

# From Weyl Conjecture to Fundamental Gap Conjecture and Beyond



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# Outline

- ★ **Eigenvalue problem** with Dirichlet BC – **Schroedinger/Laplacian** operator (**SO/LO**)
- ★ **The Weyl's law and conjecture**
  - Weyl's law for Laplacian operator in 1D/2D/3D
  - Weyl conjecture
  - Extension to cases with potentials and other BCs
  - Extension to fractional Schroedinger operator (**FSO**)
- ★ **The fundamental gap conjecture**
  - For Laplacian/Schrodinger operator (LO/SO)
  - Extension to fractional Schroedinger operator (FSO)
  - Other gaps and gaps distribution statistics
- ★ **Fundamental gaps of** constrained nonlinear eigenvalue problem (**GPE/NLSE**)
- ★ **Conclusions**

# Eigenvalue (Strum-Liouville) Problem

- 💡 Consider the **eigenvalue** problem

$$(-\Delta + V(\vec{x}))u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega \subset \mathbb{R}^d$$

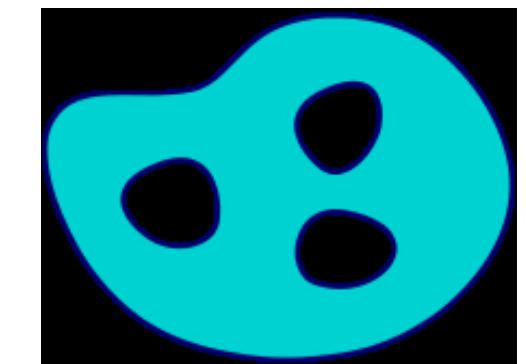
- $\Omega$  is bounded, with **Dirichlet** BC:

$$u(\vec{x}) = 0, \quad \vec{x} \in \Gamma = \partial\Omega$$

- $u(\vec{x})$  : eigenfunction (or state in physics)

- $\lambda$  : eigenvalue (spectrum or energy level)

- $V(\vec{x}) \in C^0(\Omega)$  or  $L^\infty(\Omega)$  : real-valued given potential



Hearing a shape of a drum

- 💡 Arising from **wave** equation

$$\partial_{tt}\phi(\vec{x}, t) = (\Delta - V(\vec{x}))\phi(\vec{x}, t) \quad \Rightarrow \quad (-\Delta + V(\vec{x}))u(\vec{x}) = \lambda u(\vec{x})$$

# Time-independent Schrodinger Equation

💡 The Schrodinger equation –Ewin Schrodinger, 1925

$$i\hbar \partial_t \psi(\vec{x}, t) = \left( -\frac{\hbar^2}{2m} \Delta + V(\vec{x}) \right) \psi(\vec{x}, t)$$

$$\hbar = m = 1 \Downarrow \psi(\vec{x}, t) = e^{-iEt} u(\vec{x})$$

$$\left( -\frac{1}{2} \Delta + V(\vec{x}) \right) u(\vec{x}) = E u(\vec{x}) \Rightarrow L_{SO} u := \left( -\frac{1}{2} \Delta + V(\vec{x}) \right) u(\vec{x}) = E u(\vec{x})$$



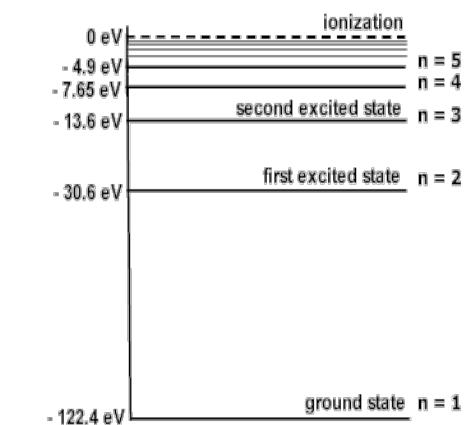
Hydrogen atom

💡 Quantum Many-body Problem – Paul Dirac

- Quantum physics/chemistry -- DFT
- Materials science– electronic structure, materials simulation & design

$$\left[ \sum_{j=1}^N \left( -\frac{\hbar^2}{2m} \Delta_j + V(\vec{r}_j) \right) + \sum_{1 \leq j < k \leq N} V_{\text{int}}(\vec{r}_j - \vec{r}_k) \right] \Phi = E \Phi$$

💡 Many other applications, .....



Spectrum of Hydrogen

# Eigenvalues & Eigenfunctions

$$(-\Delta + V(\vec{x}))u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega$$

$$u(\vec{x}) = 0, \quad \vec{x} \in \Gamma = \partial\Omega$$

## ★ Eigenvalues

$V(\vec{x}) \geq 0$  & weakly convex

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n \leq \dots \quad \Rightarrow \quad 0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n \leq \dots$$

– with the times an eigenvalue appear being its algebraic multiplicity

## ★ Eigenfunctions can be taken as orthonormal

$$u_1, u_2, \dots, u_n, \dots \Rightarrow \|u_n\|_{L^2}^2 = \int_{\Omega} u_n(\vec{x})^2 d\vec{x} = 1, \quad (u_n, u_l) = \delta_{nl}$$

★ Rayleigh quotient – variational formulation :  $E(v) = \int_{\Omega} \left( |\nabla v|^2 + V(\vec{x})v^2 \right) d\vec{x}$

$$\lambda_1 = \min_{0 \neq v \in H_0^1(\Omega)} \frac{E(v)}{\|v\|_{L^2}^2}, \quad \lambda_{n+1} = \min_{0 \neq v \in U_n^\perp} \frac{E(v)}{\|v\|_{L^2}^2}, \quad U_n = \text{span}\{u_1, \dots, u_n\}, n \geq 1$$

# Asymptotics of Eigenvalues

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n \leq \dots$$

• The number of states below a given energy

$$\lambda_n = O(n^\gamma), n \gg 1 \Rightarrow N(E) := \#\{n \in \mathbb{Z}^+ \mid \lambda_n \leq E\} = O(E^{1/\gamma}), E \gg 1$$

$$\Downarrow \exists \gamma > 0 \& C > 0$$

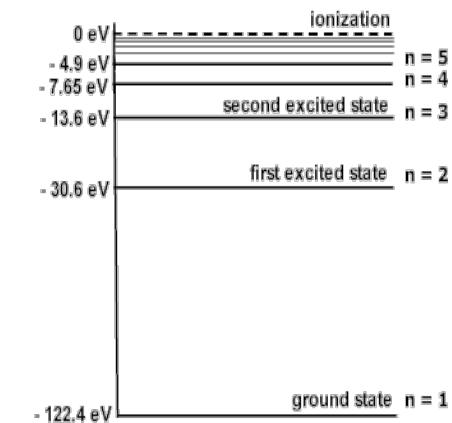
$$\lambda_n = Cn^\gamma + o(n^\gamma), n \gg 1 \Rightarrow N(E) = \left(\frac{E}{C}\right)^{1/\gamma} + o(E^{1/\gamma}), \quad E \gg 1$$

• An example in 1D:

$$-u''(x) = \lambda u(x), \quad x \in (0, S); \quad u(0) = u(S) = 0$$

– All eigenvalues

$$\lambda_n = \frac{n^2 \pi^2}{S^2}, \quad n = 1, 2, \dots \Rightarrow \lambda_n = \frac{\pi^2}{S^2} n^2, n \gg 1 \Leftrightarrow N(E) = \frac{S}{\pi} E^{1/2}, E \gg 1$$



# Asymptotics of Eigenvalues

$$0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n \leq \dots$$

Another example in 2D:

$$-\Delta u(x, y) = \lambda u(x, y), \quad (x, y) \in \Omega = (0, L_1) \times (0, L_2)$$

$$u(x, y) = 0, \quad (x, y) \in \Gamma = \partial\Omega$$

– All eigenvalues:

$$\tilde{\lambda}_{lk} = \frac{l^2 \pi^2}{L_1^2} + \frac{k^2 \pi^2}{L_2^2}, \quad l, k = 1, 2, \dots$$

– Re-arrange them and obtained by Hermann Weyl, 1911

$$0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n \leq \dots \stackrel{L_1=L_2=1}{\Rightarrow} \lambda_1 = 2\pi^2, \lambda_2 = \lambda_3 = 5\pi^2, \lambda_4 = 8\pi^2, \dots$$

$$N(E) = \frac{S}{4\pi} E + o(E), E \gg 1 \quad \stackrel{S=|\Omega|=L_1 L_2}{\Leftrightarrow} \quad \lambda_n = \frac{4\pi}{S} n + o(n), n \gg 1$$

# The Weyl's Law

$$-\Delta u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega \subset \mathbb{R}^d$$

$$u(\vec{x}) = 0, \quad \vec{x} \in \Gamma = \partial\Omega$$

• All eigenvalues:

$$0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n \leq \dots$$

• The number of states below an energy  $E$

$$N(E) := \#\{n \in \mathbb{Z}^+ \mid \lambda_n \leq E\}, \quad E > 0$$

• Hermann Weyl proved in 1D&2D&3D (1911 by counting states & 1912 by variational method):

$$\lim_{E \rightarrow +\infty} \frac{N(E)}{E^{d/2}} = \frac{\omega_d S}{(2\pi)^d} \iff \lambda_n = \frac{4\pi^2}{(\omega_d S)^{2/d}} n^{2/d} + o(n^{2/d}), \quad n \gg 1$$

$S = |\Omega|$ ,  $\omega_d$  -- the volume of the unit ball in  $\mathbb{R}^d$ ,  $\omega_1 = 2, \omega_2 = \pi, \dots$

– In 2D:  $N(E) = \frac{S}{4\pi} E + o(E), E \gg 1 \iff \lambda_n = \frac{4\pi}{S} n + o(n), n \gg 1$

# The Weyl Conjecture

$$N(E) := \#\{n \in \mathbb{Z}^+ \mid \lambda_n \leq E\}, \quad E > 0$$

– Hermann Weyl made the **conjecture** in 1912:

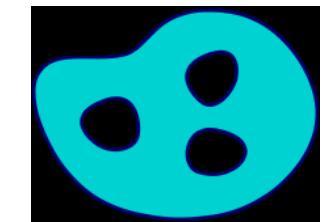
$$N(E) = \frac{\omega_d S}{(2\pi)^d} E^{d/2} - \frac{\omega_{d-1} L}{4(2\pi)^{d-1}} E^{(d-1)/2} + o(E^{(d-1)/2}), \quad E \gg 1$$

$$\Leftrightarrow \lambda_n = \frac{4\pi^2}{(\omega_d S)^{2/d}} n^{2/d} + \frac{2\pi^2 \omega_{d-1} L}{d(\omega_d S)^{(d+1)/d}} n^{1/d} + o(n^{1/d}), \quad n \gg 1$$

$$N(E) = \frac{S}{4\pi} E - \frac{L}{4\pi} E^{1/2} + o(E^{1/2}), \quad E \gg 1 \Leftrightarrow \lambda_n = \frac{4\pi}{S} n + \frac{2\sqrt{\pi} L}{S^{3/2}} n^{1/2} + o(n^{1/2}), \quad n \gg 1$$

– Some **results**:

- Richard Courant in 1922 proved a bound at :  $O(E^{(d-1)/2} \log E)$
- Boris Levitan in 1952 for compact closed domain:  $O(E^{(d-1)/2})$
- Robert Seeley in 1978 extend to general domain:
- Hans Duistermaat & Victor Guillemin in 1975 under a strong condition:  $o(E^{(d-1)/2})$
- Victor Ivrii in 1980:  $o(E^{(d-1)/2})$



area & perimeter

# A Spectral Method

$$(-\Delta + V(\vec{x}))u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega$$

💡 Variational Form:

$$u(\vec{x}) = 0, \quad \vec{x} \in \Gamma = \partial\Omega$$

Find  $0 \neq u \in H_0^1(\Omega)$  &  $\lambda \in \mathbb{R}$  s.t.

$$a(u, v) + b(u, v) = \lambda(u, v), \quad \forall v \in H_0^1(\Omega)$$

– where

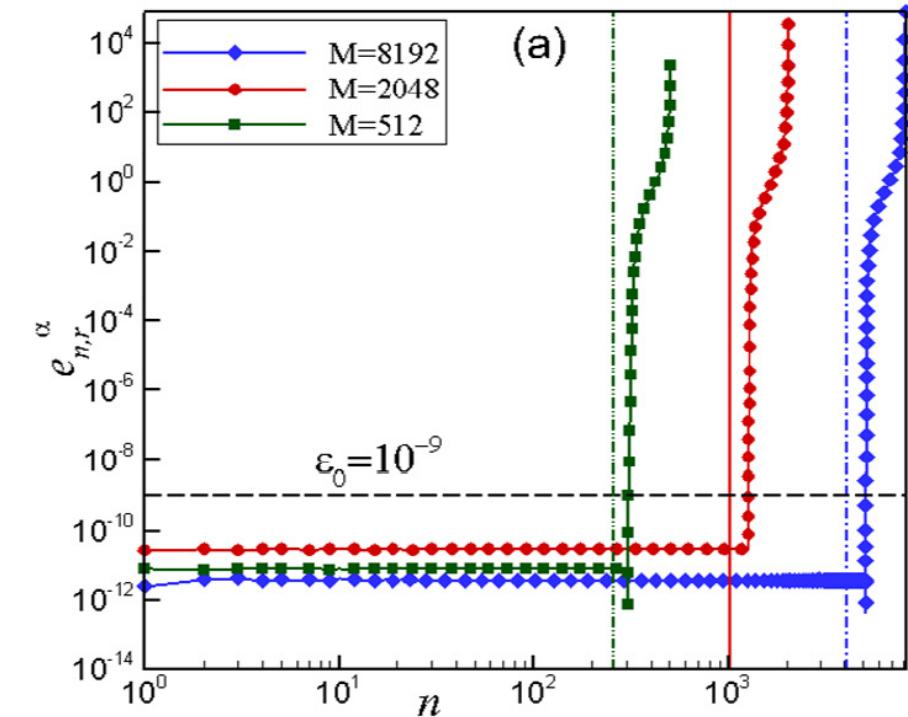
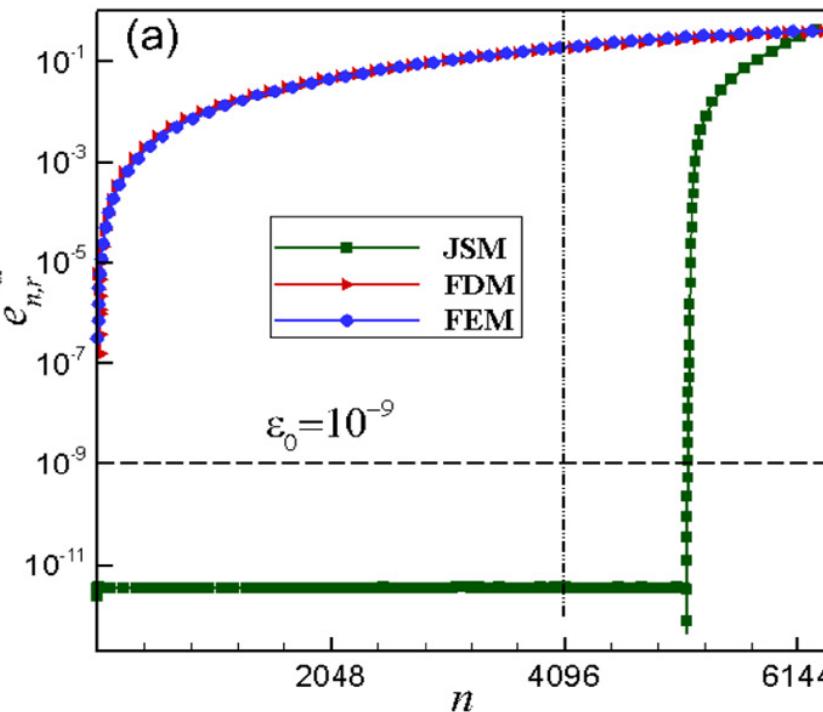
$$a(u, v) = \int_{\Omega} \nabla u(\vec{x}) \cdot \nabla v(\vec{x}) d\vec{x}, \quad b(u, v) = \int_{\Omega} V(\vec{x}) u(\vec{x}) v(\vec{x}) d\vec{x}, \quad (u, v) = \int_{\Omega} u(\vec{x}) v(\vec{x}) d\vec{x}$$

