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# On the computation of the eigenvalues of Dirac operators

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# Settings

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$$D^0 = \begin{pmatrix} 1 & -\partial_r + \frac{\kappa}{r} \\ \partial_r + \frac{\kappa}{r} & -1 \end{pmatrix} : H_0^1(0, \infty)^2 \longrightarrow L^2(0, \infty)^2$$
$$\sigma(D^0) = (-\infty, -1] \cup [1, \infty) \quad \kappa \in \mathbb{N}$$

$$\left. \begin{array}{l} V(r) \leq 0 \\ V \in C^\infty(0, \infty) \\ \sup_{r>0} |rV(r)| < \infty \end{array} \right| \Rightarrow \begin{array}{l} D^0 + V = (D^0 + V)^* \\ \sigma_{\text{ess}}(D^0 + V) = \sigma(D^0) \end{array}$$

$$H = D^0 + V$$

$$V(r) = \frac{\alpha}{r}, \quad -\frac{\sqrt{3}}{2} < \alpha < 0 \quad \text{and} \quad V(r) = \frac{\gamma}{1+r^2}, \quad \gamma < 0$$

# Motivation

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$$\mathcal{L} = \text{Span}\{b_1, \dots, b_n\} \subset D(H)$$

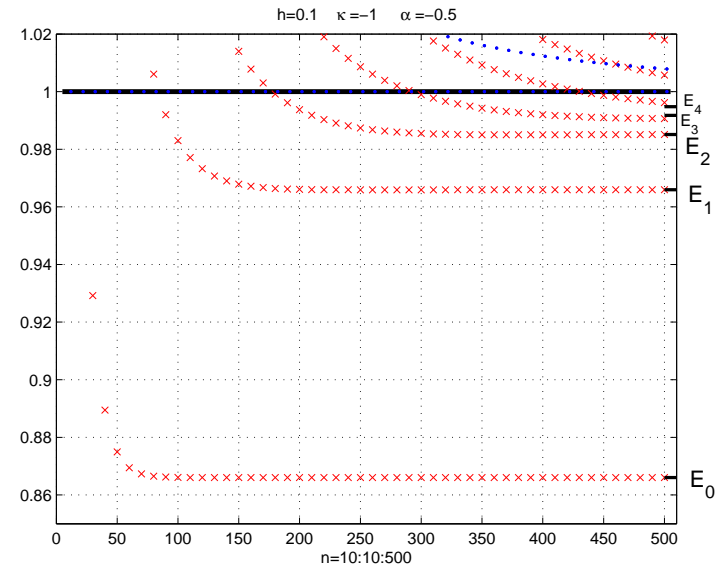
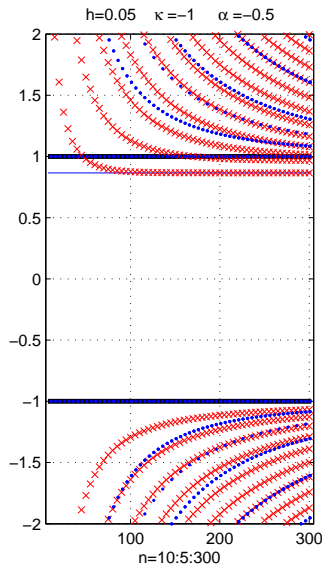
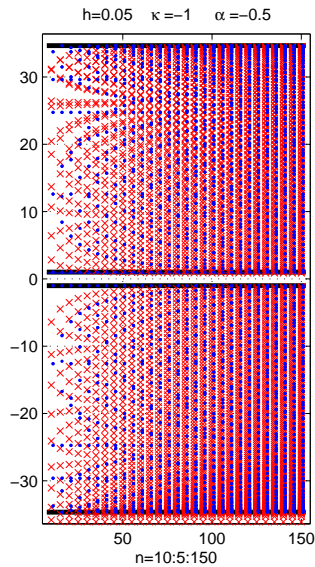
$$K_{\mathcal{L}} = [\langle Hb_j, b_k \rangle]_{jk=1}^n$$

$$B_{\mathcal{L}} = [\langle b_j, b_k \rangle]_{jk=1}^n$$

$$\mu \in \sigma(H, \mathcal{L}) \iff \exists \underline{u} \neq 0, (K_{\mathcal{L}} - \lambda B_{\mathcal{L}})\underline{u} = 0$$

$$\lim_{\mathcal{L} \uparrow D(H)} \sigma(H, \mathcal{L}) \supseteq \sigma(H) \quad (\subseteq \text{ not necessarily})$$

