# Energy spectra of compressed quantum states

arXiv: 2507.07191

**Daochen Wang, University of British Columbia**

# Quantum 101

**Quantum computing = generalization of (classical) *randomized computing***

| Deterministic | Randomized | Quantum |
|---|---|---|
| $$\begin{matrix}00 & \to \\ 01 & \to \\ 10 & \to \\ 11 & \to\end{matrix}\begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$ | $$\begin{matrix}00 & \to \\ 01 & \to \\ 10 & \to \\ 11 & \to\end{matrix}\begin{pmatrix}1/5\\1/5\\2/5\\1/5\end{pmatrix}$$ | $$\begin{matrix}00 & \to \\ 01 & \to \\ 10 & \to \\ 11 & \to\end{matrix}\begin{pmatrix}-1/2\\1/2\\-1/2\\1/2\end{pmatrix}$$ |

$n$ bits in exactly one of $2^n$ states

$n$ (qu)bits in all $2^n$ states "at the same time"

# Promise of quantum computing

Finding better

catalysts

batteries

superconductors

Ground state energy estimation problem

# Ground state energy estimation

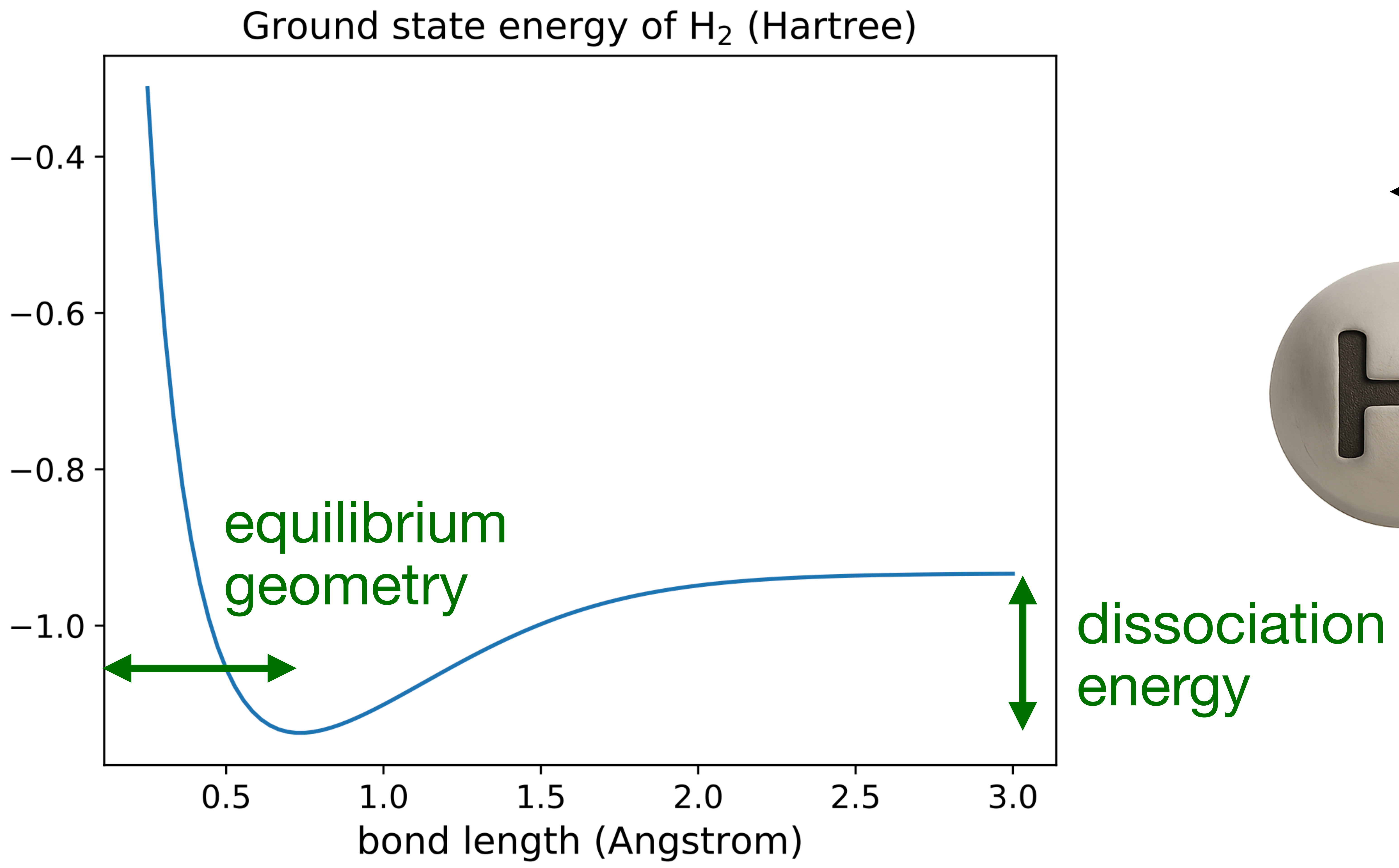
Input: Hamiltonian $H \in \mathbb{C}^{N \times N}$ (aka Hermitian matrix: $H^\dagger = H$)