💡 A **spectral** method:  $U_M := \text{span}\{\phi_1, \phi_2, \dots, \phi_M\} \subset H_0^1(\Omega)$

Find  $0 \neq u_M \in U_M$  &  $\lambda \in \mathbb{R}$  s.t.

$$a(u_M, v) + b(u_M, v) = \lambda(u_M, v), \quad \forall v \in U_M \Leftrightarrow (D + A)U = \lambda BU$$

# Comparison on Resolution



✿ Spectral method has much better resolution than FDM & FEM

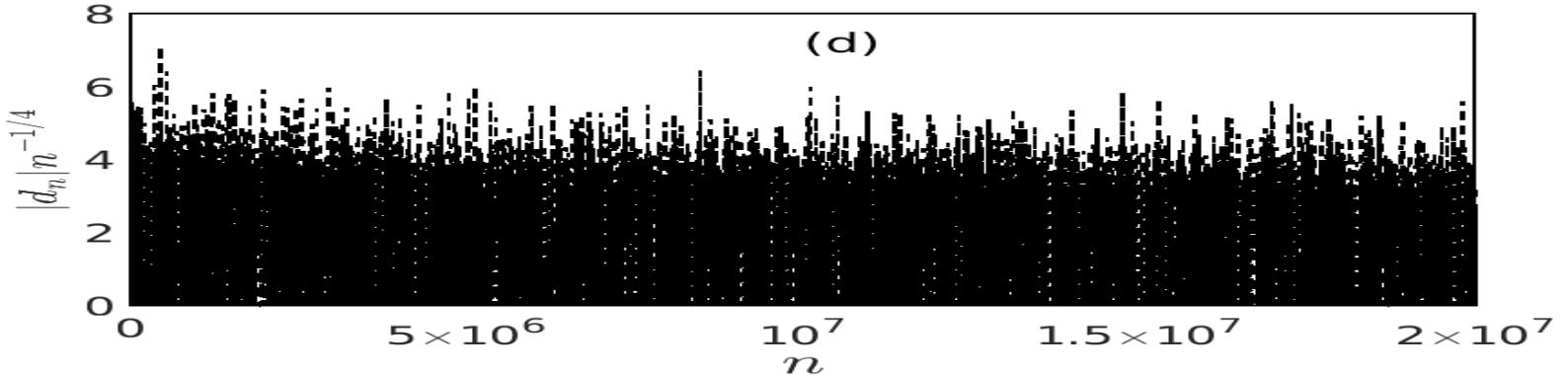
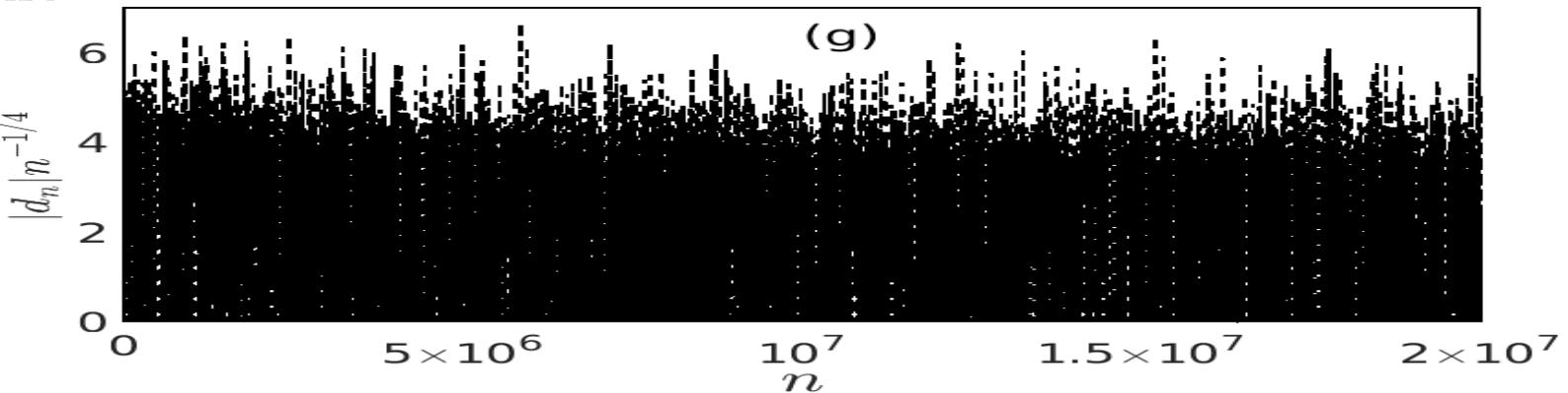
✿ Spectral method can resolve # of eigenvalues proportional to DoF

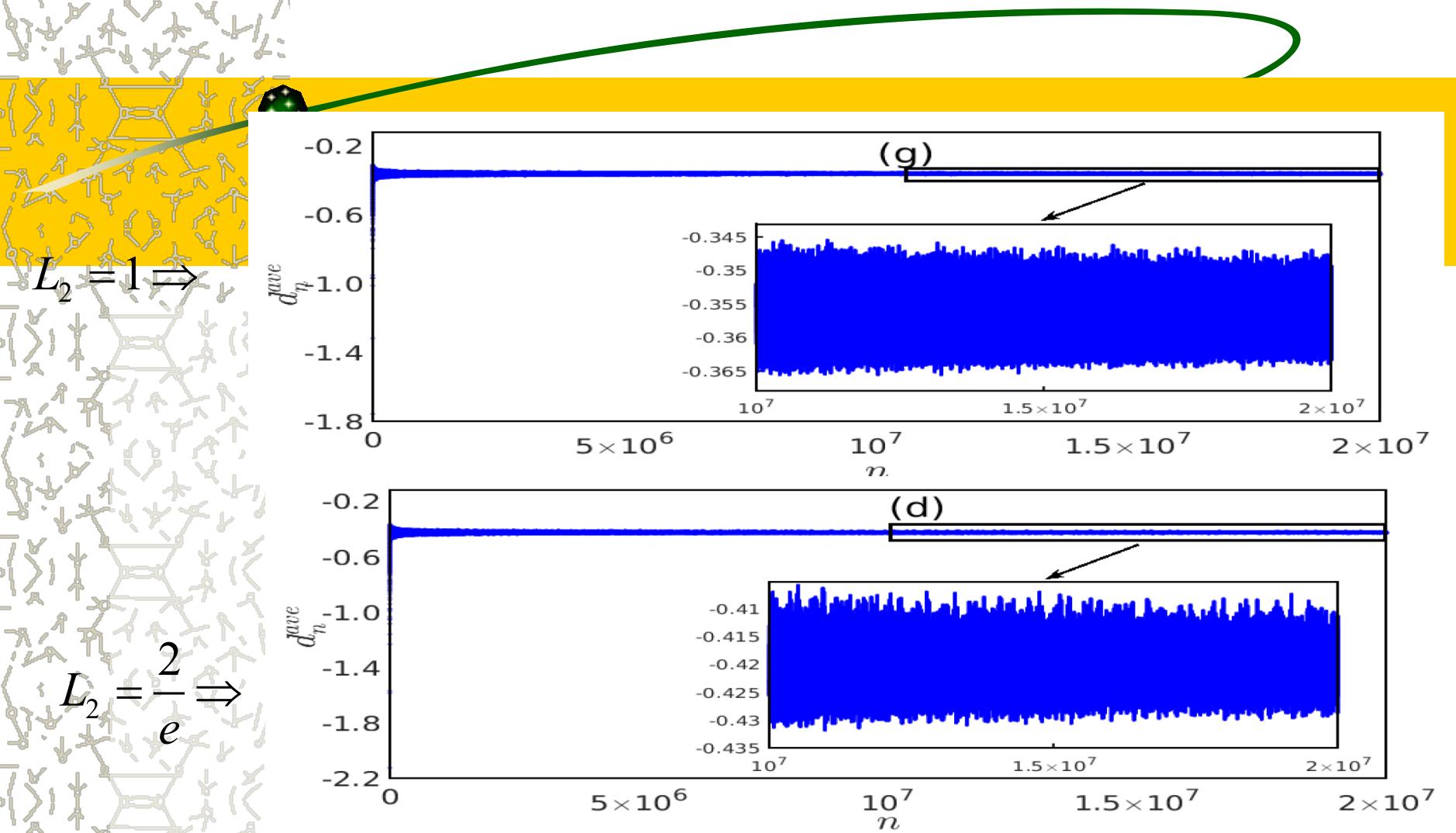
# Numerical Results in 2D

Setup:

$$d = 2, \quad V(\vec{x}) \equiv 0, \quad \Omega = (-1, 1) \times (-L_2, L_2), \quad 0 < L_2 \leq 1, \quad S = 4L_2, \quad L = 4(1 + L_2)$$

$$d_n := \lambda_n - \frac{4\pi}{S}n - \frac{2\sqrt{\pi}L}{S^{3/2}}n^{1/2}, \quad d_n^{\text{ave}} := \frac{1}{n} \sum_{m=1}^n d_m, \quad n = 1, 2, \dots$$





• Numerical observation – Bao & Chen 20'

$$\lambda_n = \frac{4\pi}{S} n + \frac{2\sqrt{\pi}L}{S^{3/2}} n^{1/2} + \alpha_n n^{1/4}, \quad n = 1, 2, \dots$$

$\alpha_n$  is oscillatory  $\lim_{n \rightarrow +\infty} \frac{\alpha_n}{n^\varepsilon} = 0, \forall \varepsilon > 0$

$d_n^{\text{ave}}$  is bounded

Hardy, 1916 showed  $N(E) - \frac{S}{4\pi}E + \frac{L}{4\pi}E^{1/2} \geq CE^{1/4}(\log E)^{1/4}$ ,  $E \gg 1$

# Extension to Laplacian Operator with Neumann BC

• The Eigenvalue Problem:

- Order of all eigenvalues:

$$0 = \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n \leq \dots$$

• In 1D with  $\Omega = (0, S)$ :

$$\lambda_n = \frac{(n-1)^2 \pi^2}{S^2}, \quad n = 1, 2, \dots \Rightarrow \lambda_n = \frac{\pi^2}{S^2} n^2 - \frac{2\pi^2}{S^2} n + \frac{\pi^2}{S^2}, \quad n \gg 1 \Leftrightarrow N(E) = \frac{S}{\pi} E^{1/2} + 1, \quad E \gg 1$$

• In 2D:

$$N(E) = \frac{S}{4\pi} E + \frac{L}{4\pi} E^{1/2} + o(E^{1/2}), \quad E \gg 1 \Leftrightarrow \lambda_n = \frac{4\pi}{S} n - \frac{2\sqrt{\pi} L}{S^{3/2}} n^{1/2} + o(n^{1/2}), \quad n \gg 1$$

- Our numerical results – Bao & Chen 20'

$$\lambda_n = \frac{4\pi}{S} n - \frac{2\sqrt{\pi} L}{S^{3/2}} n^{1/2} + \tilde{\alpha}_n n^{1/4}, \quad n = 1, 2, \dots$$

$$\begin{aligned} -\Delta u(\vec{x}) &= \lambda u(\vec{x}), \quad \vec{x} \in \Omega \\ \frac{\partial u(\vec{x})}{\partial \vec{n}} &= 0, \quad \vec{x} \in \Gamma = \partial \Omega \end{aligned}$$

$\tilde{\alpha}_n$  is oscillatory  $\lim_{n \rightarrow +\infty} \frac{\tilde{\alpha}_n}{n^\varepsilon} = 0, \forall \varepsilon > 0$

$\tilde{d}_n^{\text{ave}}$  is bounded

# Extension to Fractional Schrodinger Operator (FSO/FLO)

• The FSO in 1D:

$$L_{\text{FSO}} u := \left( (-\partial_{xx})^{\alpha/2} + V(x) \right) u(x) = \lambda u(x), \quad x \in \Omega = (0, S),$$
$$u(x) = 0, \quad x \in \Omega^c = \mathbb{R} \setminus \Omega; \quad 0 < \alpha \leq 2$$

