Energy spectra of compressed quantum states

arXiv: 2507.07191

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Quantum 101

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

Deterministic

$$\begin{array}{cc} 00 & \to \\ 01 & \to \\ 10 & \to \\ 11 & \to \end{array} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

Randomized

$$\begin{array}{cc} 00 & \to \\ 01 & \to \\ 10 & \to \\ 11 & \to \end{array} \begin{pmatrix} 1/5 \\ 1/5 \\ 2/5 \\ 1/5 \end{pmatrix}$$

Quantum

$$\begin{array}{cc} 00 & \to \\ 01 & \to \\ 10 & \to \\ 11 & \to \end{array} \begin{pmatrix} -1/2 \\ 1/2 \\ -1/2 \\ 1/2 \end{pmatrix}$$

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

catalysts

Finding better batteries

superconductors

Ground state energy estimation problem

Ground state energy estimation

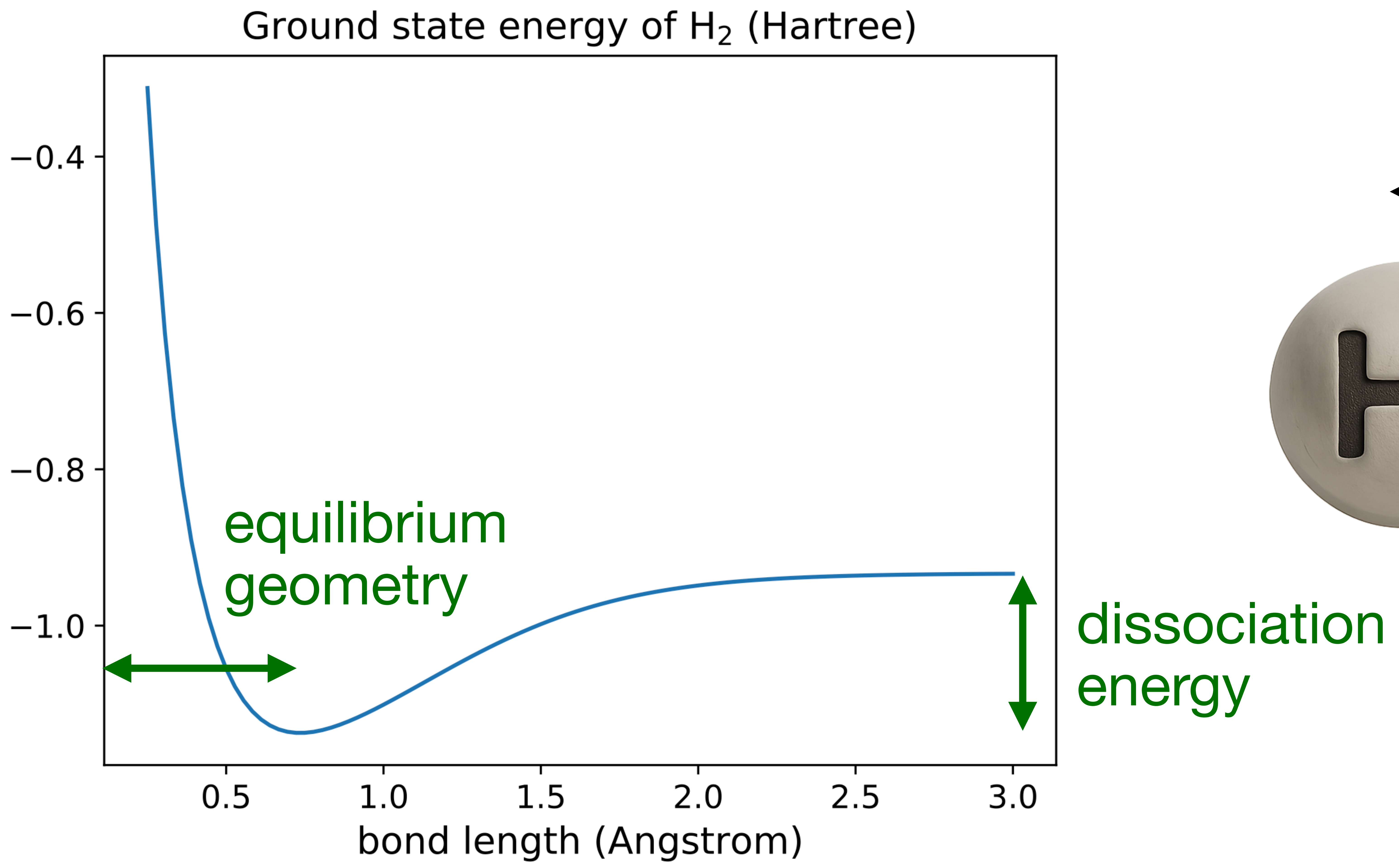
Input: Hamiltonian $H \in \mathbb{C}^{N \times N}$ (aka Hermitian matrix: $H^\dagger = H$)

