On the computation of the eigenvalues of Dirac operators

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Settings

$$D^0 = \begin{pmatrix} 1 & -\partial_r + \frac{\kappa}{r} \\ \partial_r + \frac{\kappa}{r} & -1 \end{pmatrix} : H^1_0(0,\infty)^2 \longrightarrow L^2(0,\infty)^2$$

$$\sigma(D^0) = (-\infty,-1] \cup [1,\infty) \qquad\qquad \kappa \in \mathbb{N}$$

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

$$H = D^0 + V$$

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

Motivation

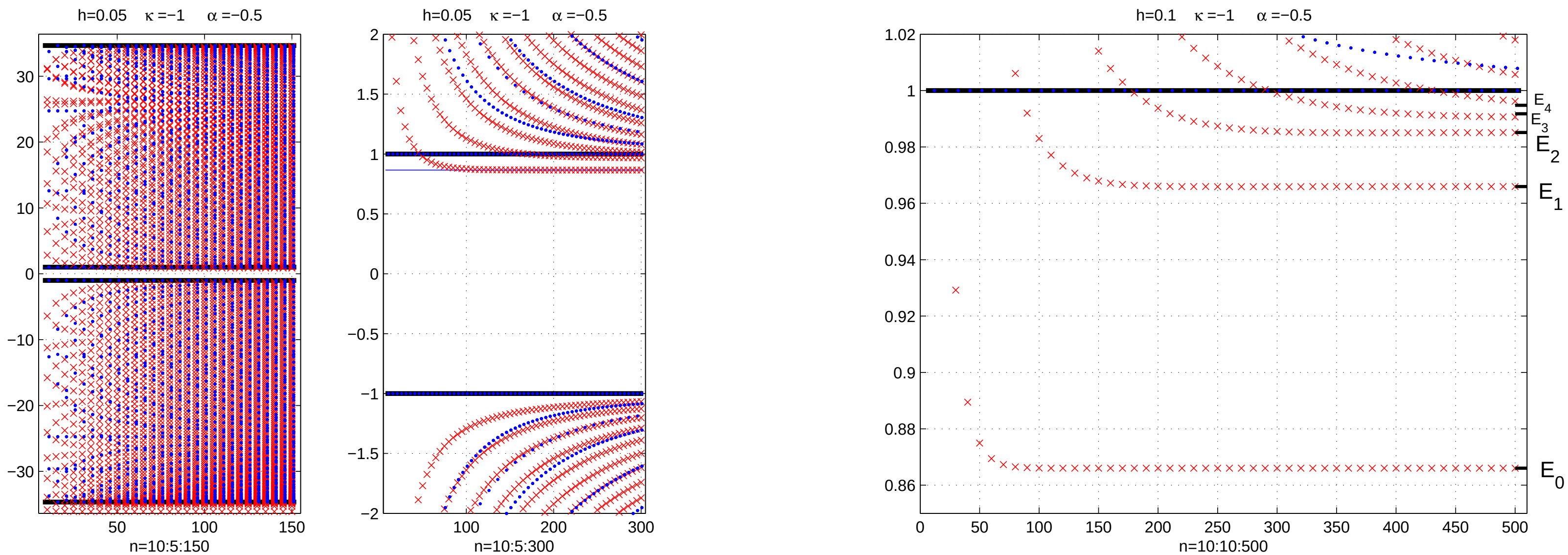
$$\mathcal{L} = \mathrm{Span}\{b_1, \ldots, b_n\} \subset \mathrm{D}(H)$$

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

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

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

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?