– Fractional derivative defined as

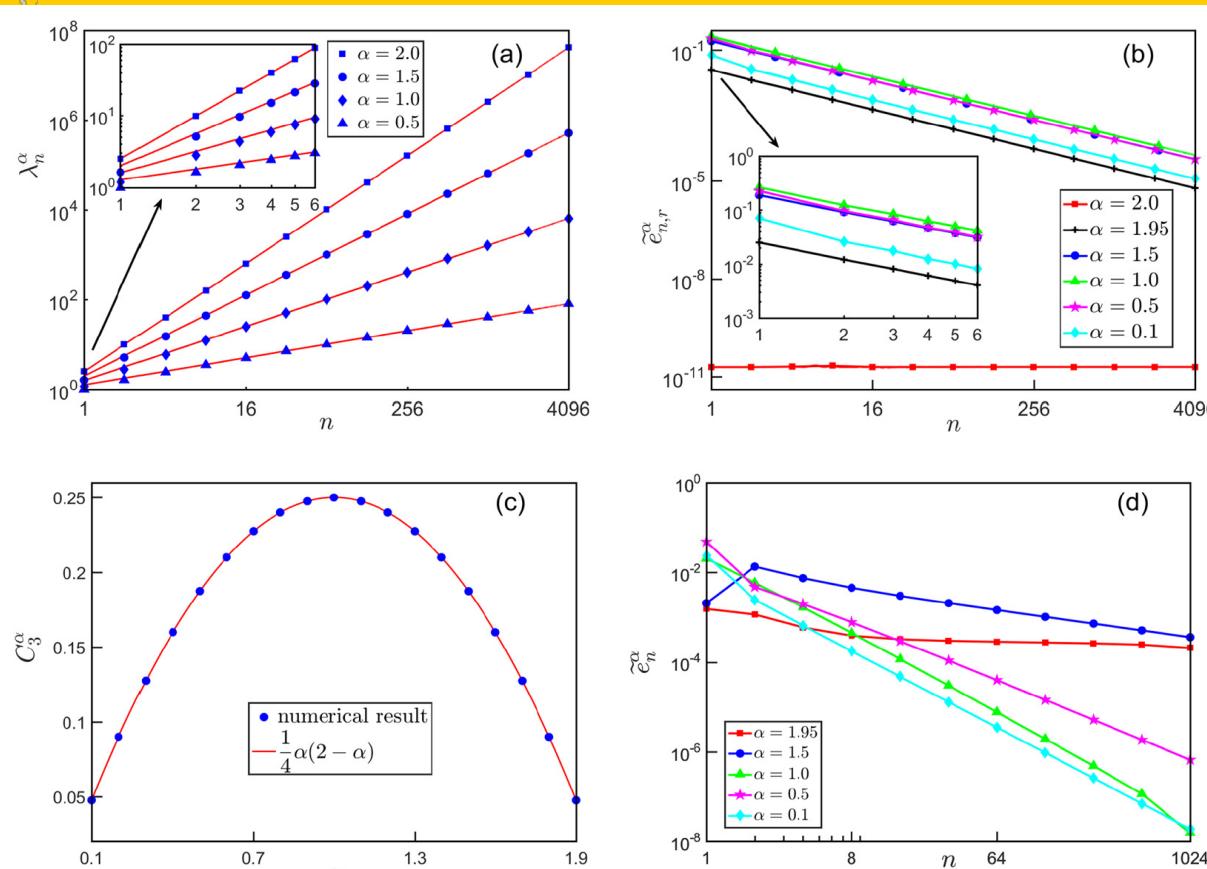
$$(-\partial_{xx})^{\alpha/2} u(x) = F^{-1}(|\xi|^\alpha (Fu)(\xi)), \quad x, \xi \in \mathbb{R}$$

• Order of all eigenvalues:

$$\lambda_1^\alpha \leq \lambda_2^\alpha \leq \dots \leq \lambda_n^\alpha \leq \dots \Rightarrow u_1^\alpha, u_2^\alpha, \dots$$

• A Jacobi spectral method:

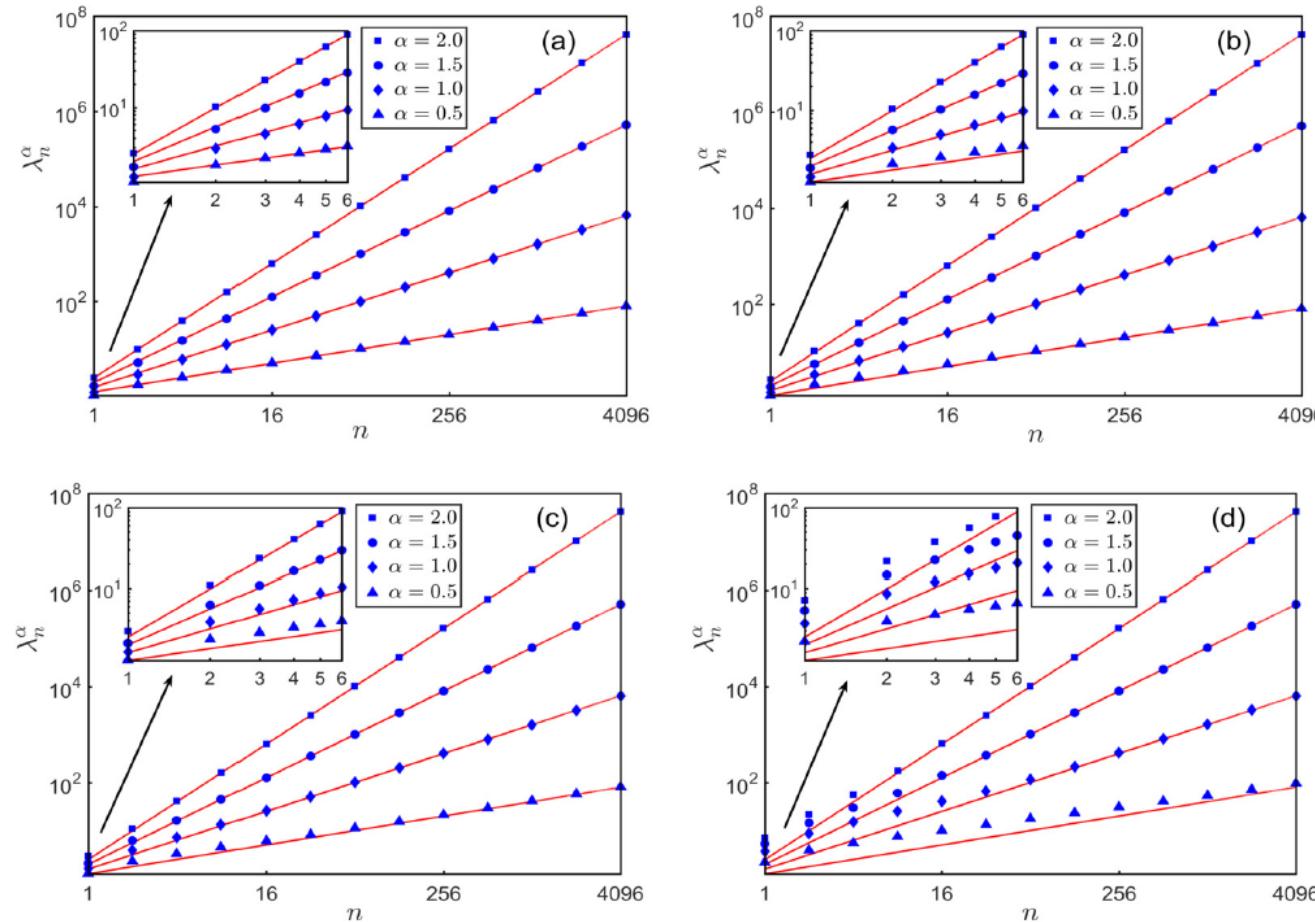
# Asymptotics of Eigenvalues of FLO



**Conjecture:**

$$\lambda_n^\alpha = \left(\frac{n\pi}{S}\right)^\alpha - \left(\frac{\pi}{S}\right)^\alpha \frac{\alpha(2-\alpha)}{4} n^{\alpha-1} + O(n^{\alpha-2}), \quad n=1, 2, \dots \quad u_n^\alpha(x) = x^{\alpha/2} (S-x)^{\alpha/2} v_n^\alpha(x), \quad 0 \leq x \leq S$$

# Asymptotics of FSO in 1D



**Fig. 12.** Eigenvalues  $\lambda_n^\alpha$  ( $n = 1, 2, \dots, 4096$ ) of (1.1) with  $\Omega = (-1, 1)$  and different  $\alpha$  for differential external potentials (symbols denote numerical results and solid lines are from fitting formulas when  $n \gg 1$ ): (a) Case I, (b) Case II, (c) Case III, and (d) Case IV.

# Asymptotics of Eigenvalues of FSO/FLO in 1D

$$[(-\partial_{xx})^{\alpha/2} + V(x)]u(x) = \lambda u(x), x \in \Omega = (0, S); \quad u(x) = 0, x \in \Omega^c = \mathbb{R} \setminus \Omega; \quad 0 < \alpha \leq 2$$

Denote eigenvalues without/with potentials:

$$0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n \leq \dots$$

$$\lambda_1^V \leq \lambda_2^V \leq \dots \leq \lambda_n^V \leq \dots$$

Define

$$\hat{d}_n := \lambda_n^V - \lambda_n, \quad n = 1, 2, \dots$$

$$\hat{d}_n^{\text{ave}} := \frac{1}{n} \sum_{m=1}^n \hat{d}_m,$$

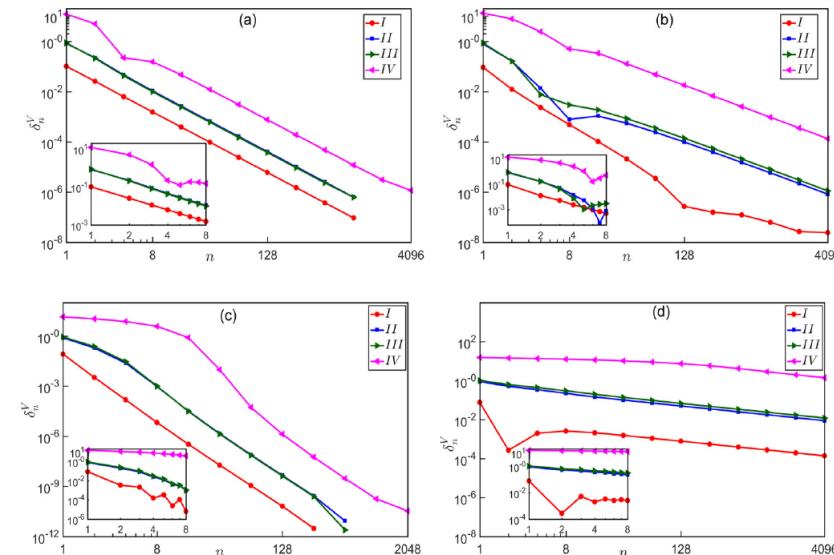


Fig. 15. Differences of the eigenvalues of (1.1) with potential  $V$  and without potential, i.e.  $\delta_n^V := \lambda_n^\alpha - \lambda_n^{\alpha,0} - C_V$  ( $1 \leq n \leq N = 4096$ ) for different potentials  $V(x)$  and  $\alpha$ : (a)  $\alpha = 2$ , (b)  $\alpha = \sqrt{2}$ , (c)  $\alpha = 1$ , and (d)  $\alpha = 0.5$ .

Numerical results – Bao, Chen, Jiang & Ma, JCP, 20' – H. Hochstadt, CPAM 1961' for  $\alpha = 2$

$$\lambda_n^V = \lambda_n + C_V + O(n^{-\tau_1(\alpha)}), \quad n \gg 1$$

$$\hat{d}_n^{\text{ave}} = C_V + O(n^{-\alpha/2}), \quad C_V = \frac{1}{|\Omega|} \int_{\Omega} V(x) dx$$

$$\tau_1(\alpha) = \begin{cases} \alpha, & 0 < \alpha \leq 2 \& \alpha \neq 1 \\ \approx 4.5, & \alpha = 1, \end{cases}$$

$$0 < \alpha < 2 \quad ????$$

# Extension to Directional FSO

★ The **directional FSO** in high dimensions:

$$L_{\text{D-FSO}} u := \left( D_{\vec{x}}^\alpha + V(\vec{x}) \right) u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega \subset \mathbb{R}^d$$

$$u(\vec{x}) = 0, \quad \vec{x} \in \Omega^c = \mathbb{R}^d \setminus \Omega; \quad 0 < \alpha \leq 2, \quad d \geq 2$$

– **Fractional derivative** defined as

$$D_{\vec{x}}^\alpha u(\vec{x}) = F^{-1} \left( \sum_{j=1}^d |\xi_j|^\alpha (Fu)(\vec{\xi}) \right), \quad \vec{x}, \vec{\xi} \in \mathbb{R}^d$$

★ Order of all **eigenvalues**:

$$\lambda_1^\alpha \leq \lambda_2^\alpha \leq \dots \leq \lambda_n^\alpha \leq \dots \Rightarrow u_1^\alpha, u_2^\alpha, \dots$$

★ A **Jacobi spectral method**:

# Asymptotics of Eigenvalues of D-FLO in 2D

**Setup:**

$$d = 2, \quad V(\vec{x}) \equiv 0, \quad \Omega = (-1,1) \times (-L_2, L_2), \quad 0 < L_2 \leq 1, \quad S = 4L_2, \quad L = 4(1+L_2)$$

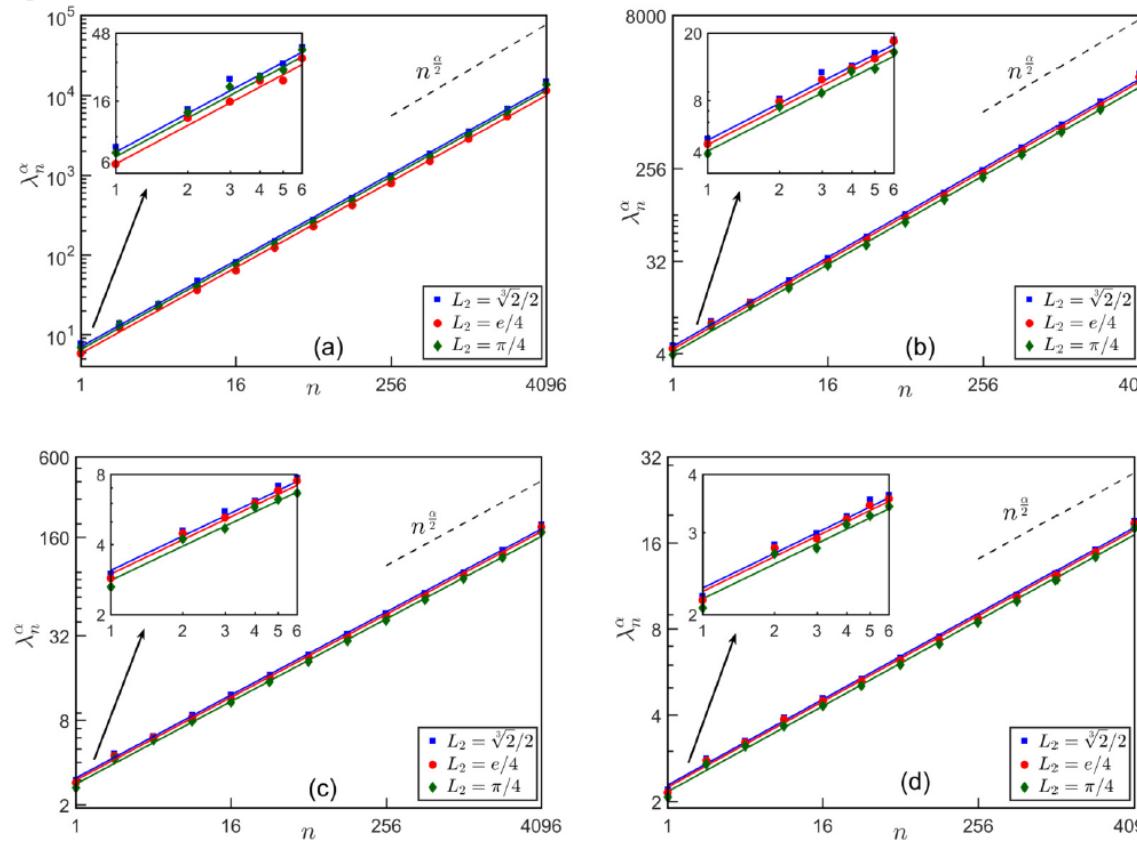


Fig. 17. Eigenvalues of (6.1) with  $d = 2$ ,  $L_1 = 1$ ,  $V(\mathbf{x}) \equiv 0$  and different  $L_2$  and  $\alpha$  (symbols denote numerical results and solid lines are from the fitting formula  $C_2^\alpha n^{\alpha/2}$  when  $n \gg 1$ ): (a)  $\alpha = 1.9$ , (b)  $\alpha = 1.5$ , (c)  $\alpha = 1.0$ , and (d)  $\alpha = 0.5$ .