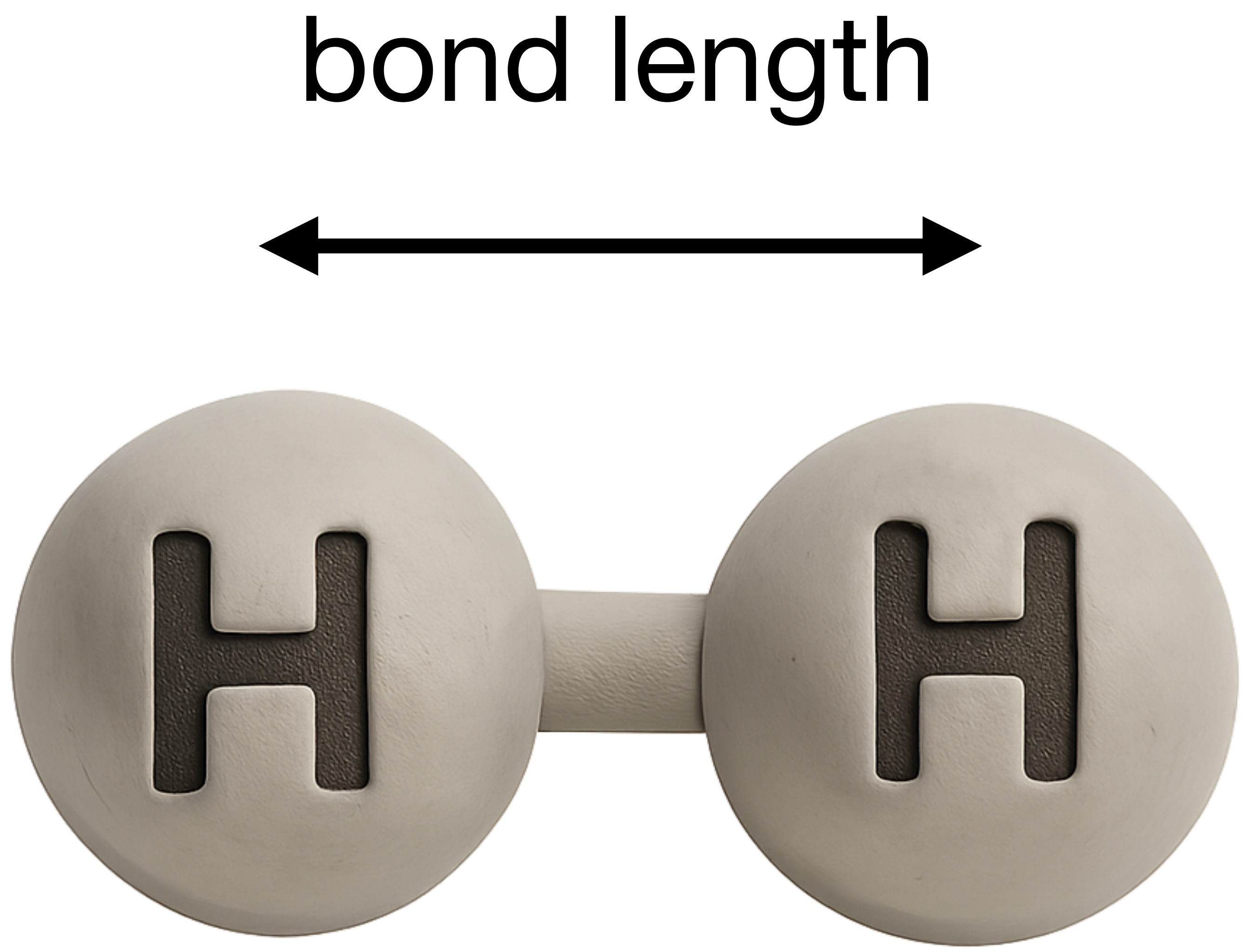
Output: smallest eigenvalue of H

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

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

Usefulness of ground state energy





Quantum algorithms for ground state energy estimation

Quantum phase estimation (QPE)

rigorous given initial state

Variational quantum eigensolver (VQE)

heuristic

Dissipative/ Lindbladian-based methods

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

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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 $O(1/|\alpha_1|^2) \Longrightarrow$ 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