ϕ_j^h - piecewise linear hat function, max at jh

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

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

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

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

Pollution is preserved under compact perturbations

Rough enclosures

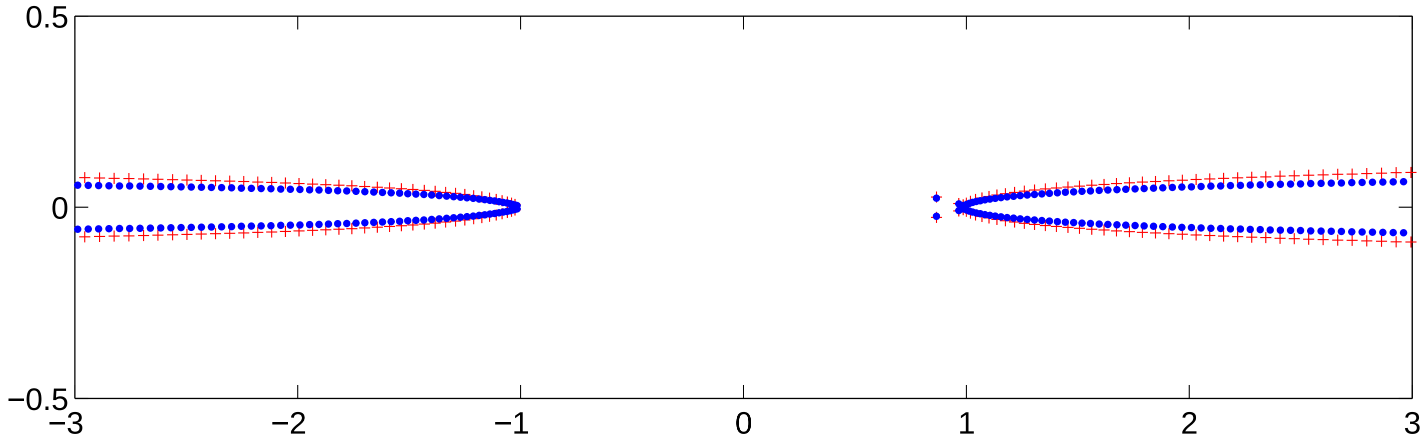
$$L_{\mathcal{L}} = [\langle Hb_j, Hb_k \rangle]_{jk=1}^{n}$$

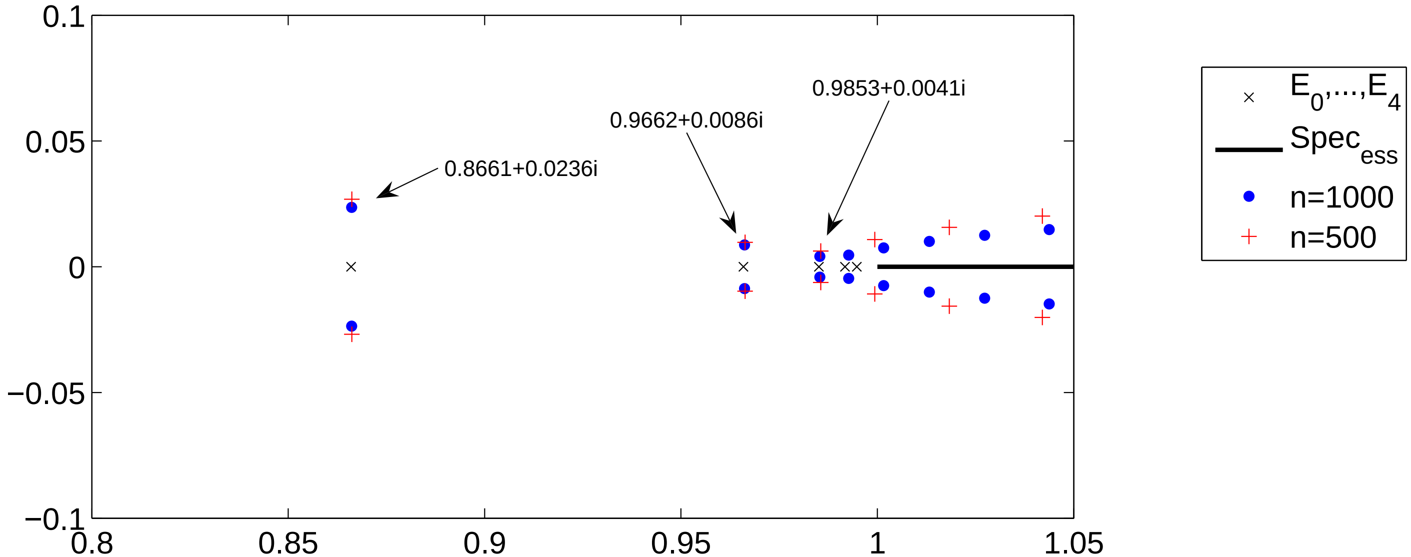
$$\lambda \in \sigma_2(H, \mathcal{L}) \quad \Longleftrightarrow \quad \exists \underline{u} \neq 0,\ (L_{\mathcal{L}} - 2\lambda K_{\mathcal{L}} + \lambda^2 B_{\mathcal{L}})\underline{u} = 0$$

