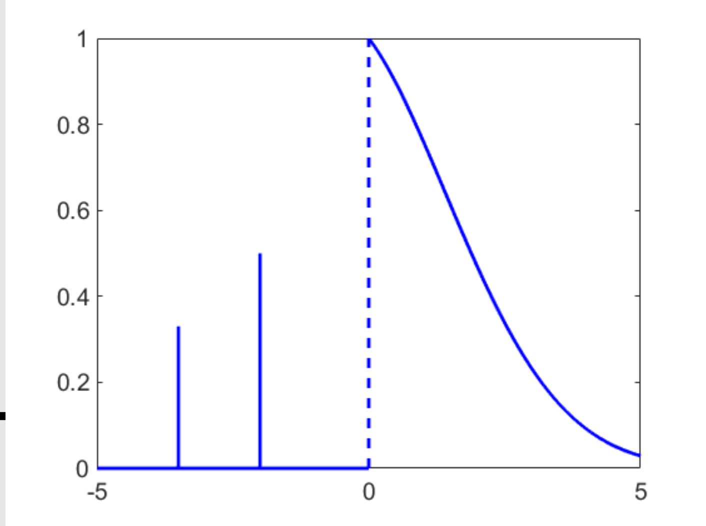
[Colbrook, H., Townsend, 2020]

Approximate

Operator

$$d\mu_f(\lambda) = \rho_f(\lambda) + \sum_k c_k\,\delta(\lambda - \lambda_k)$$

$$c_k = \langle \mathcal{P}_k f, f\rangle$$



Resolvent paradigm