# The Generalized Weyl's Law of D-FSO

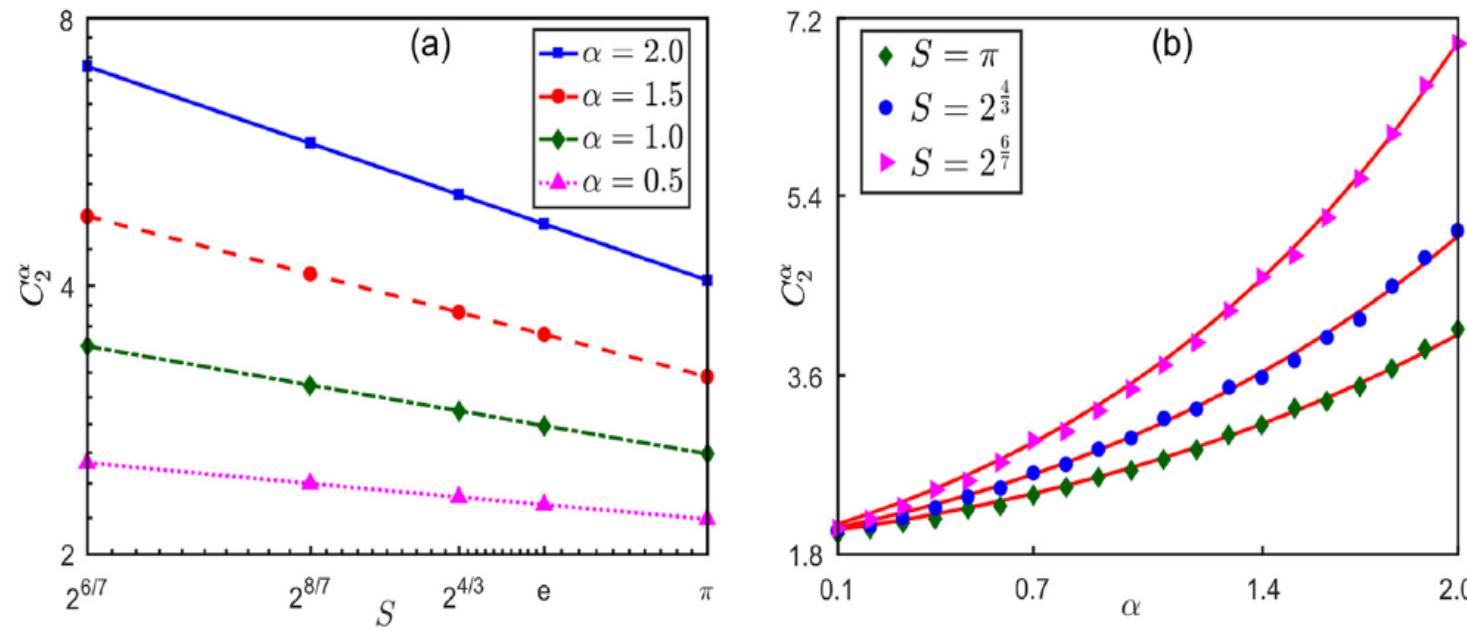


Fig. 18. Numerical results of  $C_2^\alpha$  (symbols denote numerical results and solid lines are from the fitting formula (6.7)) for different areas  $S = |\Omega| = 4L_2$  and  $\alpha$ : (a) plots of  $C_2^\alpha$  as a function of  $S$  for different  $\alpha$ , and (b) plots of  $C_2^\alpha$  as a function of  $\alpha$  for different  $S$ .

**Conjecture:** 
$$\lambda_n^\alpha = \frac{4}{2+\alpha} \left( \frac{4\pi}{S} \right)^{\alpha/2} n^{\alpha/2} + o(n^{\alpha/2}), \quad n \gg 1$$

# Asymptotics of Eigenvalues with Potentials in 2D

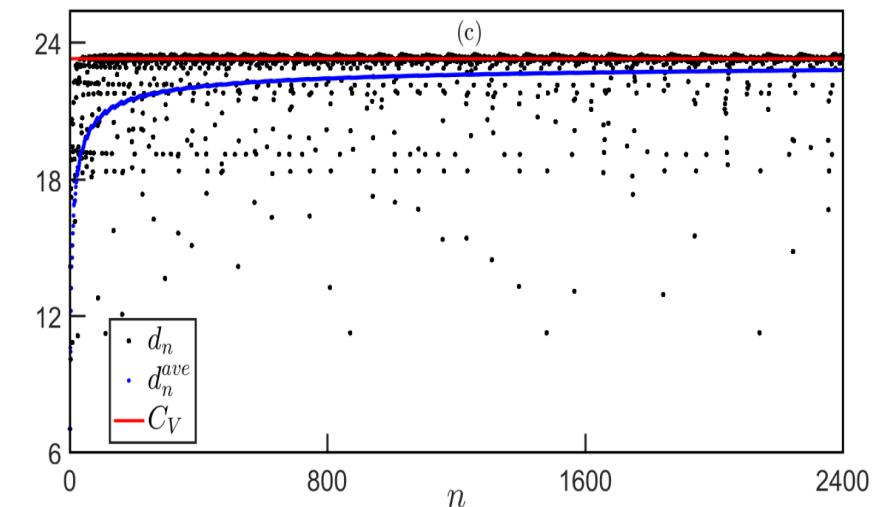
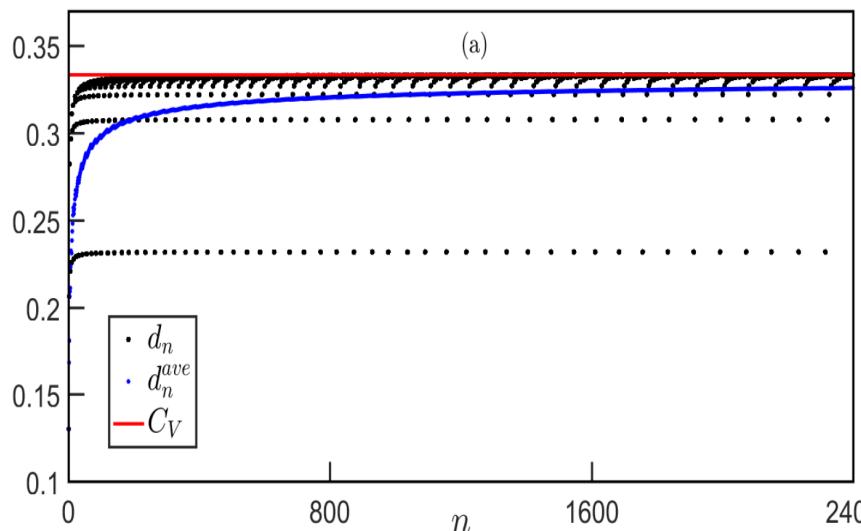
$$(-\Delta + V(\vec{x}))u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega$$

$$u(\vec{x}) = 0, \quad \vec{x} \in \Gamma = \partial\Omega$$

💡 Denote eigenvalues Without/with potentials:

$$0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n \leq \dots; \quad \lambda_1^V \leq \lambda_2^V \leq \dots \leq \lambda_n^V \leq \dots$$

💡 Define  $\hat{d}_n := \lambda_n^V - \lambda_n$ ,  $n = 1, 2, \dots$        $\hat{d}_n^{\text{ave}} := \frac{1}{n} \sum_{m=1}^n \hat{d}_m$ ,



# Asymptotics of Eigenvalues with Potentials in 2D

$$\widehat{d}_n := \lambda_n^V - \lambda_n^2, \quad n = 1, 2, \dots$$

$$\widehat{d}_n^{\text{ave}} := \frac{1}{n} \sum_{m=1}^n d_m,$$

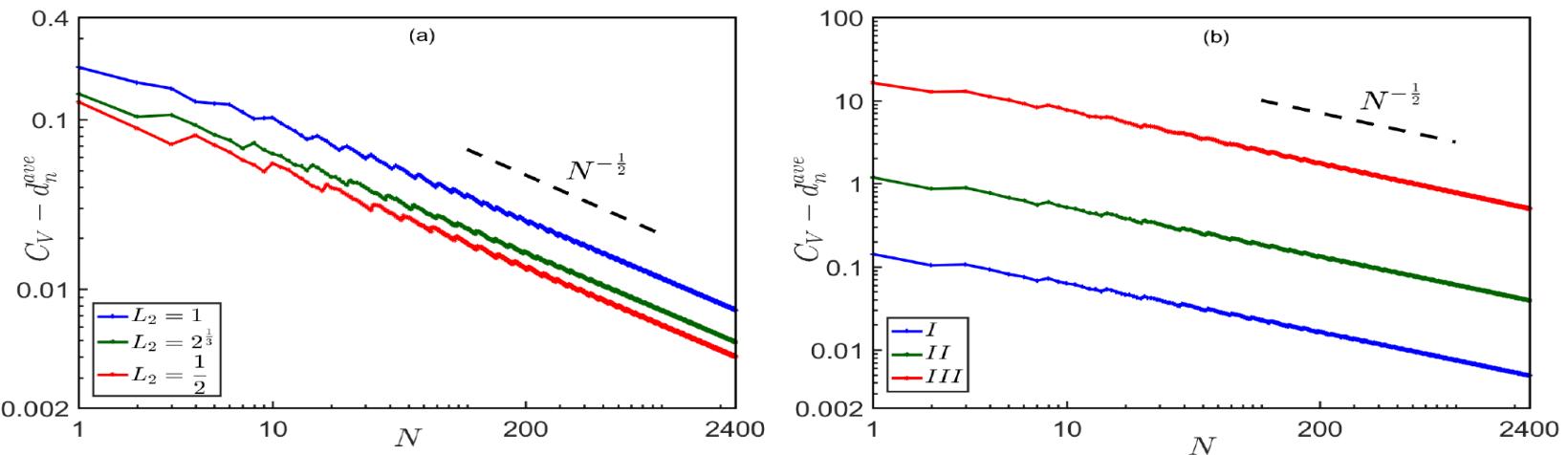


Figure 3.3: Plots of  $C_V - d_n^{\text{ave}}$  for different  $L_2$  and  $V(x, y)$ : (a) with  $V(x, y) = \frac{x^2 + y^2}{2}$  for different  $L_2$ , and (b) with  $L_2 = \frac{2^{1/3}}{2}$  for different potentials (I)  $V(x, y) = \frac{x^2 + y^2}{2}$ , (II)  $V(x, y) = 4x^2 + 4y^2 + \sin(\frac{\pi x}{2}) + \sin(\frac{\pi y}{2})$ , and (III)  $V(x, y) = 50(x^2 + y^2) + \sin(2\pi x) + \sin(2\pi y)$ .

## 💡 Numerical & analytical results – Bao, Chen & Rudnick, 20'

$\widehat{d}_n$  is oscillatory &  $\widehat{d}_n^{\text{ave}} = C_V + O(n^{-1/2})$ ,  $n \gg 1$ ,  $C_V = \frac{1}{|\Omega|} \int_{\Omega} V(\vec{x}) d\vec{x}$

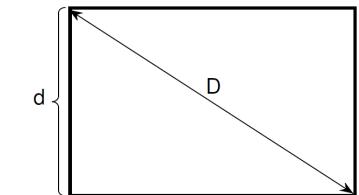
# The Fundamental Gap of SO

$$(-\Delta + V(\vec{x}))u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega$$

$$u(\vec{x}) = 0, \quad \vec{x} \in \Gamma = \partial\Omega$$

Order of all eigenvalues:

$$V(\vec{x}) \geq 0 \text{ & weakly convex} \Rightarrow 0 < \lambda_1 < \lambda_2 \leq \dots \leq \lambda_n \leq \dots$$



Fundamental gap:  $\delta_{\text{fd}} := \lambda_2 - \lambda_1 > 0$

In 1D with no potential:  $-u''(x) = \lambda u(x), \quad x \in (0, S); \quad u(0) = u(S) = 0$

$$\lambda_n = \frac{n^2 \pi^2}{S^2}, \quad n = 1, 2, \dots \Rightarrow \delta_{\text{fd}} := \lambda_2 - \lambda_1 = \frac{2^2 \pi^2}{S^2} - \frac{\pi^2}{S^2} = \frac{3\pi^2}{D^2}, \quad D - \text{diameter of } \Omega$$

In 2D on a rectangular with no potential

$$d = 2, V(\vec{x}) \equiv 0, \Omega = (-L_1, L_1) \times (-L_2, L_2)$$

$$\tilde{\lambda}_{lk} = \frac{l^2 \pi^2}{L_1^2} + \frac{k^2 \pi^2}{L_2^2}, \quad l, k = 1, 2, \dots \Rightarrow$$

$$0 < L_2 \leq L_1, \quad D = \sqrt{L_1^2 + L_2^2} \xrightarrow{L_2 \rightarrow 0} L_1$$

$$\delta_{\text{fd}} := \tilde{\lambda}_{21} - \tilde{\lambda}_{11} = \frac{2^2 \pi^2}{L_1^2} + \frac{\pi^2}{L_2^2} - \frac{\pi^2}{L_1^2} - \frac{\pi^2}{L_2^2} = \frac{3\pi^2}{L_1^2} \geq \frac{3\pi^2}{D^2} \xrightarrow{L_2 \rightarrow 0} \frac{3\pi^2}{L_1^2}$$