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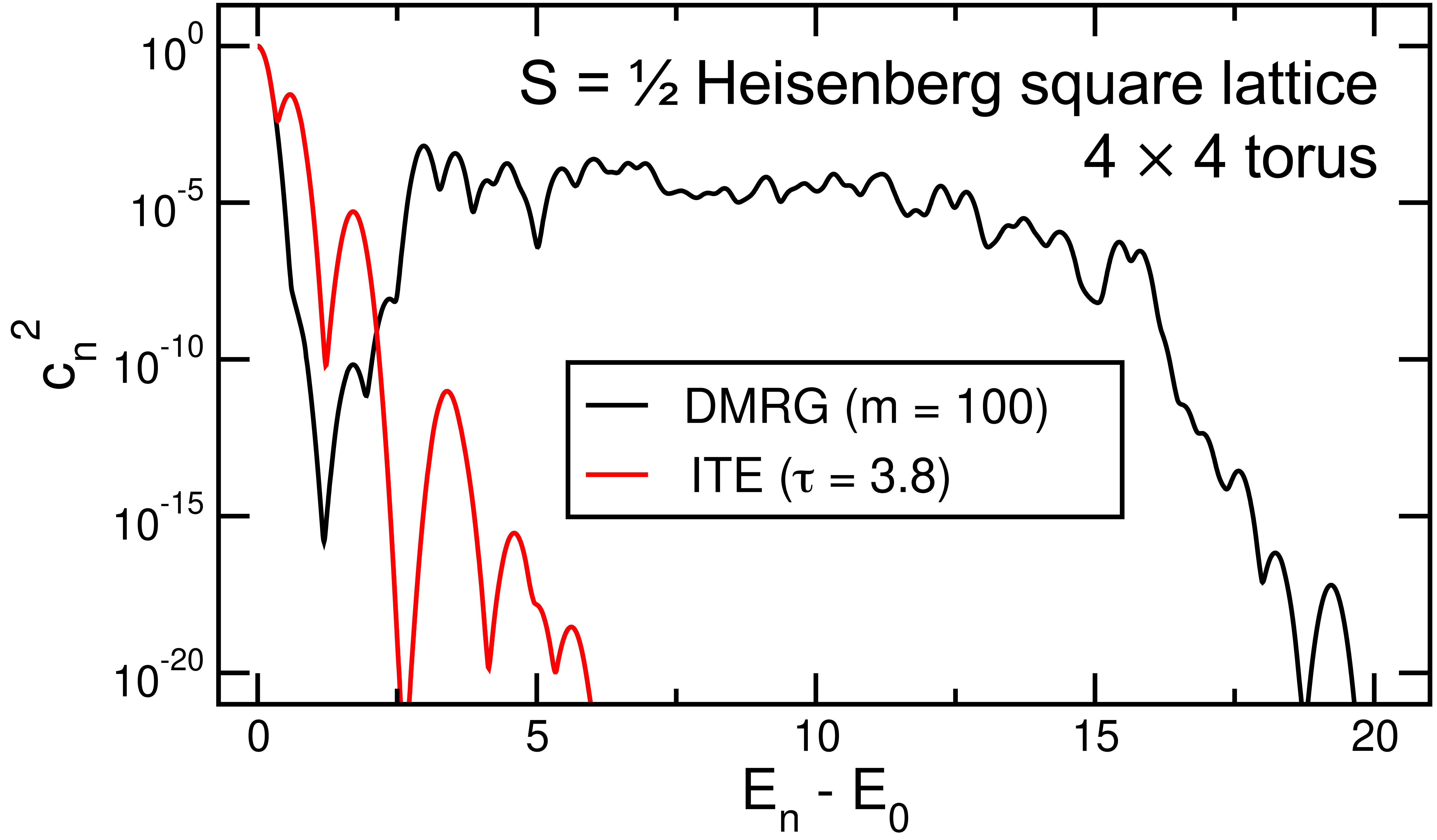
(Received 10 September 2024; accepted 27 February 2025; published 26 March 2025)