# Is pollution really an issue?



$$V(r) = \frac{\alpha}{r}$$

$\mathcal{L}_n^h$  - Lagrange elements of order 1 uniform mesh on a finite interval  
 $n$  segments of length  $h$ , same dimension in first and second component.

# Is pollution really an issue?

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$\phi_j^h$  - piecewise linear hat function, max at  $jh$

$$\mathcal{L}^h = \text{Span} \left\{ \begin{pmatrix} \phi_j^h \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \phi_j^h \end{pmatrix} \right\}_{j=1}^{\infty} \simeq \ell^2(\mathbb{N}, \mathbb{C}^2)$$

$$H = \begin{pmatrix} 1 & -\partial_r \\ \partial_r & -1 \end{pmatrix} + \frac{1}{r} \begin{pmatrix} \alpha & \kappa \\ \kappa & \alpha \end{pmatrix} = A + B$$

$A \upharpoonright \mathcal{L}^h$  - Block Toeplitz op

$B \upharpoonright \mathcal{L}^h$  - Compact

Pollution is preserved under compact perturbations

# Rough enclosures

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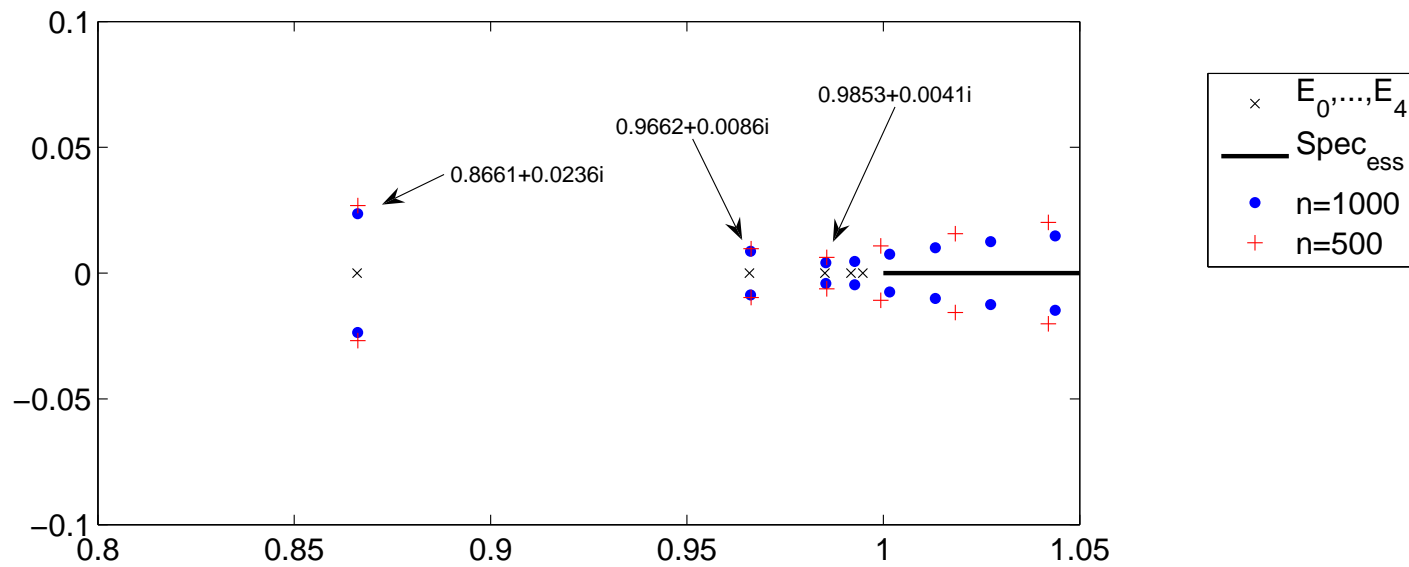
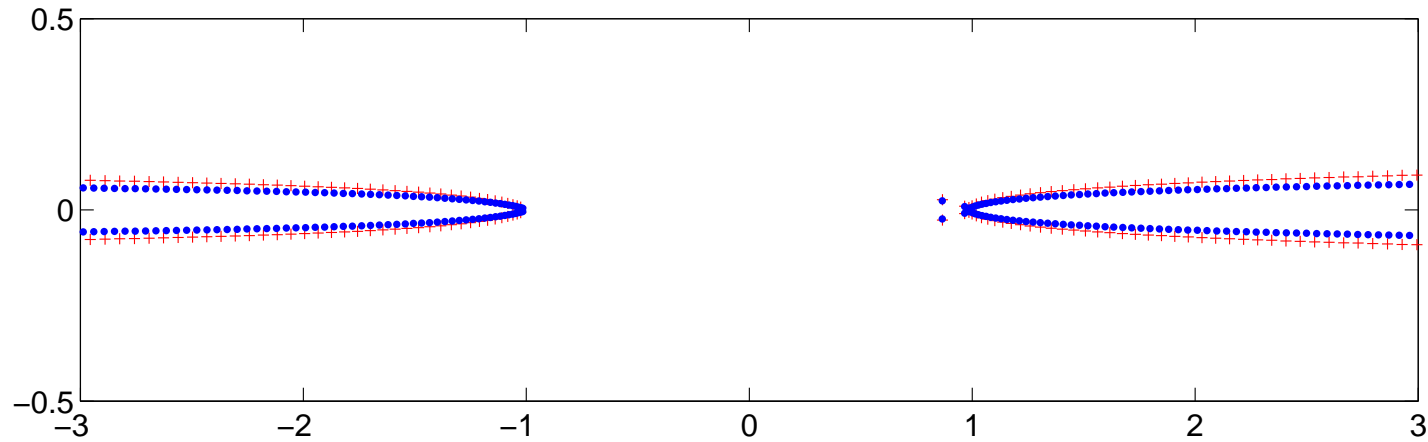
$$L_{\mathcal{L}} = [\langle Hb_j, Hb_k \rangle]_{jk=1}^n$$

$$\lambda \in \sigma_2(H, \mathcal{L}) \iff \exists \underline{u} \neq 0, (L_{\mathcal{L}} - 2\lambda K_{\mathcal{L}} + \lambda^2 B_{\mathcal{L}})\underline{u} = 0$$