# Fundamental Gap Conjecture of SO

$$(-\Delta + V(\vec{x}))u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega$$

$$u(\vec{x}) = 0, \quad \vec{x} \in \Gamma = \partial\Omega$$

• Fundamental Gap conjecture – convex domain & weak convex potential

$$\delta_{\text{fd}} := \lambda_2 - \lambda_1 \geq \frac{3\pi^2}{D^2}$$

$$D := \max_{\vec{x}, \vec{y} \in \bar{\Omega}} |\vec{x} - \vec{y}|$$

$$r_0 := \max_{\vec{x} \in \bar{\Omega}} \sup \{ r > 0 \mid B_r(\vec{x}) \subseteq \bar{\Omega} \}$$

- Observed by Michiel van Den Berg, J. Stat. Phys. 1983
- Suggested by S. T. Yau, 86'
- For  $d=1$ , partial result by Ashbaugh & Benguria 89'; & proved by Levine 94'
- For  $d>1$ , partial results by Qi Huang Yu & **JiaQing Zhong** 86', Li & Yau, ...
- Completely **proved** by Ben Andrews & Julie Clutterbuck, **JAMS** 2011!!!!
  - Gradient flow, geometric analysis, sharp estimates of ODE, etc.
  - Results for whole space with sub-harmonic potential

$$\delta_{\text{fd}} := \lambda_2 - \lambda_1 \geq \frac{3\pi^2}{D^2} \left( 1 + \frac{(d-1)r_0^2}{D^2} \right) ???$$

# Extension to FSO

## • Fractional Schrodinger operator (FSO)

$$L_{\text{FSO}} u := \left( (-\Delta)^{\alpha/2} + V(\vec{x}) \right) u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega \subset \mathbb{R}^d$$

$$u(\vec{x}) = 0, \quad \vec{x} \in \Omega^c = \mathbb{R}^d \setminus \Omega; \quad 0 < \alpha \leq 2$$

– Fractional derivative

$$(-\Delta)^{\alpha/2} u(\vec{x}) = F^{-1}(|\vec{\xi}|^\alpha (Fu)(\vec{\xi})), \quad \vec{x}, \vec{\xi} \in \mathbb{R}^d$$

– Order of all eigenvalues:  $0 < \lambda_1^\alpha < \lambda_2^\alpha \leq \dots \leq \lambda_n^\alpha \leq \dots$

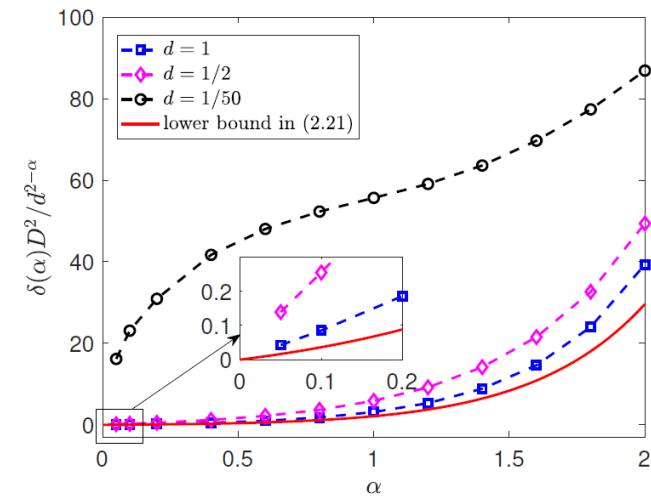
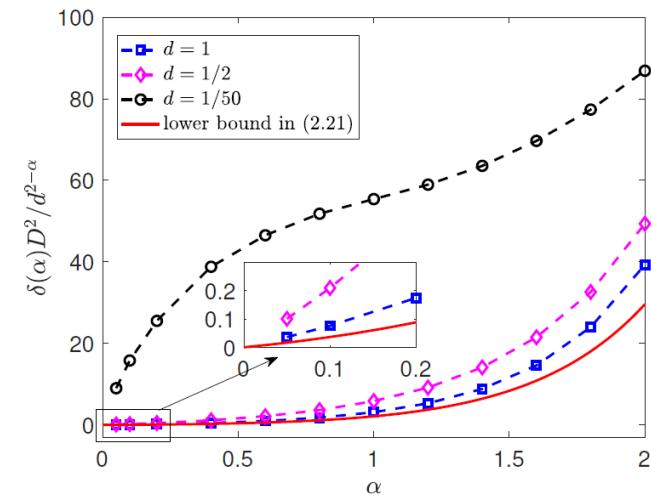
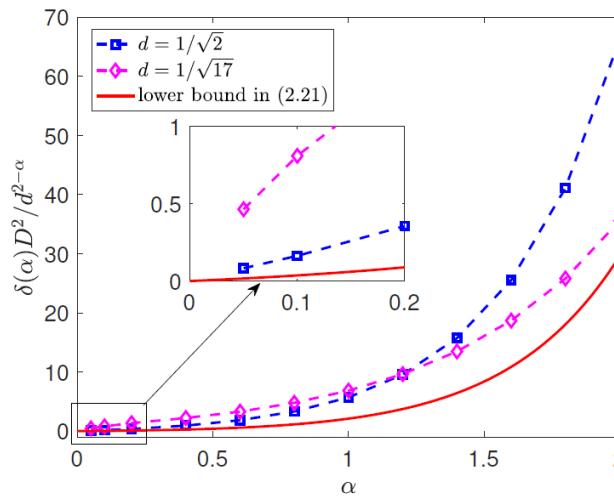
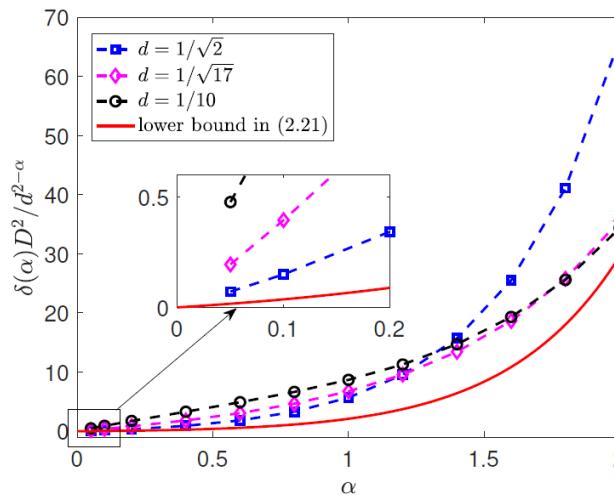
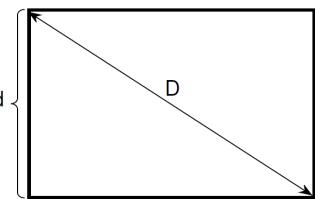
## • Fundamental gap conjecture:

$$\delta_{\text{fd}}(\alpha) := \lambda_2^\alpha - \lambda_1^\alpha \geq \frac{3\alpha\pi^\alpha}{2(d+3)^{1-\alpha/2}} \frac{r_0^{2-\alpha}}{D^2}$$

$$D := \max_{\vec{x}, \vec{y} \in \bar{\Omega}} |\vec{x} - \vec{y}|$$

$$r_0 := \max_{\vec{x} \in \bar{\Omega}} \sup \{ r > 0 \mid B_r(\vec{x}) \subseteq \bar{\Omega} \}$$

# Numerical Results



# Other Gaps and their Statistics

$$L_{\text{FSO}} u := ((-\Delta)^{\alpha/2} + V(\vec{x}))(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in \Omega \subset \mathbb{R}^d$$

$$u(\vec{x}) = 0, \quad \vec{x} \in \Omega^c = \mathbb{R}^d \setminus \Omega; \quad 0 < \alpha \leq 2$$

Order of eigenvalues:

$$0 < \lambda_1^\alpha < \lambda_2^\alpha \leq \dots \leq \lambda_n^\alpha \leq \dots$$

Ratio of repeated eigenvalues:  $R(n) := \frac{\#\{1 \leq l \leq n \mid \lambda_l^\alpha = \lambda_{l+1}^\alpha\}}{n}, \quad n = 1, 2, \dots$

Nearest neighbor gaps  $\delta_{\text{nn}}(n) := \lambda_{n+1} - \lambda_n, \quad n = 1, 2, \dots$

Average gaps  $\delta_{\text{ave}}(n) := \frac{1}{n} \sum_{l=1}^n \delta_{\text{nn}}(l) = \frac{1}{n} (\lambda_{n+1} - \lambda_1), \quad n = 1, 2, \dots$

Minimal gaps:  $\delta_{\text{min}}(n) := \min_{1 \leq l \leq n} \delta_{\text{nn}}(l), \quad n = 1, 2, \dots$

Normalized gaps (or "unfolding" local statistics in physics)

$$\text{If } \lim_{n \rightarrow +\infty} \frac{\lambda_n}{n^\gamma} = C > 0 \quad \Rightarrow \quad \tilde{\lambda}_n = (\lambda_n / C)^{1/\gamma} \quad \delta_{\text{norm}}(n) := \tilde{\lambda}_{n+1} - \tilde{\lambda}_n, \quad n = 1, 2, \dots$$

Gaps distribution statistics

$$\frac{\#\{1 \leq l \leq n \mid \delta_{\text{norm}}(l) < x\}}{n} \xrightarrow{n \rightarrow +\infty} \int_0^x P(s) ds, \quad x \geq 0$$

# For Laplacian Operator (LO) in 1D

$$-u''(x) = \lambda u(x), \quad x \in (0, S);$$

$$u(0) = u(S) = 0$$

• All eigenvalues:

$$\lambda_n = \frac{n^2\pi^2}{S^2}, \quad n = 1, 2, \dots$$

• Different gaps and statistics:

– Ratio of repeated eigenvalues:  $R(n) \equiv 0, \quad n = 1, 2, \dots$

– Nearest neighbour gaps:  $\delta_{nn}(n) := \frac{\pi^2(2n+1)}{S^2}, \quad n = 1, 2, \dots$

– Averages gaps:  $\delta_{ave}(n) = \frac{\pi^2(n+2)}{S^2}, \quad n = 1, 2, \dots$

– Minimal gaps:  $\delta_{min}(n) \equiv \frac{3\pi^2}{S^2}, \quad n = 1, 2, \dots$

– Normalized gaps:  $\delta_{norm}(n) := \tilde{\lambda}_{n+1} - \tilde{\lambda}_n = \frac{\tilde{\lambda}_n - n}{\tilde{\lambda}_n} = n + 1 - n = 1, \quad n = 1, 2, \dots$

– Gaps distribution statistics:

$$P(s) = \delta(s-1), \quad s \geq 0$$

# For Fractional Laplacian Operator (**FLO**) in 1D

$$(-\partial_{xx})^{\alpha/2} u(x) = \lambda u(x), x \in \Omega = (0, S);$$

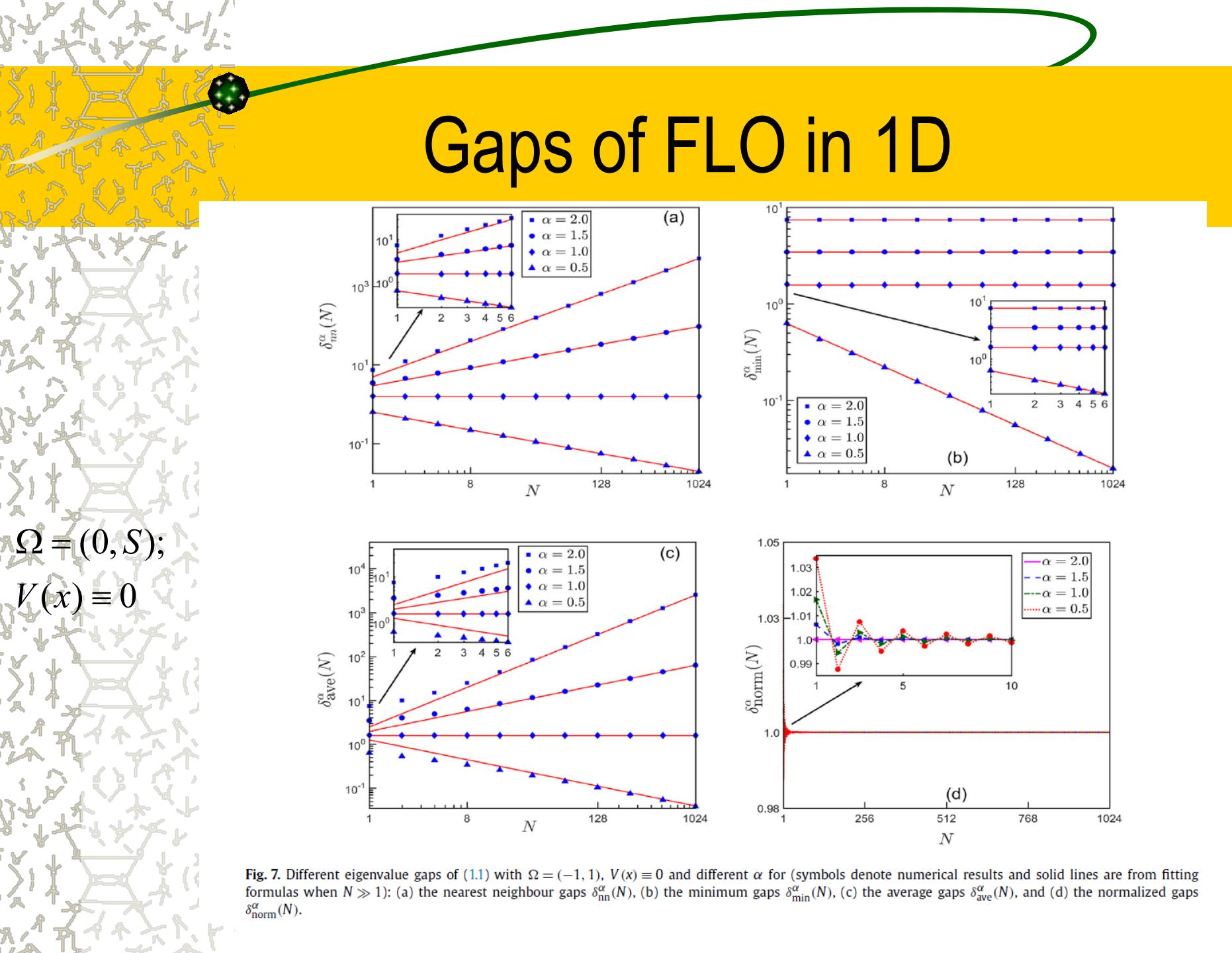
💡 All eigenvalues:  $u(x) = 0, x \in \Omega^c = \mathbb{R} \setminus \Omega; \quad 0 < \alpha \leq 2$

$$\lambda_n^\alpha = \left(\frac{n\pi}{S}\right)^\alpha - \left(\frac{\pi}{S}\right)^\alpha \frac{\alpha(2-\alpha)}{4} n^{\alpha-1} + O(n^{\alpha-2}), \quad n = 1, 2, \dots$$

💡 Different gaps and statistics:

- Ratio of repeated eigenvalues:  $R(n) \equiv 0, \quad n = 1, 2, \dots$
- Nearest neighbour gaps:  $\delta_{nn}(n) := \left(\frac{\pi}{S}\right)^\alpha \left[ \alpha n^{\alpha-1} + \frac{\alpha(\alpha-1)(\alpha+2)}{4} n^{\alpha-2} + O(n^{\alpha-3}) \right] + O(n^{\alpha-2}), \quad n = 1, 2, \dots$
- Averages gaps:  $\delta_{ave}(n) = \left(\frac{\pi}{S}\right)^\alpha n^{\alpha-1} + O(n^{\alpha-2}), \quad n = 1, 2, \dots$
- Normalized gaps:  $\delta_{norm}(n) := 1 + O(n^{-2}), \quad n = 1, 2, \dots$
- Gaps distribution statistics:  $P(s) = \delta(s-1), \quad s \geq 0$

# Gaps of FLO in 1D



**Fig. 7.** Different eigenvalue gaps of (1.1) with  $\Omega = (-1, 1)$ ,  $V(x) \equiv 0$  and different  $\alpha$  for (symbols denote numerical results and solid lines are from fitting formulas when  $N \gg 1$ ): (a) the nearest neighbour gaps  $\delta_{nn}^\alpha(N)$ , (b) the minimum gaps  $\delta_{\min}^\alpha(N)$ , (c) the average gaps  $\delta_{ave}^\alpha(N)$ , and (d) the normalized gaps  $\delta_{norm}^\alpha(N)$ .