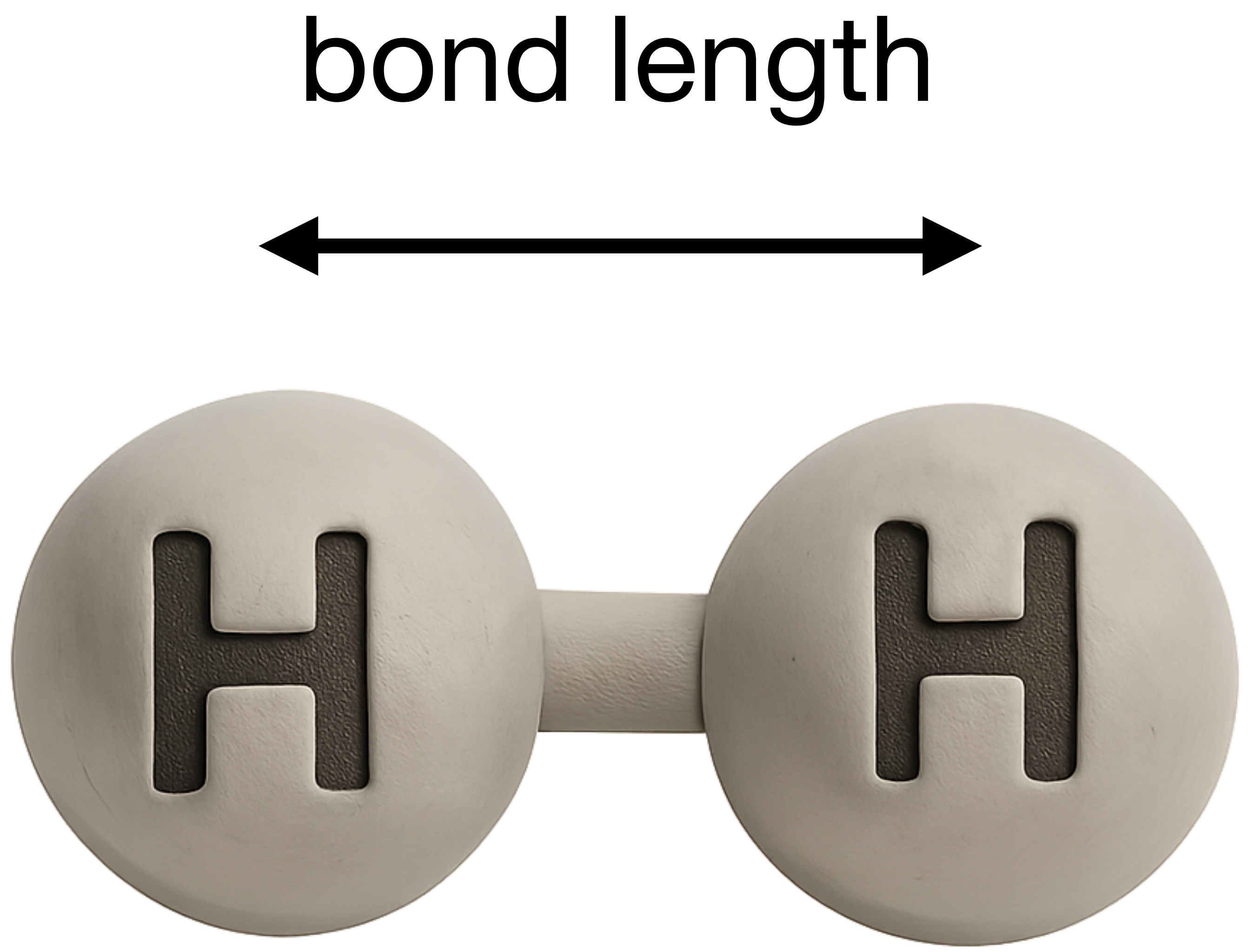
Output: smallest eigenvalue of $H$

Example: $H = \begin{pmatrix} 0 & 1 - i \\ 1 + i & 0 \end{pmatrix}$

Solution: $\det(\lambda I - H) = \lambda^2 - 2 = 0 \implies \lambda = \pm 2 \implies$ Output: $-2$

# Usefulness of ground state energy



# Quantum algorithms for ground state energy estimation

| Quantum phase estimation (QPE) | Variational quantum eigensolver (VQE) | Dissipative/ Lindbladian-based methods |
|---|---|---|
| rigorous given initial state | heuristic | rigorous given mixing time |

# Quantum phase estimation (QPE)

Input: Hamiltonian $H \in \mathbb{C}^{N\times N}$, quantum state $|\psi\rangle \in \mathbb{C}^N$

Output: $E_i$ with probability $|\alpha_i|^2$, where $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$ and $|v_i\rangle$ is an eigenvector of $H$ with eigenvalue $E_i$

Complexity: efficient – $\mathrm{poly}(\log(N))$

[Kitaev '95]

# QPE for ground state energy estimation

Notation: Hamiltonian $H \in \mathbb{C}^{N \times N}$ eigenvalues: $E_1 \leq E_2 \leq \ldots \leq E_N$,
eigenvectors $|v_1\rangle, |v_2\rangle, \ldots, |v_N\rangle$

Step 1: prepare $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$

Step 2: run QPE $O(1/|\alpha_1|^2)$ times with $H, |\psi\rangle$ and take smallest output

# What is $|\psi\rangle$?

Typically a classically-accessible quantum state

Examples:

1. Product state: $|\psi\rangle = |\psi_1\rangle \otimes \ldots \otimes |\psi_n\rangle$

aka Hartree-Fock/mean-field states in quantum chemistry

2. Matrix product state
3. Tensor network state
4. Stabilizer state
5. Neural network state…

# Quantum advantage = good overlap *and* bad energy

Notation: Hamiltonian $H \in \mathbb{C}^{N \times N}$ eigenvalues: $E_1 \leq E_2 \leq \ldots \leq E_N$,

eigenvectors $|v_1\rangle, |v_2\rangle, \ldots, |v_N\rangle$; $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$

***"Proof"***

Quantum advantage = quantumly easy *and* classically hard

Quantumly easy: QPE runtime $O(1/|\alpha_1|^2) \implies$ need high $|\alpha_1|^2$ — **good overlap**

Classically hard: $\sum_{i=1}^{N} |\alpha_i|^2 E_i$ far from $E_1$ — **bad energy**

Is good overlap and bad energy plausible?