**Theorem** [Levitin & Shargorodsky]

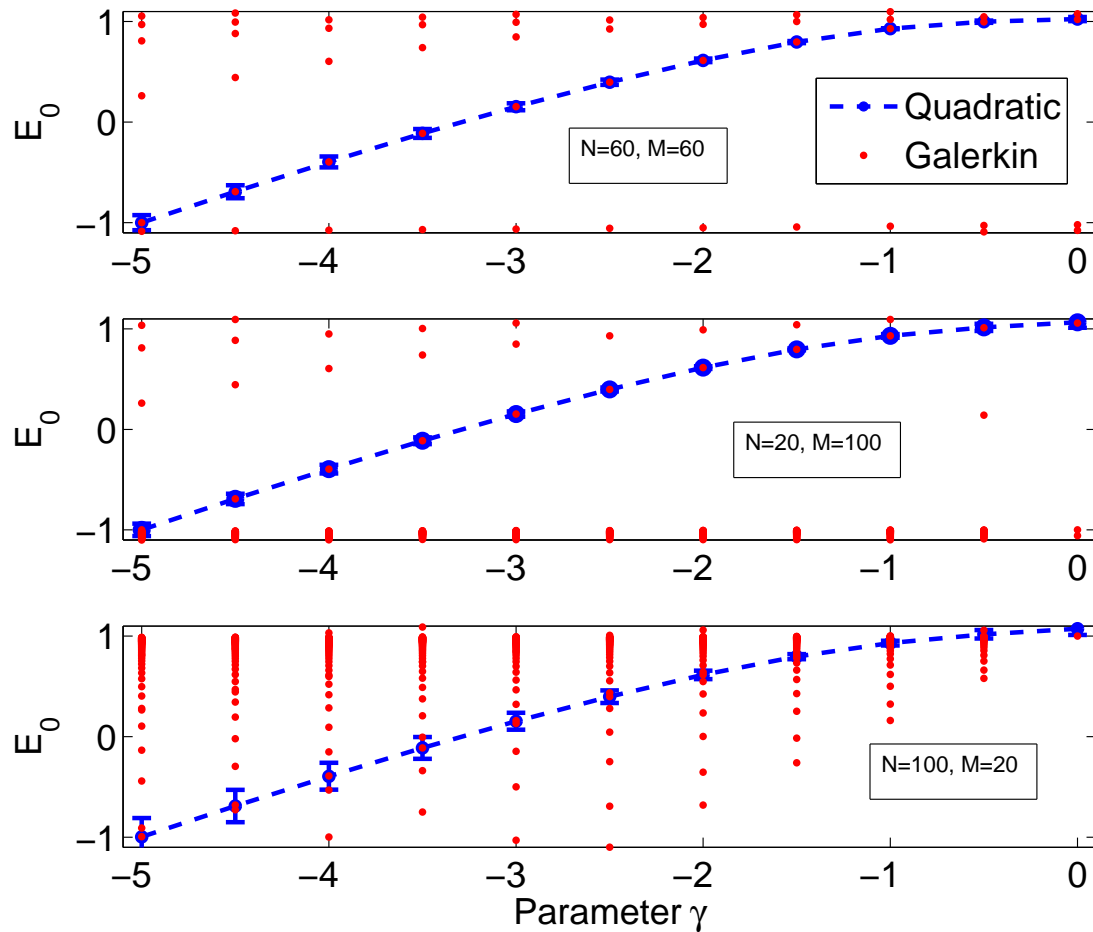
$$\lambda \in \sigma_2(H, \mathcal{L}) \Rightarrow \begin{aligned} & [\alpha, \beta] \cap \sigma(H) \neq \emptyset \\ & \alpha = \operatorname{Re}\lambda - |\operatorname{Im}\lambda|, \beta = \operatorname{Re}\lambda + |\operatorname{Im}\lambda| \end{aligned}$$

# Rough enclosures



$$V(r) = -\frac{1}{2r} \quad \kappa = -1 \quad \mathcal{L}_n \text{ - balanced odd Hermite basis}$$

# Rough enclosures



$$V(r) = \frac{\gamma}{1+r^2}$$

$$e_j(r) = h_{2j+1}(r)e^{-r^2/2}$$

$$\mathcal{L}_{NM} = \text{Span} \left\{ \left( \begin{array}{c} e_j \\ 0 \end{array} \right), \left( \begin{array}{c} 0 \\ e_k \end{array} \right) \right\}_{\substack{j=0:N \\ k=0:M}}$$