# Gaps Statistics of FLO in 1D

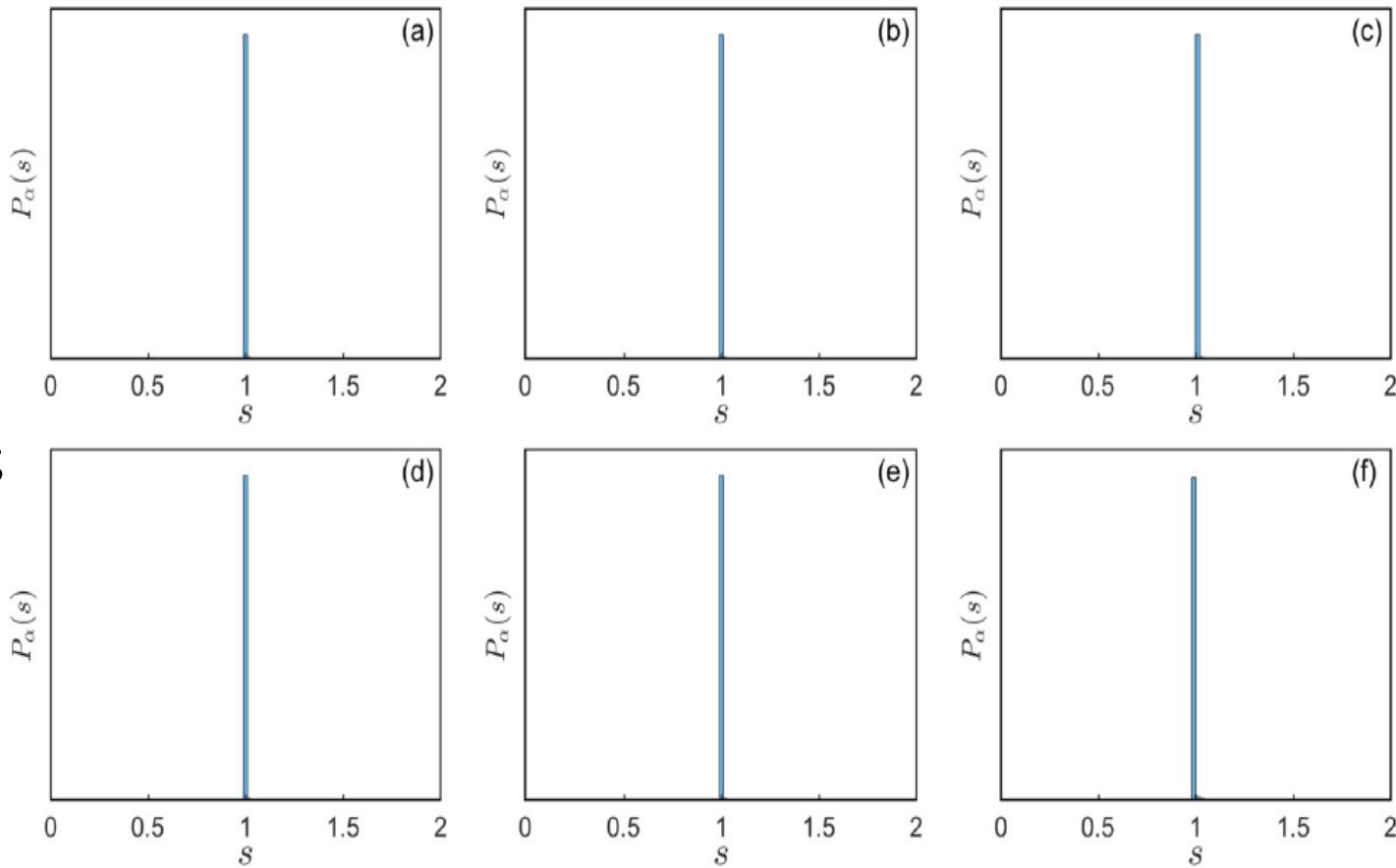
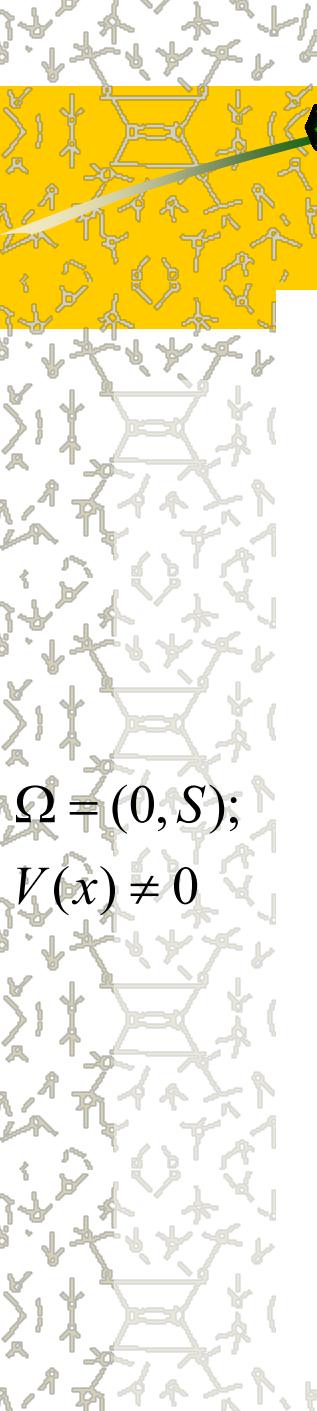
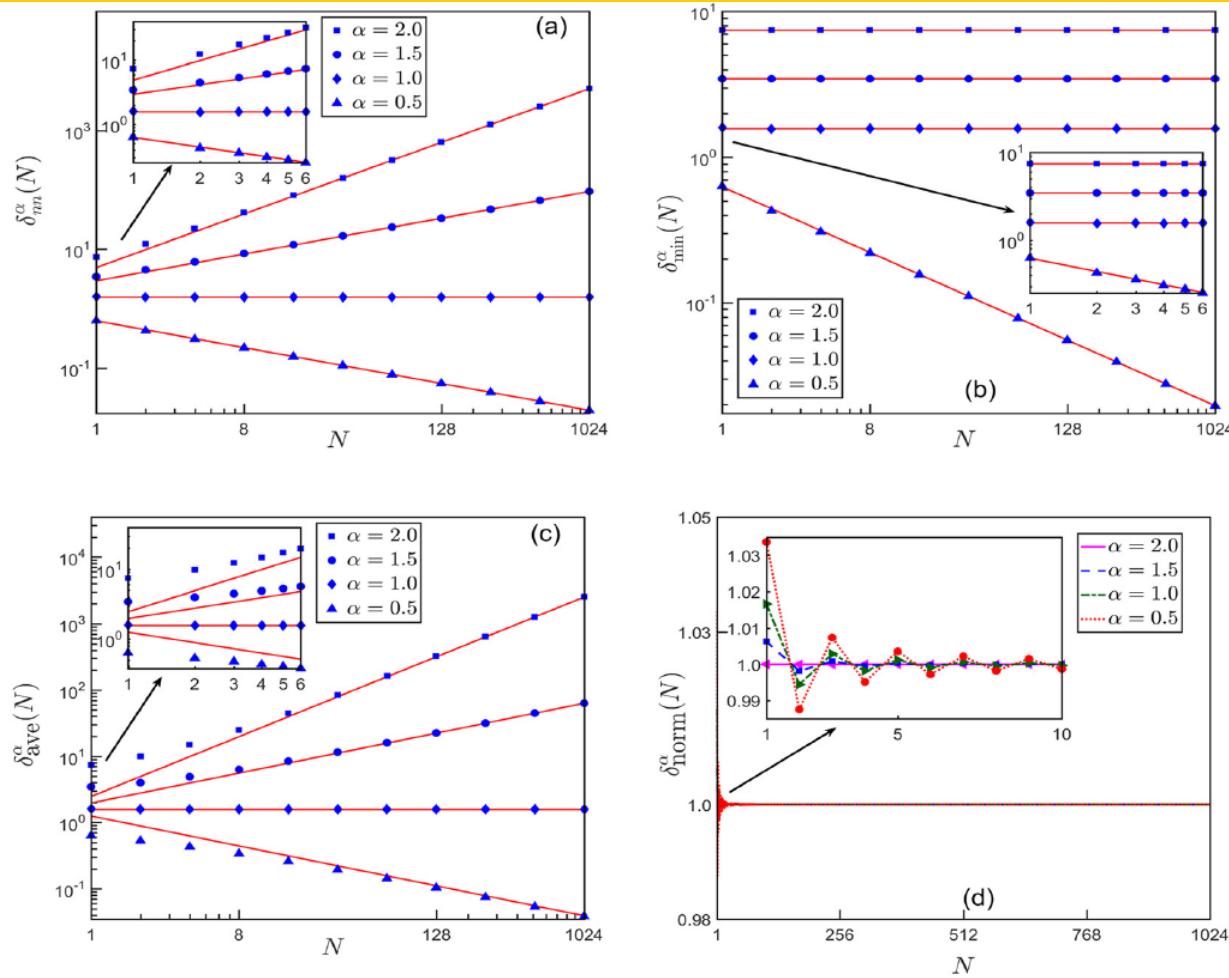


Fig. 8. The histogram of the normalized gaps  $\{\delta_{\text{norm}}^\alpha(n) \mid 1 \leq n \leq N = 4096\}$  of (1.1) with  $\Omega = (-1, 1)$  and  $V(x) \equiv 0$  for different  $\alpha$ : (a)  $\alpha = 2.0$ , (b)  $\alpha = 1.9$ , (c)  $\alpha = \sqrt{3}$ , (d)  $\alpha = 1.5$ , (e)  $\alpha = 1.0$ , and (f)  $\alpha = 0.5$ .