# Energy spectra of quantum states

Notation: Hamiltonian $H \in \mathbb{C}^{N \times N}$ eigenvalues: $E_1 \leq E_2 \leq \ldots \leq E_N$,

eigenvectors $|v_1\rangle, |v_2\rangle, \ldots, |v_N\rangle$; $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$

The sequence $|\alpha_1|^2, \ldots, |\alpha_N|^2$ is known as the energy spectrum of $|\psi\rangle$

Good overlap and bad energy $\iff$ $|\alpha_1|^2$ high

$|\alpha_2|^2, \ldots, |\alpha_N|^2$ non-negligible

(assume $E_1 < E_2$)

# Enter Silvester, Carleo, and White

PHYSICAL REVIEW LETTERS **134,** 126503 (2025)

Editors' Suggestion

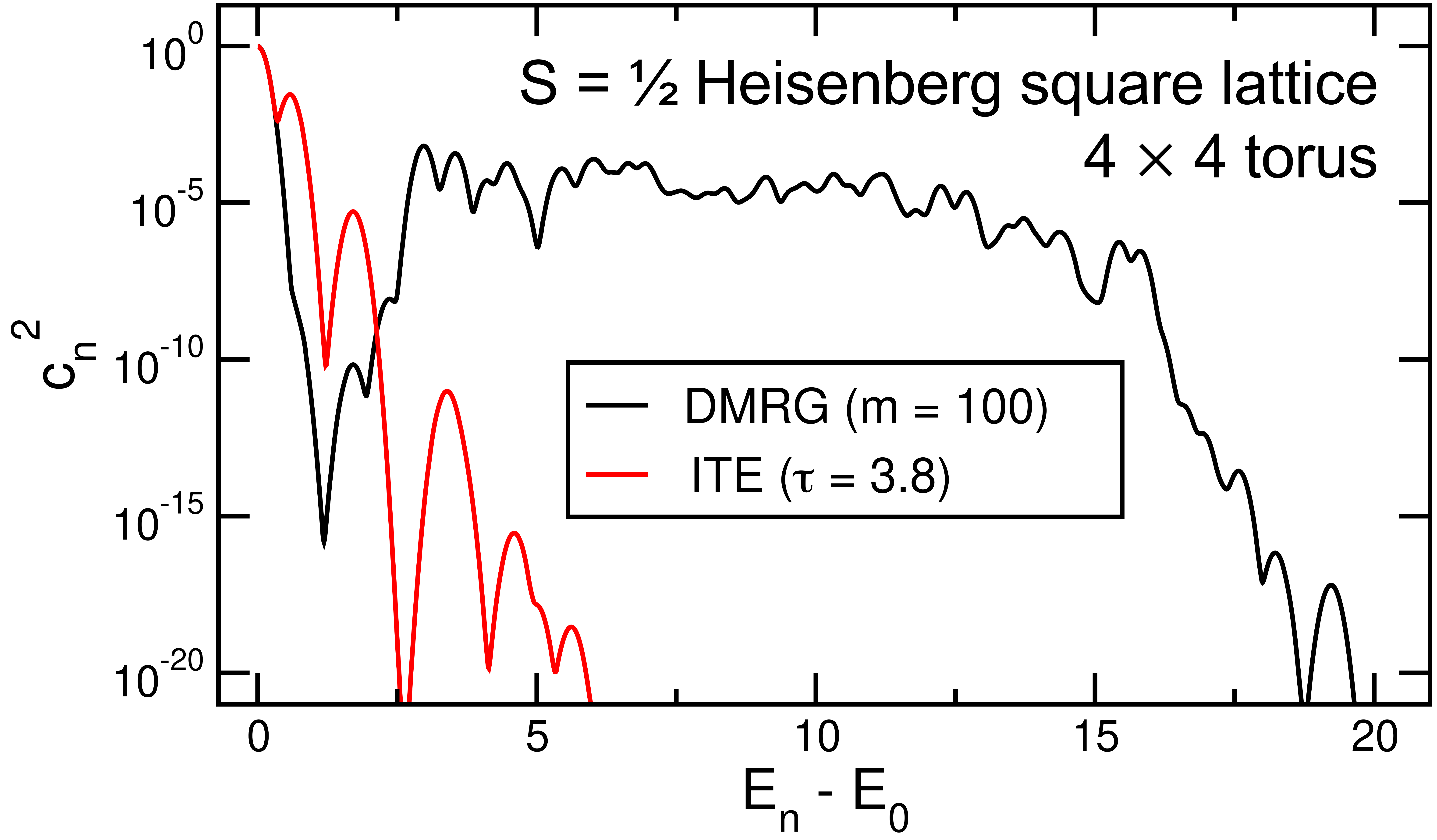
## Unusual Energy Spectra of Matrix Product States