Theorem [Levitin & Shargorodsky]

$$\lambda \in \sigma_2(H, \mathcal{L}) \Rightarrow \begin{array}{l} [\alpha, \beta] \cap \sigma(H) \neq \varnothing \\ \alpha = \mathrm{Re}\lambda - |\mathrm{Im}\lambda|,\ \beta = \mathrm{Re}\lambda + |\mathrm{Im}\lambda| \end{array}$$

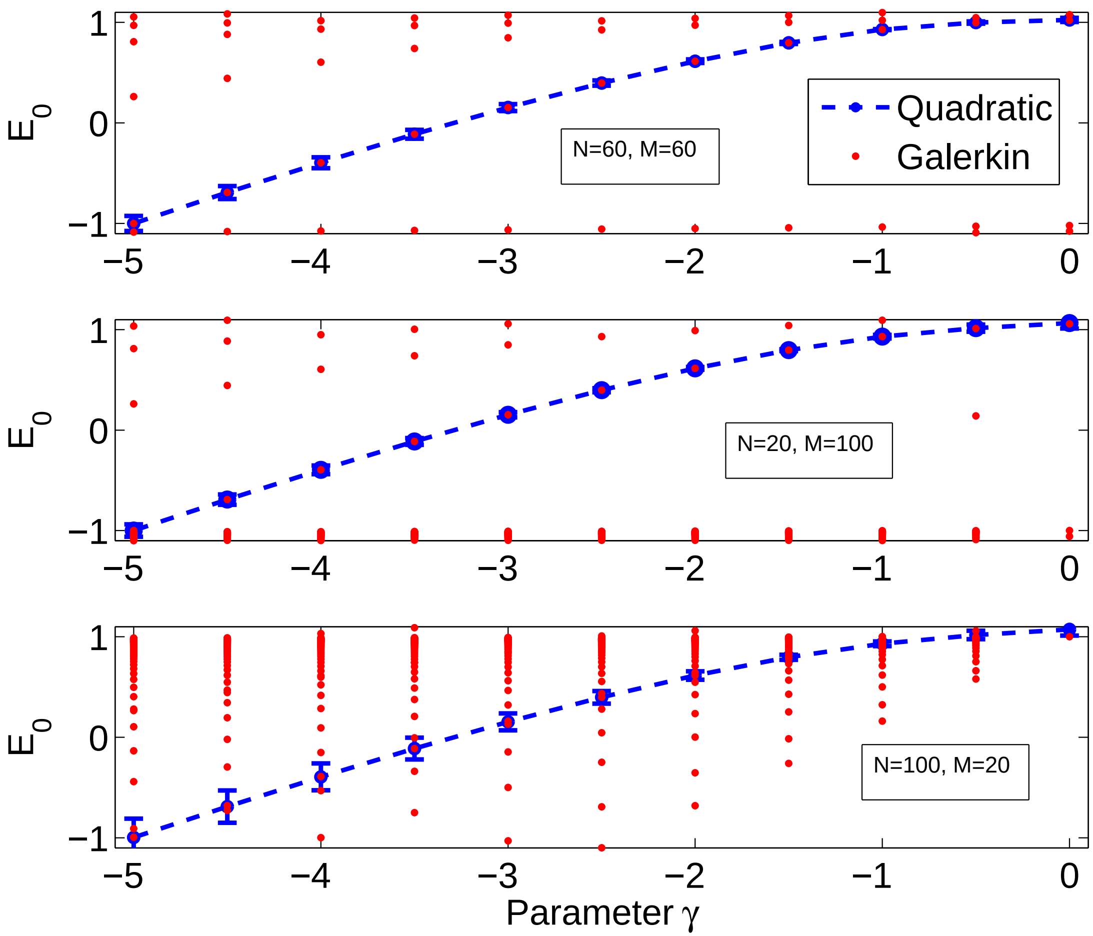
Rough enclosures





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

Rough enclosures



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

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

$$\mathcal{L}_{NM} = \text{Span}\left\{ \begin{pmatrix} e_j \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ e_k \end{pmatrix} \right\}_{k=0:M}^{j=0:N}$$