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

entanglement limited by "bond dimension"

4. Stabilizer state
5. Neural network state…

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

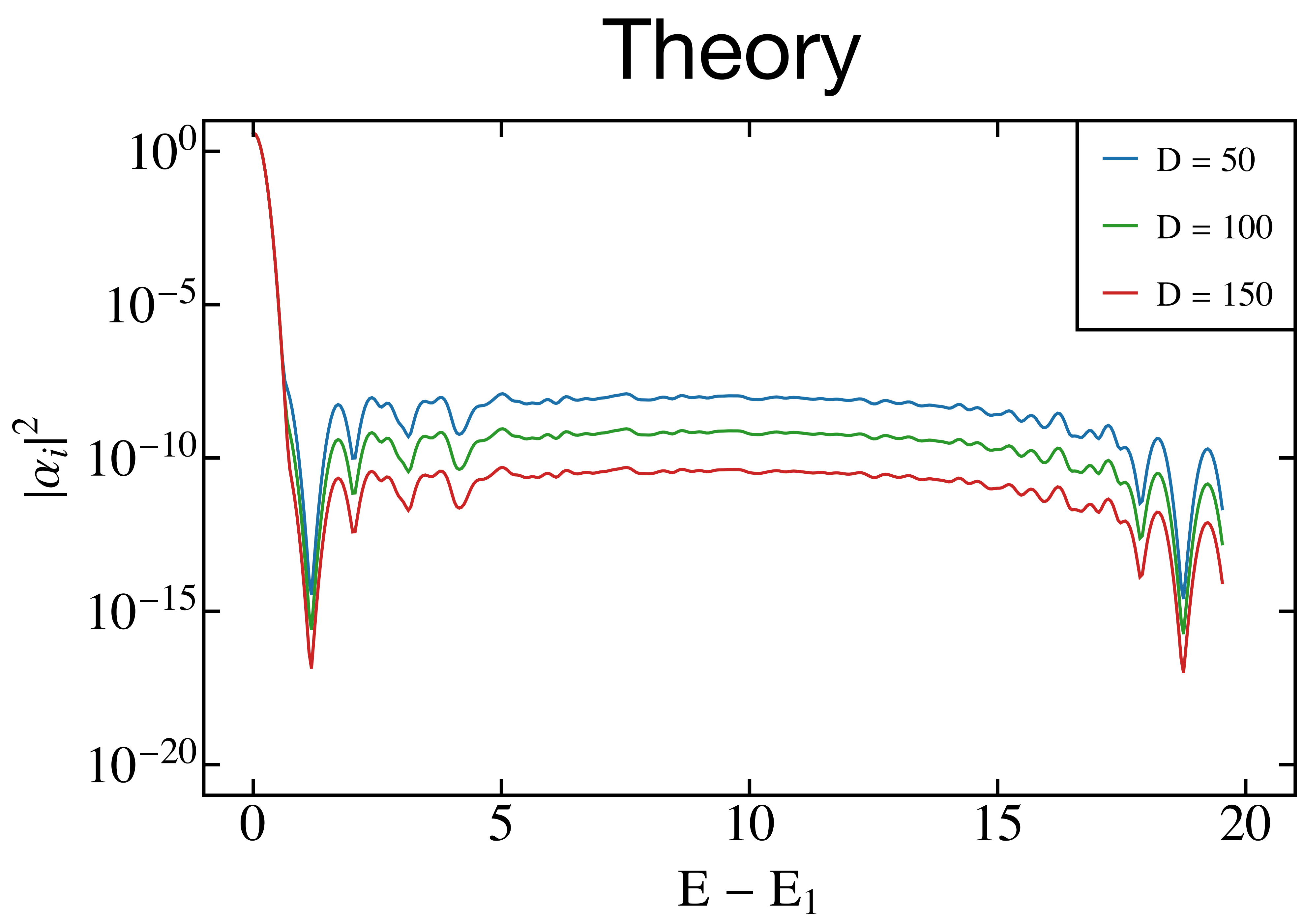
Lemma: if $|\psi\rangle = \sum_{i=1}^{N} \alpha_i |v_i\rangle$ then $1/\sqrt{\chi(\psi)} \leq \sum_{i=1}^{N} |\alpha_i|/\sqrt{\chi(v_i)}$