J. Maxwell Silvester,[1] Giuseppe Carleo,[2] and Steven R. White[1]
[1]*Department of Physics and Astronomy, University of California, Irvine, California 92667, USA*
[2]*Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

(Received 10 September 2024; accepted 27 February 2025; published 26 March 2025)

In approximate ground states obtained from imaginary-time evolution, the spectrum of the state—its decomposition into exact energy eigenstates—falls off exponentially with the energy. Here we consider the energy spectra of approximate matrix product ground states, such as those obtained with the density matrix renormalization group. Despite the high accuracy of these states, contributions to the spectra are roughly constant out to surprisingly high energy, with an increase in the bond dimension reducing the amplitude but not the extent of these high-energy tails. The unusual spectra appear to be a general feature of compressed wavefunctions, independent of boundary or dimensionality, and are also observed in neural network wavefunctions. The unusual spectra can have a strong effect on sampling-based methods, yielding large fluctuations. The energy variance, which can be used to extrapolate observables to eliminate truncation error, is subject to these large fluctuations when sampled. Nevertheless, we devise a sampling-based variance approach which gives excellent and efficient extrapolations.

# Unusual energy spectra




$$H = \frac{1}{4} \sum_{\langle i,j \rangle} X_i X_j + Y_i Y_j + Z_i Z_j$$

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

[ earlier: $X + Y$ ]

# Compressed quantum states

Definition: a quantum state is compressed if its entanglement is limited

Entanglement measures how “uncertain” a state is a product state

Examples:

$|0\rangle|0\rangle$ has zero entanglement

$\sqrt{0.9}|0\rangle|0\rangle + \sqrt{0.1}|1\rangle|1\rangle$ has more entanglement

$\sqrt{1/2}|0\rangle|0\rangle + \sqrt{1/2}|1\rangle|1\rangle$ has even more entanglement

# Compressed quantum states

Classically accessible states

1. Product state: $|\psi\rangle = |\psi_1\rangle \otimes \ldots \otimes |\psi_n\rangle$ ← zero entanglement
2. Matrix product state
3. Tensor network state

   (2–3) entanglement limited by "bond dimension"

4. Stabilizer state
5. Neural network state…

   (4–5) can have low or high entanglement

# Measuring entanglement

| | Entanglement entropy: $-\sum_i p_i \log_2(p_i)$ |
|---|---|
| $\|0\rangle\|0\rangle$ | $0$ |
| $\sqrt{0.9}\,\|0\rangle\|0\rangle + \sqrt{0.1}\,\|1\rangle\|1\rangle$ | $-0.9 \cdot \log_2(0.9) - 0.1 \cdot \log_2(0.1) \approx 0.47$ |
| $\sqrt{1/2}\,\|0\rangle\|0\rangle + \sqrt{1/2}\,\|1\rangle\|1\rangle$ | $-(1/2) \cdot (-1) \cdot 2 = 1$ |

# A new measure: stable Schmidt rank

| | Entanglement min-entropy: $-\log_2(p_{\max})$ |
|---|---|
| $\|0\rangle\|0\rangle$ | $0$ |
| $\sqrt{0.9}\|0\rangle\|0\rangle + \sqrt{0.1}\|1\rangle\|1\rangle$ | $-\log_2(0.9) \approx 0.15$ |
| $\sqrt{1/2}\|0\rangle\|0\rangle + \sqrt{1/2}\|1\rangle\|1\rangle$ | $1$ |