# Rough enclosures

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## Theorem

Let  $V$  be as above and such that  $r^\alpha V(r)$  is locally bounded for some  $0 < \alpha < 1$ . Let  $E \in \sigma_{\text{disc}}(H)$ . For any  $1 < q < 5/4$ , there exists  $b > 0$  and  $\lambda_{NM} \in \sigma_2(H, \mathcal{L}_{NM})$  such that

$$|\lambda_{NM} - E| < b(N^{-\frac{q-1}{2}} + M^{-\frac{q-1}{2}}).$$

# A variational principle

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$$H \begin{pmatrix} \phi \\ \psi \end{pmatrix} = E \begin{pmatrix} \phi \\ \psi \end{pmatrix} \iff \begin{aligned} L_E \phi &= 0 \\ \psi &= -(V - 1 - E)^{-1} (\partial_r + \frac{\kappa}{r}) \phi \end{aligned}$$

$$L_\lambda = (-\partial_r + \frac{\kappa}{r})(1 + \lambda - V)^{-1}(\partial_r + \frac{\kappa}{r}) + V + 1 - \lambda$$

$$V \text{ - "reasonable"} \Rightarrow \min \sigma_{\text{ess}}(L_\lambda) = 1 - \lambda \geq 0, \lambda \in (-1, 1)$$

$$E \in \sigma_{\text{disc}}(H) \iff 0 \in \sigma_{\text{disc}}(L_E)$$

Dolbeault, Esteban, Séré

# A variational principle

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$$\mu_\lambda \in \sigma_{\text{disc}}(L_\lambda) \quad \left. \frac{\partial \mu_\lambda}{\partial \lambda} \right|_{\lambda=E} \leq -1$$

$$A(E)\phi = 0$$

$$A(\lambda)\phi = \int_0^\infty \frac{|(r^\kappa \phi(r))'|^2}{r^{2\kappa}(1 + \lambda - V(r))} + (V(r) + 1 - \lambda)|\phi(r)|^2$$

$$\tilde{A}_{\mathcal{L}}(\lambda) = [\langle A(\lambda)b_j, b_k \rangle]_{jk=1}^n$$

# The $F_n$ method

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$$L = L^* \quad (\alpha, \beta) \cap \sigma(L) = \{E\}$$

$$\min_{0 \neq \phi \in \mathcal{L}} \frac{\langle L\phi, \phi \rangle}{\langle \phi, \phi \rangle} < \alpha < \beta < \max_{0 \neq \phi \in \mathcal{L}} \frac{\langle L\phi, \phi \rangle}{\langle \phi, \phi \rangle}$$

$$\tau_- = \min_{0 \neq \phi \in \mathcal{L}} \frac{\langle (L-\beta)\phi, \phi \rangle}{\langle (L-\beta)\phi, (L-\beta)\phi \rangle} < 0 \quad \tau_+ = \max_{0 \neq \phi \in \mathcal{L}} \frac{\langle (L-\alpha)\phi, \phi \rangle}{\langle (L-\alpha)\phi, (L-\alpha)\phi \rangle} > 0$$

**Theorem [Davies & Plum]**

$$\beta + \frac{1}{\tau_-} \leq E \leq \alpha + \frac{1}{\tau_+}$$

# The $F_n$ method

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$$(*) \quad (Q_{\mathcal{L}} - \tau R_{\mathcal{L}})\underline{u} = 0 \quad \underline{u} \neq 0$$