Rough enclosures

Theorem

Let V be as above and such that $r^{\alpha}V(r)$ is locally bounded for some $0 < \alpha < 1$. Let $E \in \sigma_{\mathrm{disc}}(H)$. 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

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

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

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

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

Dolbeault, Esteban, Séré

A variational principle

$\mu_\lambda \in \sigma_{\mathrm{disc}}(L_\lambda)$ $\qquad \frac{\partial \mu_\lambda}{\partial \lambda}\Big|_{\lambda=E} \leq -1$

$A(E)\phi = 0$

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

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

The F_n method

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

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

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

Theorem [Davies & Plum]

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

Davies & Plum, Mertins & Zimmermann

The F_n method

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

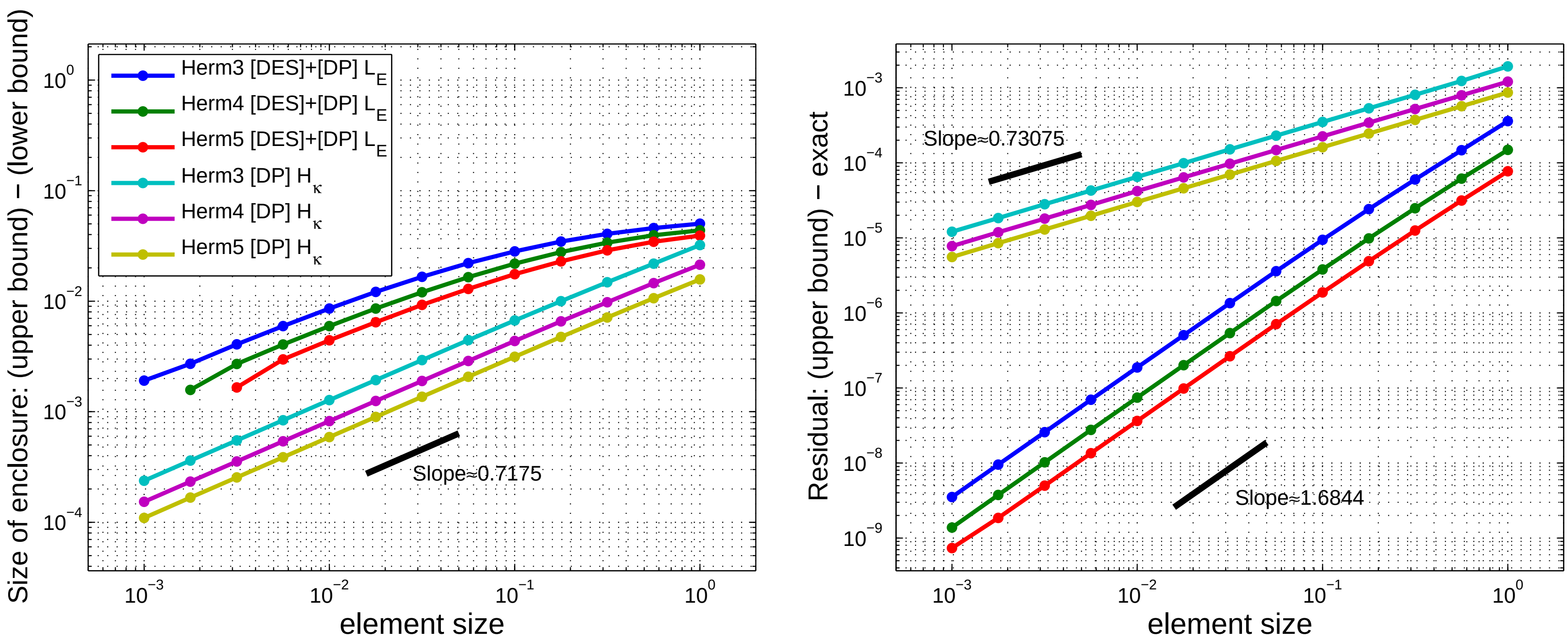
$$R_{\mathcal{L}} = [\langle (L-\delta)b_j, b_k \rangle]_{jk=1}^{n} \qquad Q_{\mathcal{L}} = [\langle (L-\delta)b_j, (L-\delta)b_k \rangle]_{jk=1}^{n}$$