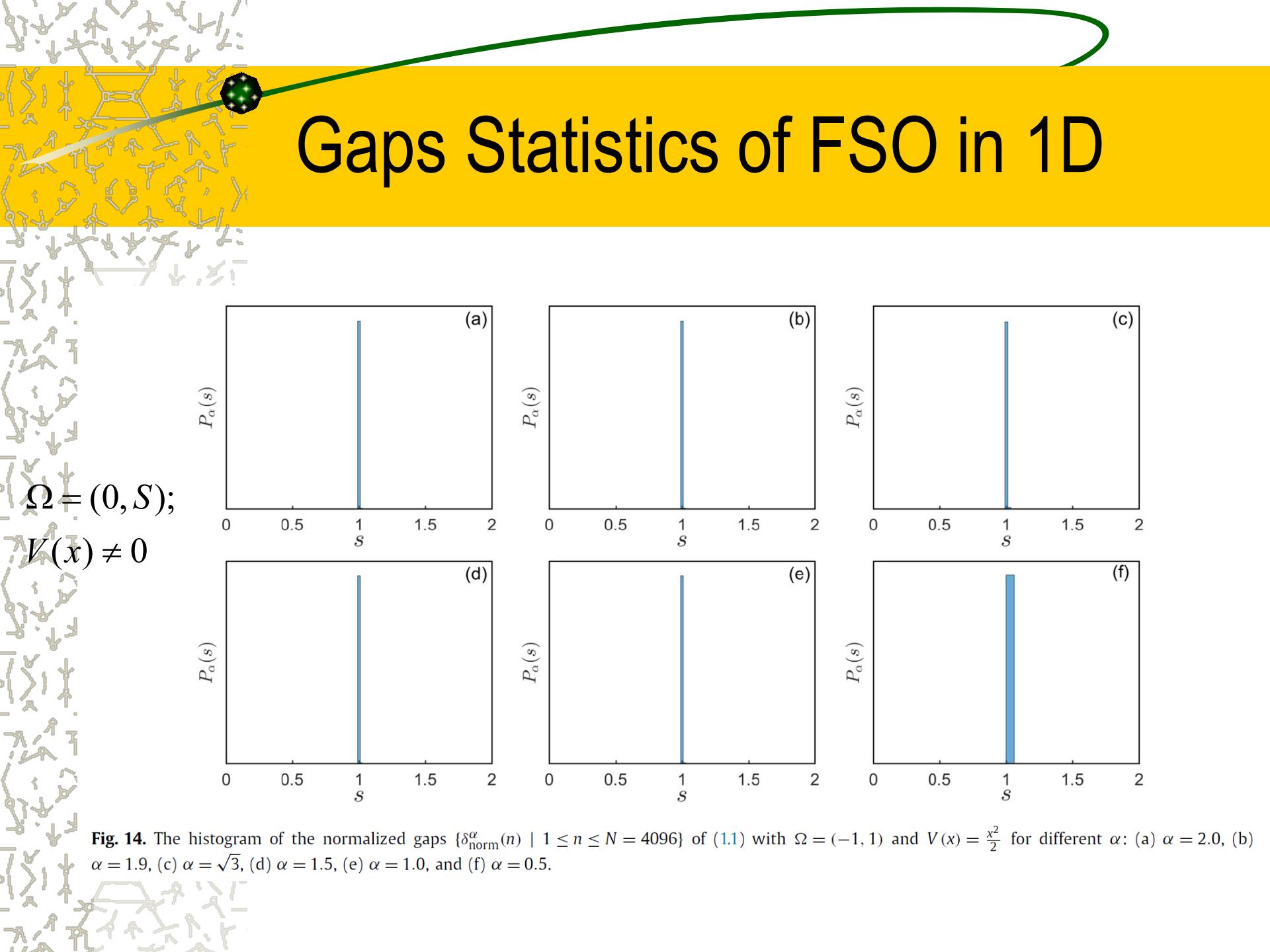
# Gaps of FSO in 1D



$$\Omega = (0, S); \\ V(x) \neq 0$$



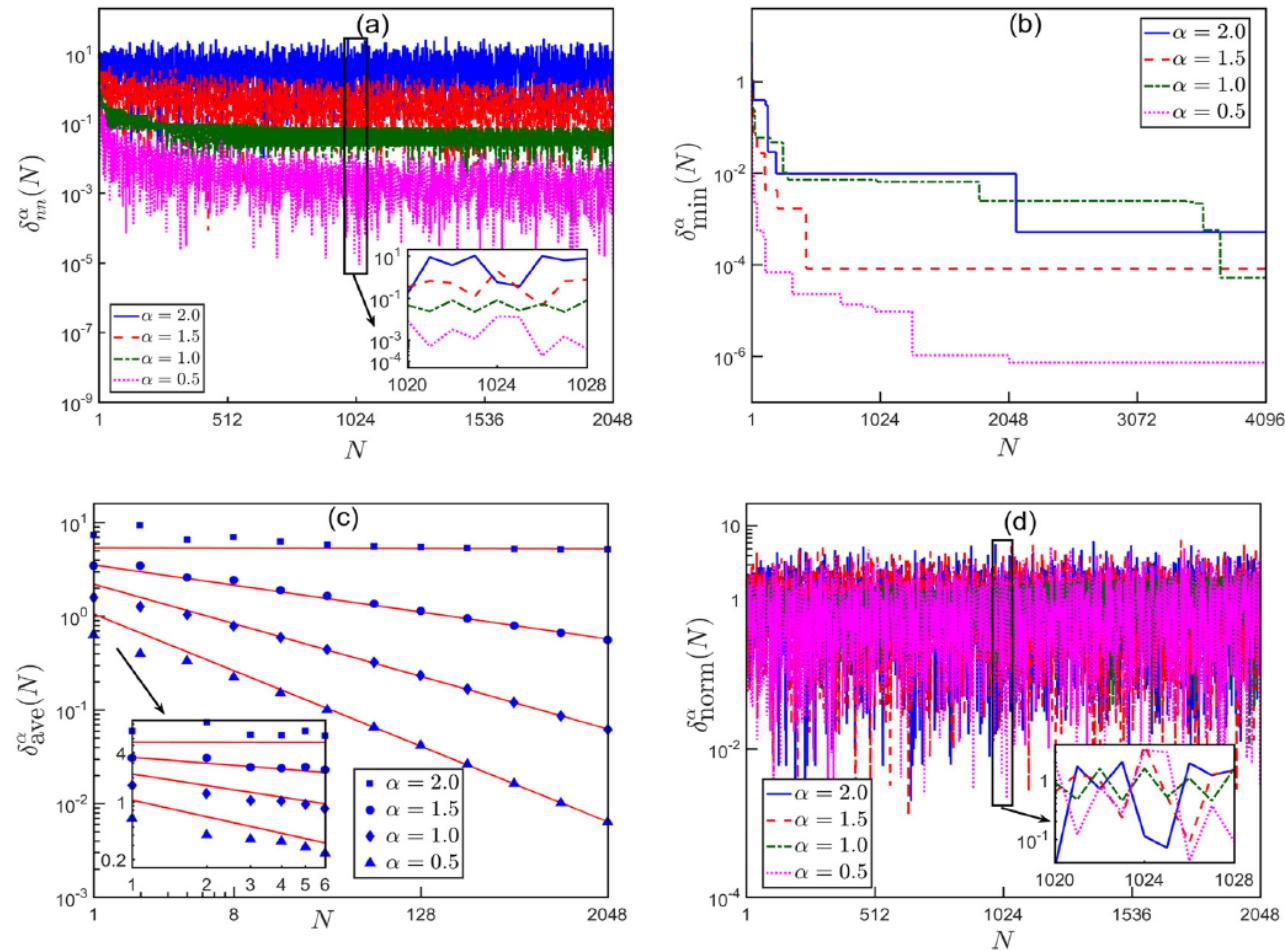
**Fig. 7.** Different eigenvalue gaps of (1.1) with  $\Omega = (-1, 1)$ ,  $V(x) \equiv 0$  and different  $\alpha$  for (symbols denote numerical results and solid lines are from fitting formulas when  $N \gg 1$ ): (a) the nearest neighbour gaps  $\delta_{nn}^\alpha(N)$ , (b) the minimum gaps  $\delta_{\min}^\alpha(N)$ , (c) the average gaps  $\delta_{\text{ave}}^\alpha(N)$ , and (d) the normalized gaps  $\delta_{\text{norm}}^\alpha(N)$ .



# Gaps of D-FLO in 2D

$$\Omega = (-1, 1) \times (-L_2, L_2)$$

$$V(x, y) \equiv 0$$

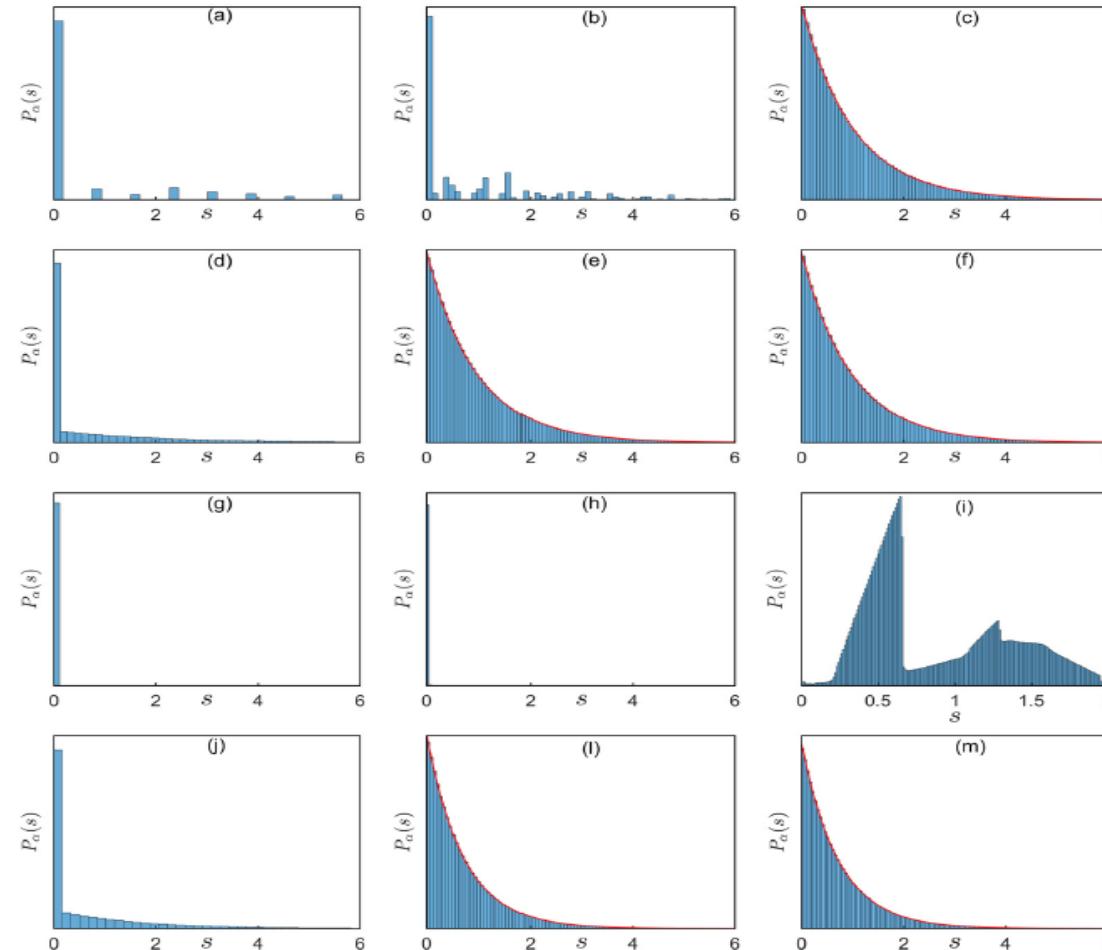


**Fig. 19.** Different eigenvalue gaps of (6.1) with  $d = 2$ ,  $L_1 = 1$ ,  $V(\mathbf{x}) \equiv 0$ ,  $L_2 = \frac{\sqrt[3]{2}}{2}$  and different  $\alpha$  for: (a) the nearest neighbour gaps  $\delta_{nn}^\alpha(N)$ , (b) the minimum gaps  $\delta_{\min}^\alpha(N)$ , (c) the average gaps  $\delta_{\text{ave}}^\alpha(N)$  (symbols denote numerical results and solid lines are from fitting formulas when  $N \gg 1$ ), and (d) the normalized gaps  $\delta_{\text{norm}}^\alpha(N)$ .

# Gaps Statistics of D-FLO in 2D

$$\Omega = (-1, 1) \times (-L_2, L_2)$$

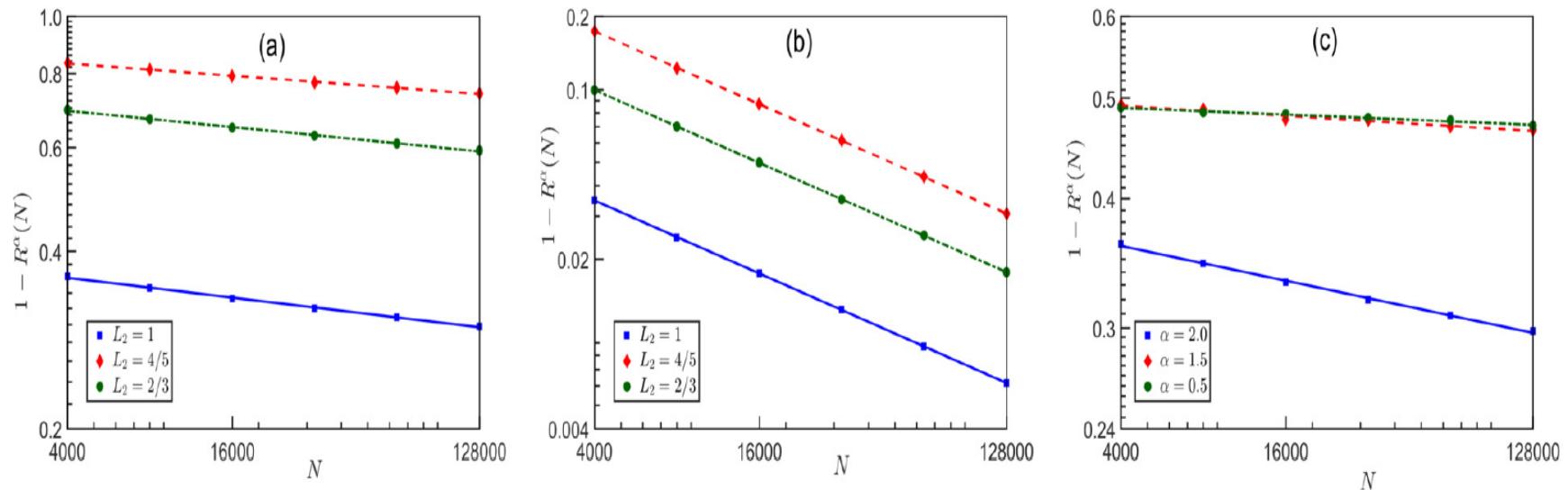
$$V(x, y) \equiv 0$$



**Fig. 20.** The histogram of the normalized gaps ( $\delta_{\text{norm}}^{\alpha} | 1 \leq n \leq N = 4000000$ ) of (6.1) with  $d = 2$ ,  $L_1 = 1$  and  $V(\mathbf{x}) \equiv 0$  for different  $0 < \alpha \leq 2$  and  $0 < L_2 \leq 1$ : (a)  $\alpha = 2.0$  and  $L_2 = 1$ , (b)  $\alpha = 2.0$  and  $L_2 = 2/3$ , (c)  $\alpha = 2.0$  and  $L_2 = \frac{\sqrt{3}}{2}$ ; (d)  $\alpha = 1.5$  and  $L_2 = 1$ , (e)  $\alpha = 1.5$  and  $L_2 = 2/3$ , (f)  $\alpha = 1.5$  and  $L_2 = \frac{\sqrt{3}}{2}$ ; (g)  $\alpha = 1.0$  and  $L_2 = 1$ , (h)  $\alpha = 1.0$  and  $L_2 = 2/3$ , (i)  $\alpha = 1.0$  and  $L_2 = \frac{\sqrt{3}}{2}$ ; (j)  $\alpha = 0.5$  and  $L_2 = 1$ , (l)  $\alpha = 0.5$  and  $L_2 = 2/3$ , (m)  $\alpha = 0.5$  and  $L_2 = \frac{\sqrt{3}}{2}$ . Solid lines are fitting curves for the gaps distribution statistics  $P_{\alpha}(s)$ .