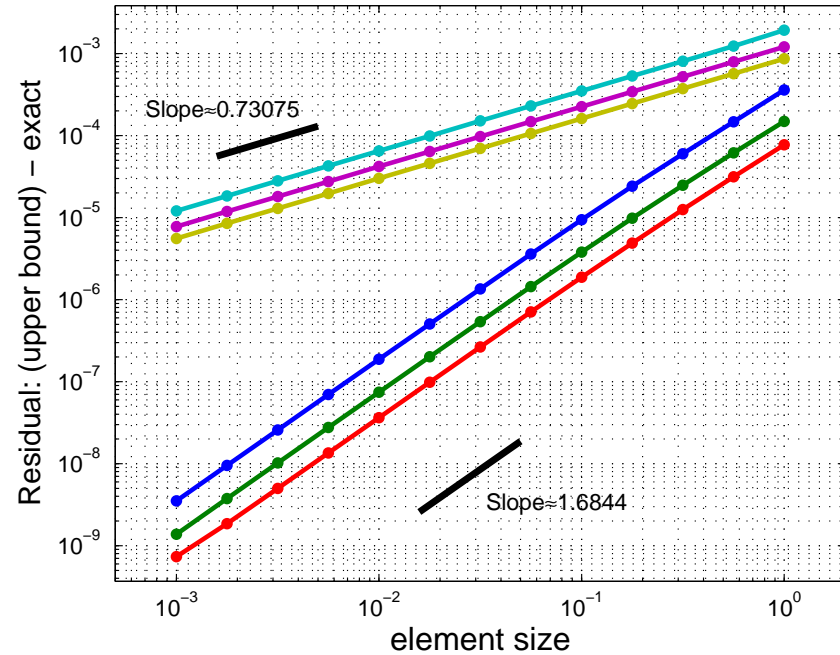
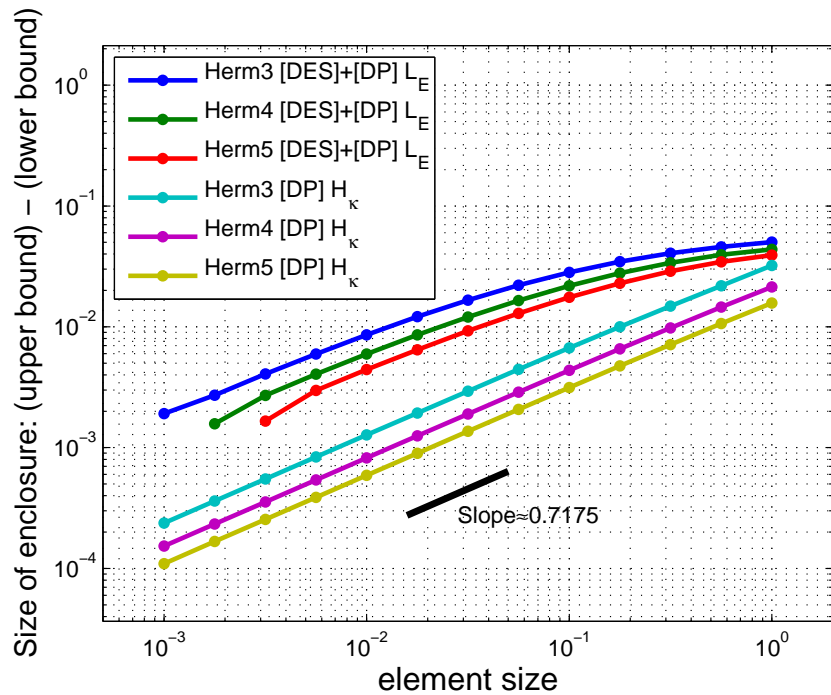
$$R_{\mathcal{L}} = [\langle (L - \delta)b_j, b_k \rangle]_{jk=1}^n \quad Q_{\mathcal{L}} = [\langle (L - \delta)b_j, (L - \delta)b_k \rangle]_{jk=1}^n$$