Stable Schmidt rank: $2^{-\log_2(p_{\max})} = 1/p_{\max}$

inspired by [Rudelson & Vershynin '07]

# A key property of stable Schmidt rank

Notation: $\chi(\cdot)$ = stable Schmidt rank

Lemma: if $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$ then $1/\sqrt{\chi(\psi)} \leq \sum_{i=1}^{N} |\alpha_i| / \sqrt{\chi(v_i)}$

Example: $N = 2$, $\chi(\psi) = 1$, $\chi(v_1) = \chi(v_2) = 2$, then

$$\sqrt{2} \leq |\alpha_1| + |\alpha_2| \implies |\alpha_1| = |\alpha_2| = \sqrt{2}/2 \text{ if } |\alpha_1|^2 + |\alpha_2|^2 = 1$$

# A key property of stable Schmidt rank

Notation: $\chi(\cdot)$ = stable Schmidt rank

Lemma: if $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$ then $1/\sqrt{\chi(\psi)} \leq \sum_{i=1}^{N} |\alpha_i| / \sqrt{\chi(v_i)}$

*Proof:* write $|\psi\rangle = \sum_{x,y} \Gamma_{x,y} |x\rangle|y\rangle$, $|v_i\rangle = \sum_{x,y} (\Gamma_i)_{x,y} |x\rangle|y\rangle$,

can verify $\|\Gamma\| = 1/\sqrt{\chi(\psi)}$ and $\|\Gamma_i\| = 1/\sqrt{\chi(v_i)}$, and so

$$\Gamma = \sum_i \alpha_i \Gamma_i \implies \|\Gamma\| = \|\sum_i \alpha_i \Gamma_i\| \implies \|\Gamma\| \leq \sum_i |\alpha_i| \|\Gamma_i\|$$

# From key property to energy spectra

Notation: $\chi(\,\cdot\,)$ = stable Schmidt rank

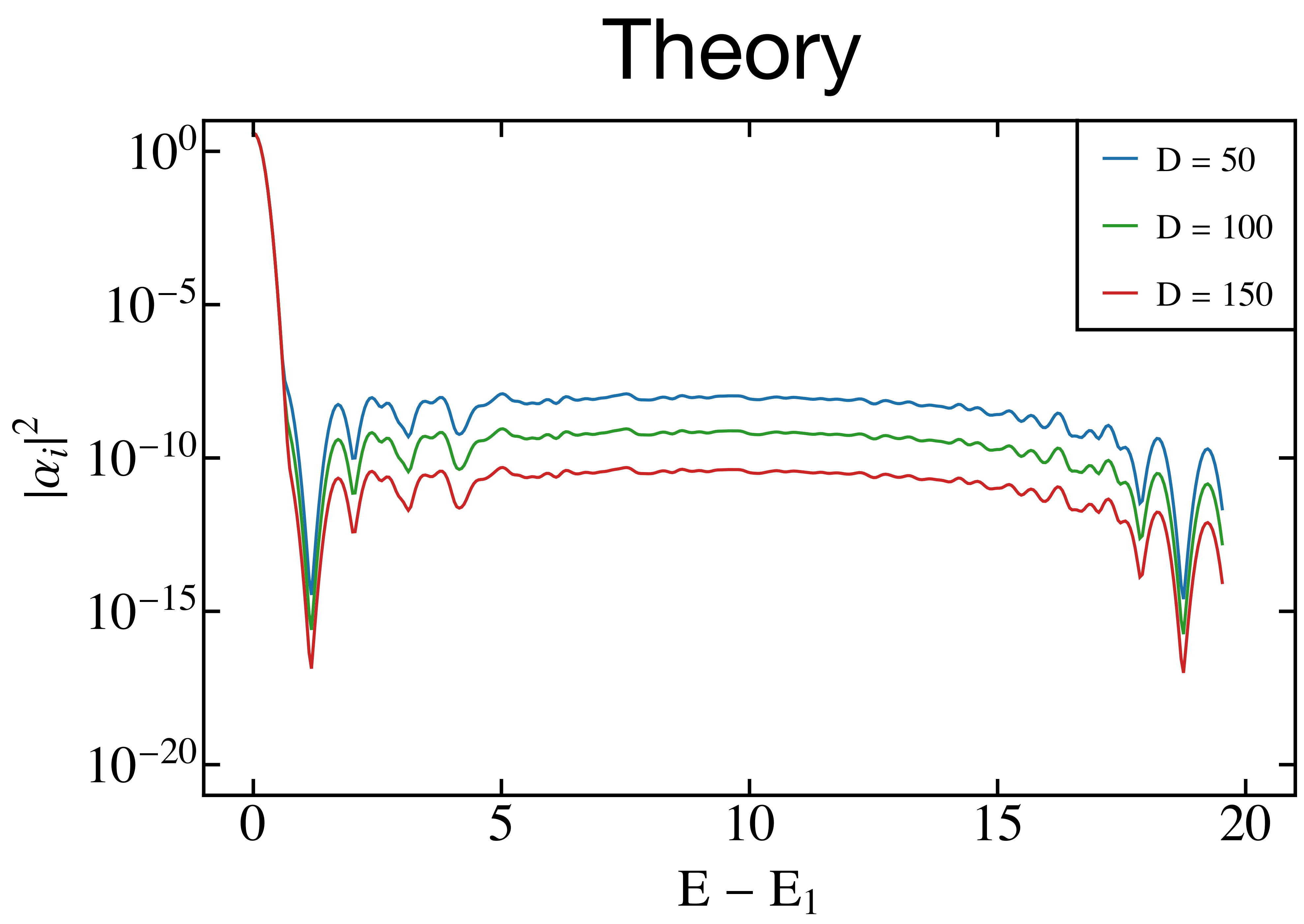
Lemma: if $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$ then $1/\sqrt{\chi(\psi)} \leq \sum_{i=1}^{N} |\alpha_i|/\sqrt{\chi(v_i)}$