# Ratio of Repeated Eigenvalues

$$\Omega = (-1,1) \times (-L_2, L_2), \quad V(x, y) \equiv 0, \quad L_2^2 \in \mathbb{Q}$$



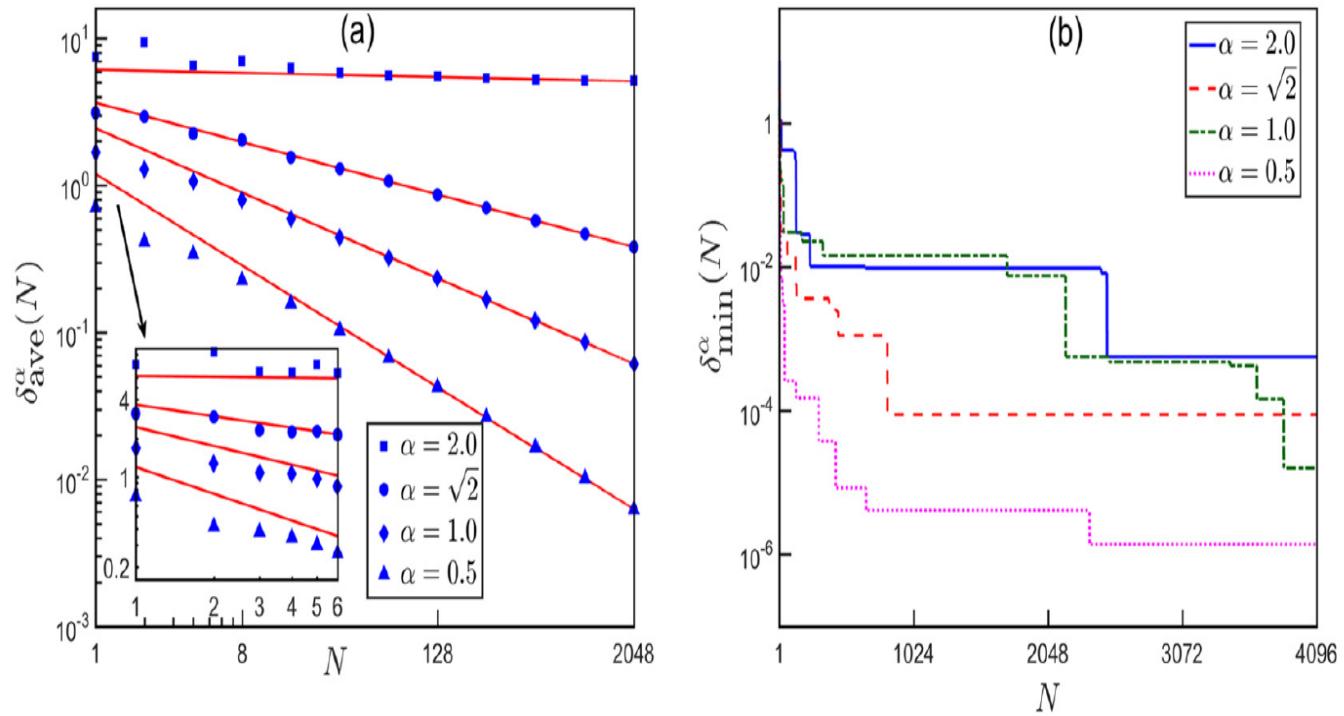
**Fig. 21.** Plots of  $1 - R^\alpha(N)$  vs  $N$  ( $N \gg 1$ ) for different  $\alpha$  and  $L_2$ : (a)  $\alpha = 2$  for different  $L_2 \in \mathbb{Q}$ ; (b)  $\alpha = 1$  for different  $L_2 \in \mathbb{Q}$ ; and (c)  $L_2 = 1$  for different  $0 < \alpha \leq 2$ .

$$R(n) := \frac{\#\{1 \leq l \leq n \mid \lambda_l^\alpha = \lambda_{l+1}^\alpha\}}{n}, \quad n = 1, 2, \dots \Rightarrow \quad R(n) \xrightarrow{n \rightarrow +\infty} 1$$

# Gaps of D-FSO in 2D

$$\Omega = (-1, 1) \times (-L_2, L_2)$$

$$V(x, y) \neq 0$$

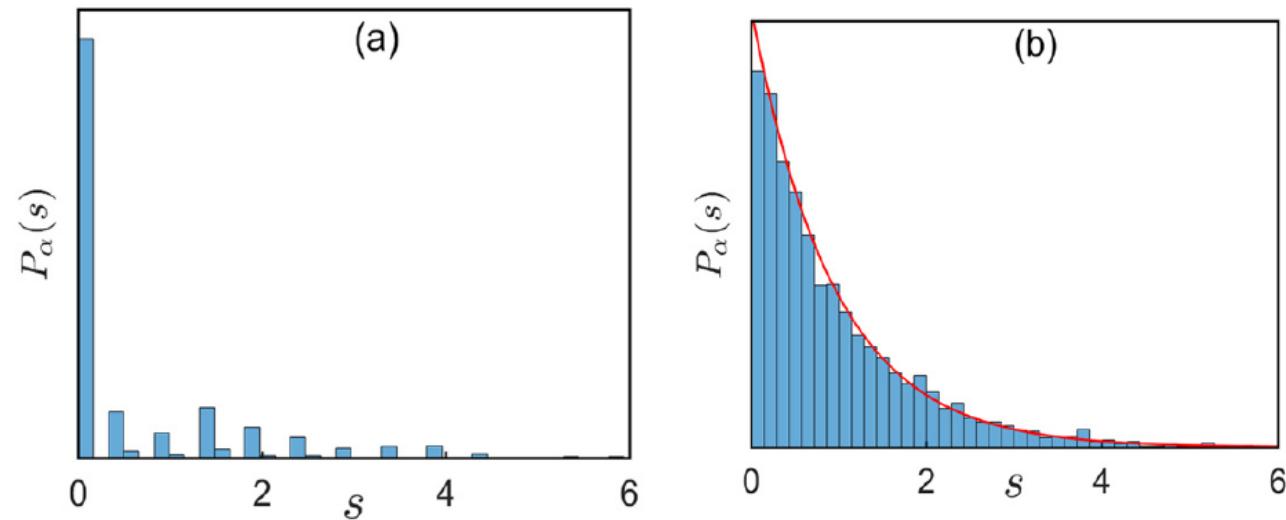


**Fig. 24.** Different gaps of (6.1) with  $d = 2$ ,  $L_1 = 1$ ,  $L_2 = \sqrt[3]{2}/2$  and  $V(x, y) = \frac{x^2+y^2}{2}$ : (a) the average gaps  $\delta_{\text{ave}}^{\alpha}(N)$  (symbols denote numerical results and solid lines are from fitting formulas when  $N \gg 1$ ), and (b) the minimum gaps  $\delta_{\min}^{\alpha}(N)$ .

# Gaps Statistics of D-FSO in 2D

$$\Omega = (-1, 1) \times (-L_2, L_2)$$

$$V(x, y) \neq 0$$



**Fig. 25.** The histogram of the normalized gaps  $\{\delta_{\text{norm}}^\alpha(n) \mid 1 \leq n \leq N = 4096\}$  of (6.1) with  $d = 2$  and  $V(x, y) = \frac{x^2+y^2}{2}$ : (a)  $\alpha = 2$  and  $L_2 = 1$ ; and (b)  $\alpha = \sqrt{2}$  and  $L_2 = \sqrt[3]{2}/2$  (the solid line is a fitting curve by the Poisson distribution).

# Summary of Gaps Statistics of D-FSO in 2D

$$d = 2, \quad \Omega = (-L_1, L_1) \times (-L_2, L_2)$$

	$\frac{L_2}{L_1} = 1$	$1 \neq \frac{L_2}{L_1} \in \mathbb{Q}$	$\frac{L_2}{L_1} \notin \mathbb{Q} \text{ & } \frac{L_2^2}{L_1^2} \in \mathbb{Q}$	$\frac{L_2^2}{L_1^2} \notin \mathbb{Q}$
$\alpha = 2$	$\delta(s)$	$\delta(s)$	$\delta(s)$	Poisson
$1 < \alpha < 2$	$\delta(s)$	Poisson	Poisson	Poisson
$\alpha = 1$	$\delta(s)$	$\delta(s)$	Bimodal distribution	Bimodal distribution
$0 < \alpha < 1$	$\delta(s)$	Poisson	Poisson	Poisson

# Time-independent GPE/NLSE

$$H\phi := -\frac{1}{2} \nabla^2 \phi(\vec{x}) + V(\vec{x})\phi(\vec{x}), \quad H\phi + \beta |\phi(\vec{x})|^2 \phi(\vec{x}) = \mu \phi(\vec{x}), \quad \vec{x} \in \mathbb{R}^d$$

with  $\|\phi\|^2 := \int_{\mathbb{R}^d} |\phi(\vec{x})|^2 d\vec{x} = 1$

💡 **Eigenfunctions** are

- Orthogonal in linear case & Superposition is valid for dynamics!!
- Not orthogonal in nonlinear case !!!! No superposition for dynamics!!!

💡 **The eigenvalue** is also called as **chemical potential**

$$\mu := \mu(\phi) = E(\phi) + \frac{\beta}{2} \int_{\mathbb{R}^d} |\phi(\vec{x})|^4 d\vec{x}$$

– With energy  $E(\phi) = \int_{\mathbb{R}^d} \left[ \frac{1}{2} |\nabla \phi(\vec{x})|^2 + V(\vec{x}) |\phi(\vec{x})|^2 + \frac{\beta}{2} |\phi(\vec{x})|^4 \right] d\vec{x}$

💡 **Ground states** -- **nonconvex** minimization problem

$$E_g^\beta := E(\phi_g^\beta) = \min_{\phi \in S} E(\phi), \quad S = \left\{ \phi \mid \|\phi\| = 1, \quad E(\phi) < \infty \right\}, \quad \mu_g^\beta = \mu(\phi_g^\beta)$$

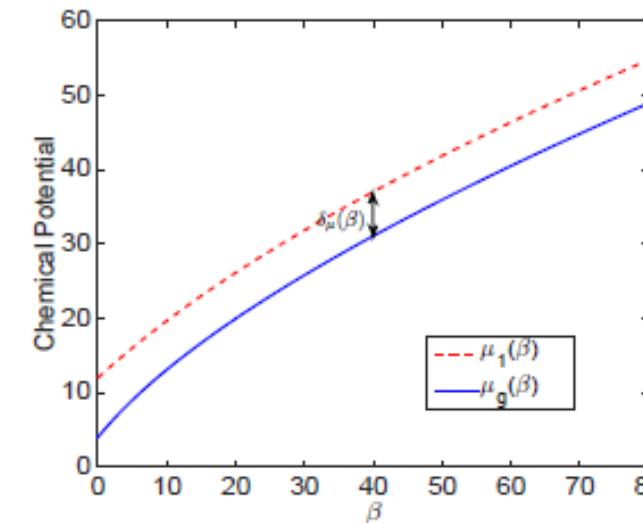
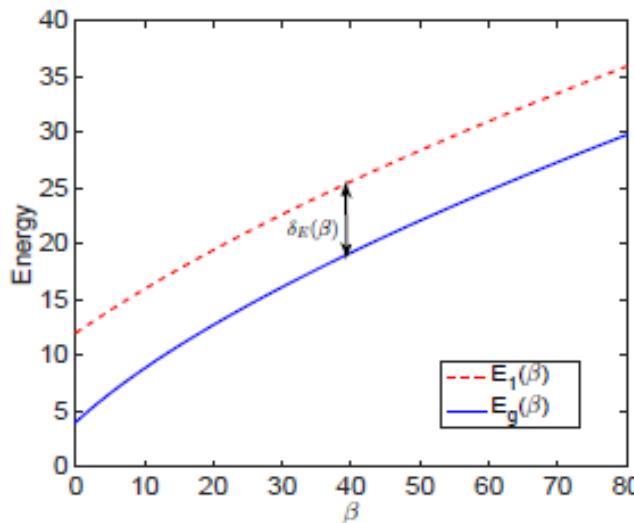
💡 **First excited state:**  $\phi_1^\beta$ ,  $E_1^\beta := E(\phi_1^\beta) > E_g^\beta$ ,  $\mu_1^\beta := \mu(\phi_1^\beta) > \mu_g^\beta$ ,

# Fundamental gaps of GPE

$$\delta_E(\beta) := E(\phi_1^\beta) - E(\phi_g^\beta) > 0, \quad \delta_\mu(\beta) := \mu(\phi_1^\beta) - \mu(\phi_g^\beta) > 0, \quad \beta \geq 0$$

Gaps:

$$\delta_E^\infty := \inf_{\beta \geq 0} \delta_E(\beta), \quad \delta_\mu^\infty := \inf_{\beta \geq 0} \delta_\mu(\beta),$$



Eigenspace of the first excited space of SO:  $H := -\frac{1}{2}\nabla^2 + V(\vec{x})$

$$W_1 = \{\phi(\mathbf{x}) : \Omega \rightarrow \mathbb{C} | H\phi = E_1\phi, \phi|_{\partial\Omega} = 0 \text{ if } \Omega \text{ is bounded}\}$$

# Fundamental Gaps of GPE

$$H\phi := -\frac{1}{2}\nabla^2\phi(\vec{x}) + V(\vec{x})\phi(\vec{x}), \quad H\phi + \beta |\phi(\vec{x})|^2 \phi(\vec{x}) = \mu \phi(\vec{x}), \quad \vec{x} \in \Omega \subset \mathbb{R}^d$$

$$\phi|_{\partial\Omega} = 0; \quad \|\phi\|^2 := \int_{\Omega} |\phi(\vec{x})|^2 d\vec{x} = 1$$

## Fundamental gaps

– Bao & Ruan, Asymp. Anal. 18'

– In the non-degenerate case, i.e.  $\dim(W_1) = 1$

$$\delta_E(\beta) = \begin{cases} \frac{3\pi^2}{2L_1^2} + o(\beta), \\ \frac{4A_0}{3L_1}\beta^{\frac{1}{2}} + A_1 + o(1), \end{cases} \quad \delta_\mu(\beta) = \begin{cases} \frac{3\pi^2}{2L_1^2} + o(\beta), \\ \frac{2A_0}{L_1}\beta^{\frac{1}{2}} + \frac{6}{L_1^2} + o(1), \quad \beta \gg 1. \end{cases} \quad 0 \leq \beta \ll 1$$

$$\delta_E^\infty := \inf_{\beta \geq 0} \delta_E(\beta) \geq \frac{3\pi^2}{2D^2}, \quad \delta_\mu^\infty := \inf_{\beta \geq 0} \delta_\mu(\beta) \geq \frac{3\pi^2}{2D^2}$$

– In the degenerate case, i.e.  $\dim(W_1) \geq 2$

- Weak nonlinearity

$$\delta_E(\beta) = \frac{3\pi^2}{2L^2} - \frac{5dA_0^2}{32}\beta + o(\beta), \quad \delta_\mu(\beta) = \frac{3\pi^2}{2L^2} - \frac{5dA_0^2}{16}\beta + o(\beta)$$

- Strong nonlinearity

$$\delta_E(\beta) = \frac{\pi}{2L^2} \ln(\beta) + \mathcal{O}(1), \quad \delta_\mu(\beta) = \frac{\pi}{2L^2} \ln(\beta) + \mathcal{O}(1)$$

$$\delta_E^\infty := \inf_{\beta \geq 0} \delta_E(\beta) \geq \frac{\pi^2}{2D^2}, \quad \delta_\mu^\infty := \inf_{\beta \geq 0} \delta_\mu(\beta) \geq \frac{3\pi^2}{8D^2}$$

# Conclusions

## • The Weyl's law and conjecture

- Laplacian operator in 1D/2D/3D
- Schrodinger operator in 1D/2D/3D
- Extension to Fractional Laplacian/directional Schrodinger operator

## • Fundamental gap conjecture

- For Laplacian/Schrodinger operator
- Extension to fractional Schrodinger operator
- Different gaps and gaps statistics

## • Future challenges

- Other BCs, singular/random potentials, on manifold/graph (data science)
- Other type operators – Dirac operator, relativistic Schrodinger operator, .....