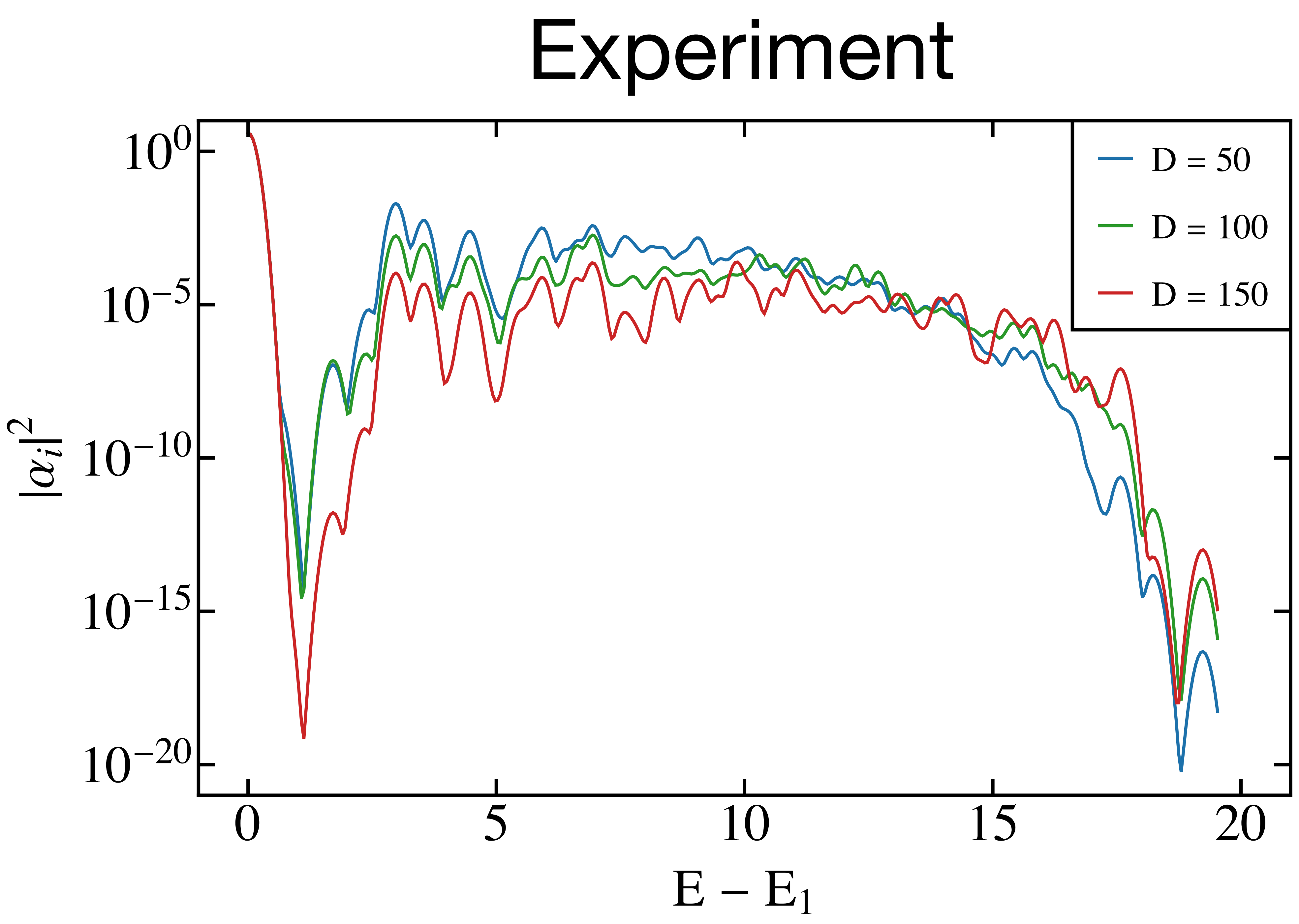
Theorem: suppose $\chi(\psi) = m, \chi(v_i) = M_i$, $\sum_{i=1}^{n} |\alpha_i|^2 = 1$ and $\sum_{i=1}^{N} |\alpha_i|^2 E_i$ is minimized, then $|\alpha_i|^2 \propto \dfrac{1}{M_i(E_i - E^*)^2}$, for the unique $E^* < \min_i E_i$ satisfying

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

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