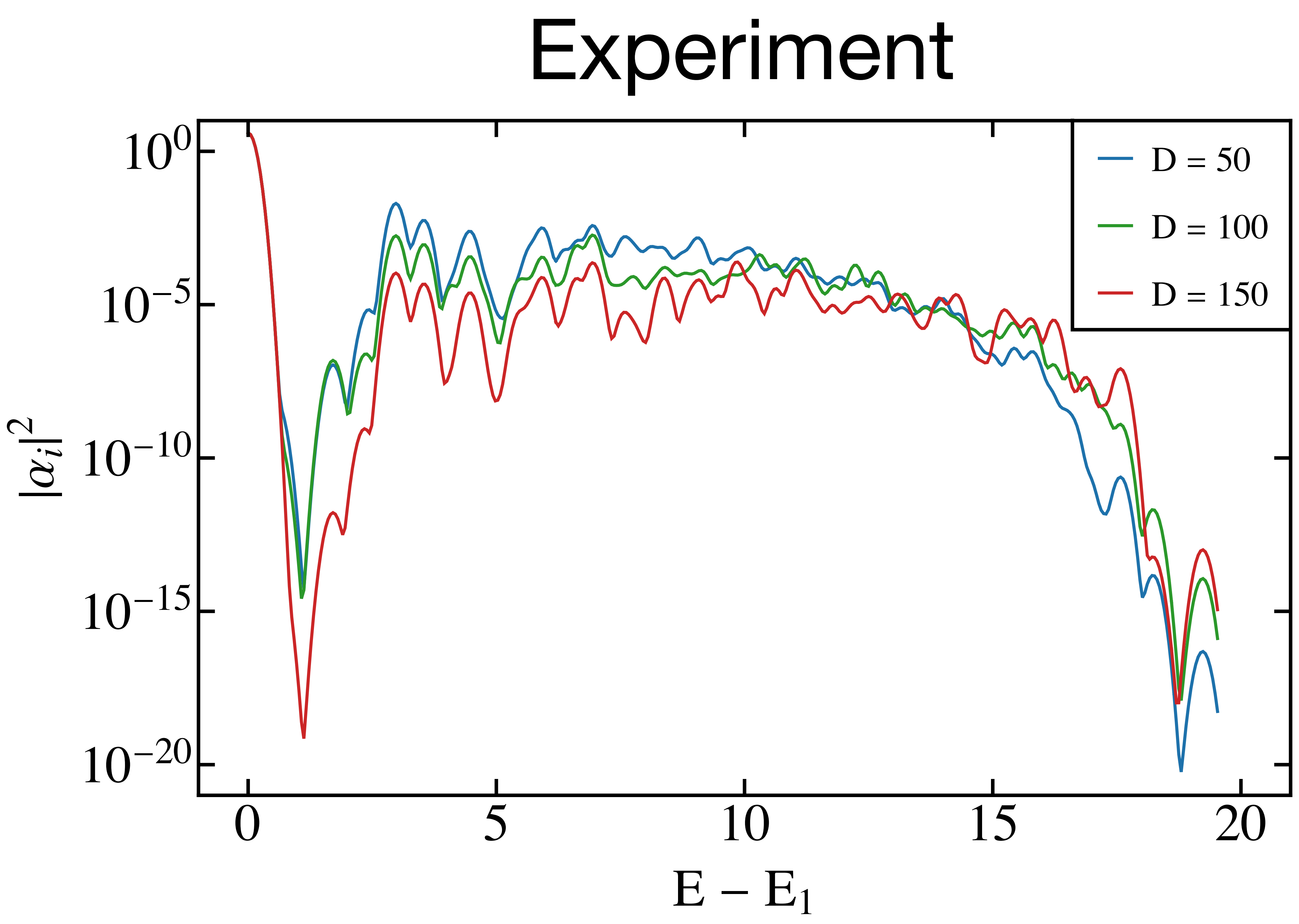
**Theorem:** suppose $\chi(\psi) = m, \chi(v_i) = M_i$, $\sum_{i=1}^{N} |\alpha_i|^2 = 1$ and $\sum_{i=1}^{N} |\alpha_i|^2 E_i$ is minimized, then $|\alpha_i|^2 \propto \dfrac{1}{M_i(E_i - E^*)^2}$, for the unique $E^* < \min_i E_i$ satisfying

