Probing Thermalization Through Spectral Analysis with Matrix Product Operators

Y. Yang[1] S. Iblisdir[2] J. I. Cirac[1,4] M. C. Bañuls[1,4]

[1]Max-Planck-Institut für Quantenoptik

[2]Departament de Física Quàntica i Astronomia & Institut de Ciències del Cosmos,
Universitat de Barcelona

[3]Departamento de Análisis y Matemática Aplicada,
Universidad Complutense de Madrid & Instituto de Ciencias Matemáticas

[4]Munich Center for Quantum Science and Technology (MCQST)

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Method

Chebyshev expansion

Expand continuous function $f(x)$ in $(-1, 1)$ with Chebyshev polynomials $T_n(x)$:

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_{n+2}(x) = 2xT_{n+1}(x) - T_n(x);$$

$$f(x) \approx \frac{1}{\pi\sqrt{1-x^2}}[\gamma_0\mu_0 + 2\sum_{n=1}^{M-1}\gamma_n\mu_n T_n(x)], \ \mu_n = \int_{-1}^{1} f(x)T_n(x)\mathrm{d}x.$$

Many Body Spectral Property

Target function: *generalized density of states (DOS)* for Hamiltonian with spectral decomposition $\hat{H} = \sum_k E_k |k\rangle\langle k|$:

$$g(E;\hat{O}) = \sum_k \delta(E - E_k)\langle k|\hat{O}|k\rangle.$$

Approximate with Chebyshev expansion and matrix product operator (MPO):

$$\mu_n(\hat{H};\hat{O}) = \mathrm{Tr}\,(\hat{O}T_n(\hat{H})).$$

(Local) density of states

- Access to thermodynamic quantities:

  – DOS ($\hat{O} = \mathbb{1}$) $\xrightarrow{\text{Laplace transform}}$ partition function

  – LDOS ($\hat{O} = |\psi\rangle\langle\psi|$) $\xrightarrow{\text{Fourier transform}}$ survival probability.

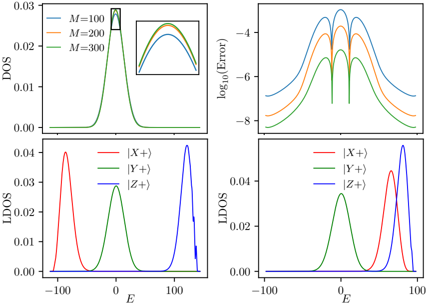
- Models: Ising and PXP models.

$$\hat{H}_{\text{Ising}} = J\sum_{i=1}^{N-1}\sigma_i^z\sigma_{i+1}^z + \sum_{i=1}^{N}(g\sigma_i^x + h\sigma_i^z),$$

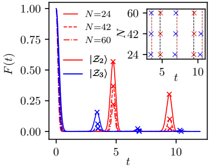
$(J, g, h) = (1, -1.05, 0.5)$ (non-integrable) and $(1, 0.8.0)$ (integrable);

$$\hat{H}_{\text{PXP}} = \sum_{i=2}^{N-1} P_{i-1}\sigma_i^x P_{i+1} + \sigma_1^x P_2 + P_{N-1}\sigma_N^x,$$

projector $P_i = (1 - \sigma_i^z)/2$.



Ising model. Left: non-integrable; right: integrable. $N = 80$.



Survival probability of PXP model.

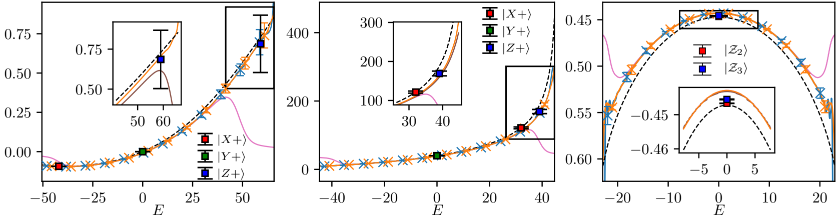
Thermalization probe

Assume eigenstate thermalization hypothesis (ETH), microcanonical ensemble expectation value of $\hat{O}$ given by the ratio $O(E) = g(E; \hat{O})/g(E; \mathbb{1})$ would be same as thermal value:

$$O(E) \overset{\text{ETH}}{\approx} \mathrm{Tr}\,(\rho_{\beta(E)}\hat{O}).$$

For a non-degenerate system, the long time averaged expectation value of a state $|\psi\rangle$ is the diagonal ensemble expectation $O_{\text{diag}}(\psi) = \sum_k \langle k|O|k\rangle\, |\langle k|\psi\rangle|^2$ and if it thermalizes,

$$O_{\text{diag}}(\psi) = \int \mathrm{d}E O(E) g(E; \psi) \approx \mathrm{Tr}\,(\rho_{\beta(E_\psi)}\hat{O}).$$



Thermalization probes: non-integrable and integrable Ising model, PXP model (from left to right). $N = 40$. $\hat{O} = \sigma^z_{N/2}$ (left / right) and $\hat{O} = (\sum_i \sigma^z_i)^2$ (middle). Black line dashed line: thermal value; orange line: $O(E)$.