$\tau_-$  - negative eva of smallest modulus of  $(*)$  for  $\delta = \beta$

$\tau_+$  - positive eva of smallest modulus of  $(*)$  for  $\delta = \alpha$

We can take  $L = L_\mu, E \lesssim \mu$       or       $L = H$

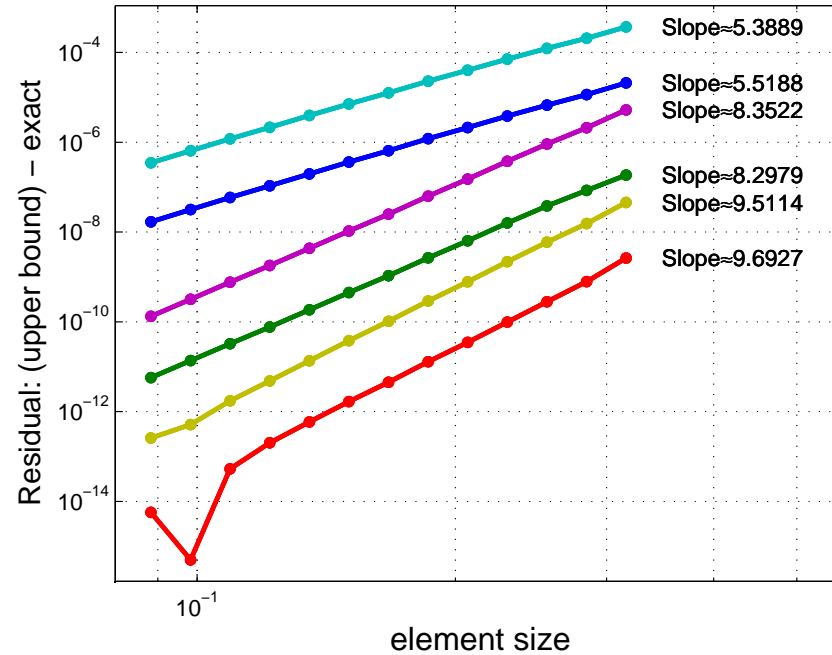
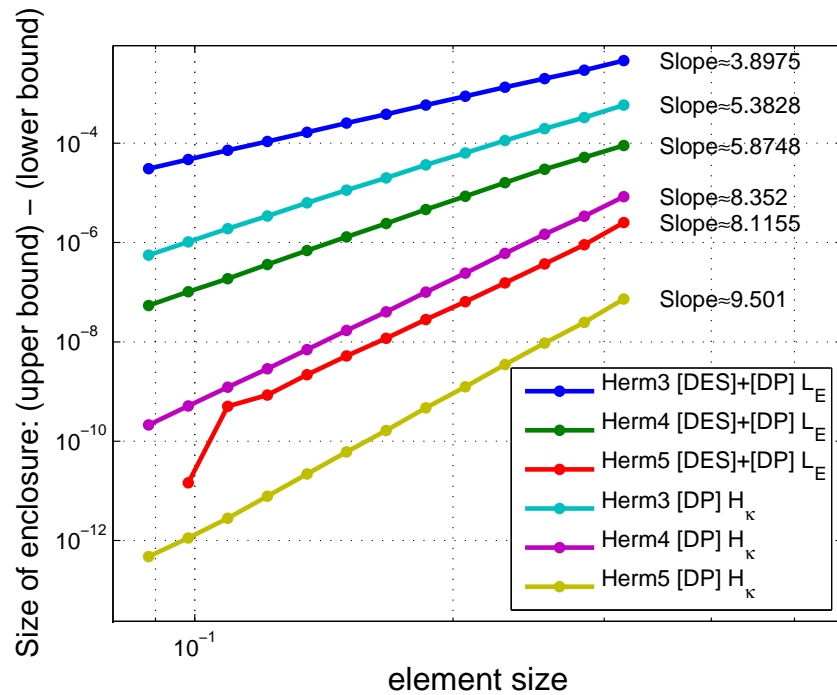
# Numerical experiments



$$V(r) = -\frac{1}{2r} \quad \kappa = -1 \quad E = E_0$$

$\mathcal{L}^h$  - Hermite elements on a uniform mesh of max el size  $h$  in  $[0, 128]$ .

# Numerical experiments



$$V(r) = -\frac{4}{1+r^2} \quad \kappa = -1 \quad E = E_0$$

$\mathcal{L}^h$  - Hermite elements on a uniform mesh of max el size  $h$  in  $[0, 128]$ .

# Open questions

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$$H_B = \alpha \cdot (-i\nabla + \frac{1}{2}B(-x_2, x_1, 0)) + \beta - \frac{\nu}{|x|}$$

$$\alpha = (\alpha_1, \alpha_2, \alpha_3)$$

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} \quad \beta = \begin{pmatrix} I_{\mathbb{C}^2} & 0 \\ 0 & -I_{\mathbb{C}^2} \end{pmatrix}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$