$$\frac{1}{m} \sum_{i=1}^{N} \frac{1}{M_i(E_i - E^*)^2} = \left(\sum_{i=1}^{N} \frac{1}{M_i(E_i - E^*)}\right)^2.$$

Power law decay!

# Theory vs experiment: 2D Heisenberg model




*"contributions to the spectra are roughly constant out to surprisingly high energy, with an increase in the bond dimension (D) reducing the amplitude but not the extent of these high-energy tails"*

# Expect theory to lower bound experiment

Lemma: if $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$ then $1/\sqrt{\chi(\psi)} \leq \sum_{i=1}^{N} |\alpha_i| / \sqrt{\chi(v_i)}$

*Proof:* write $|\psi\rangle = \sum_{x,y} \Gamma_{x,y} |x\rangle|y\rangle$, $|\psi_i\rangle = \sum_{x,y} (\Gamma_i)_{x,y} |x\rangle|y\rangle$,

can verify $\|\Gamma\| = 1/\sqrt{\chi(\psi)}$ and $\|\Gamma_i\| = 1/\sqrt{\chi(v_i)}$, and so

$$\Gamma = \sum_i \alpha_i \Gamma_i \implies \|\Gamma\| = \|\sum_i \alpha_i \Gamma_i\| \implies \|\Gamma\| \leq \sum_i |\alpha_i| \|\Gamma_i\|$$

*Lossy!* $1/\sqrt{\chi(\psi)} \leq \|\sum_i \alpha_i \Gamma_i\|$ is more constrained

Is good overlap and bad energy plausible?

Yes, for compressed quantum states, it is enforced by entanglement!

Thank you for your attention