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

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

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

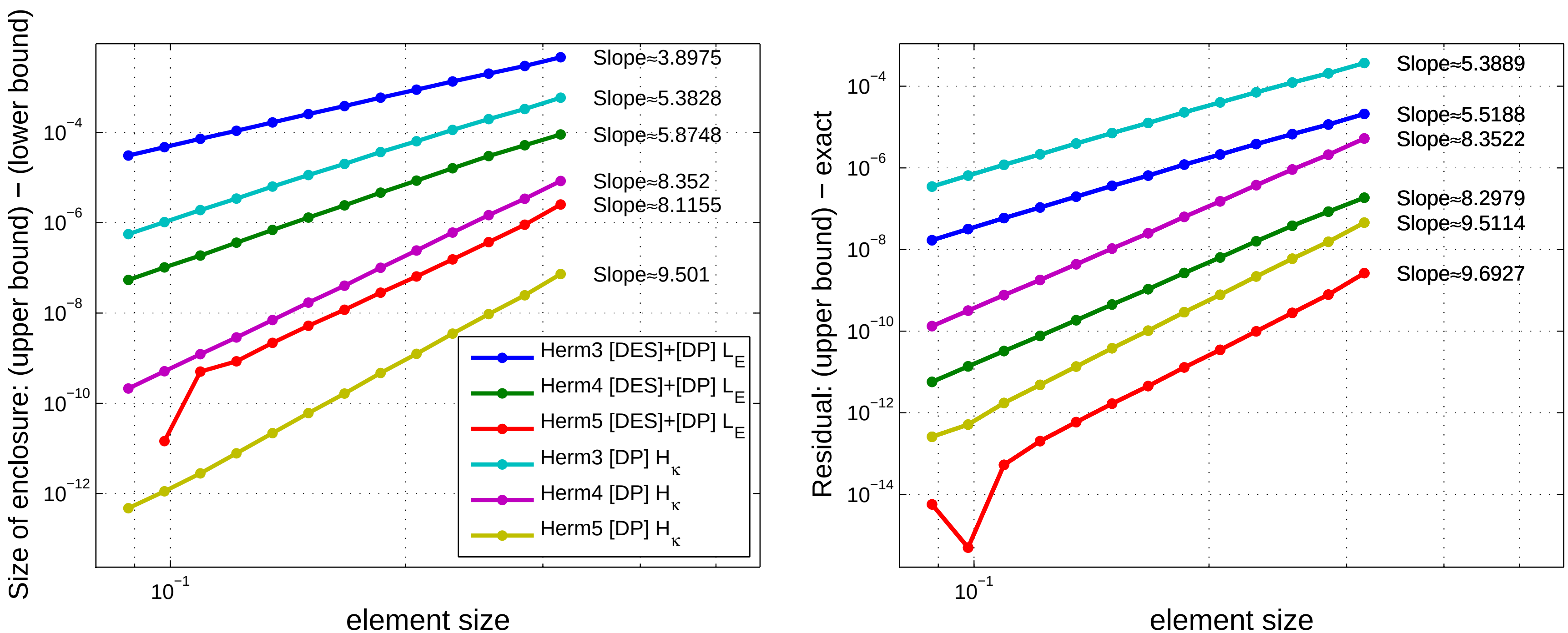
Numerical experiments



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

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

Numerical experiments



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

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

Open questions

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

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

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

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