Tensor Networks and spectral properties: probing ETH

Mari-Carmen Bañuls

Maxine Luo, Yilun Yang, Rahul Trivedi, Siri Lu,

J. Ignacio Cirac

PRB 109, 134304 (2024)
PRB 106, 024307 (2022)
PRX Quantum 2, 020321 (2021)
PRL124, 100602 (2020)

MAX PLANCK INSTITUTE
OF QUANTUM OPTICS

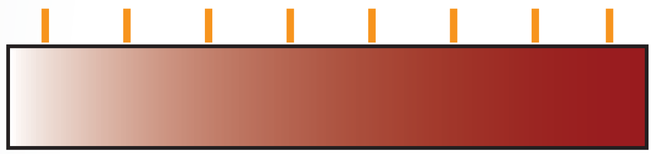
MCQST

DFG FOR 5522

DFG TRR 360

IHP 17.10.2024

arbitrary many-body state



d^N

$$|\Psi\rangle = \sum_{i_j} c_{i_1 \ldots i_N} |i_1 \ldots i_N\rangle$$

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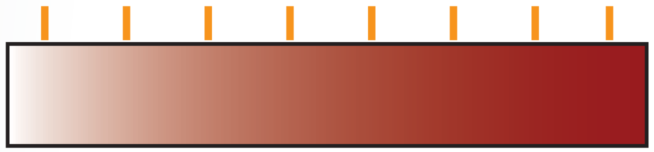

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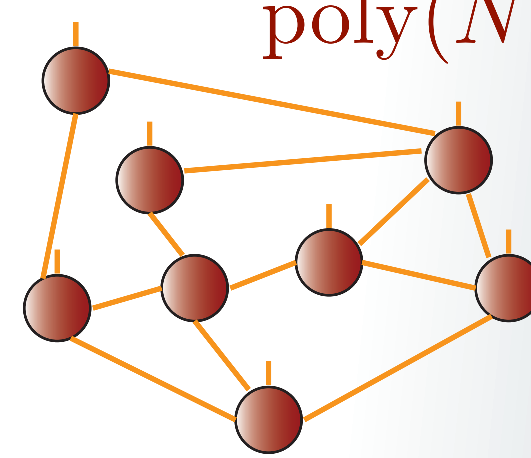
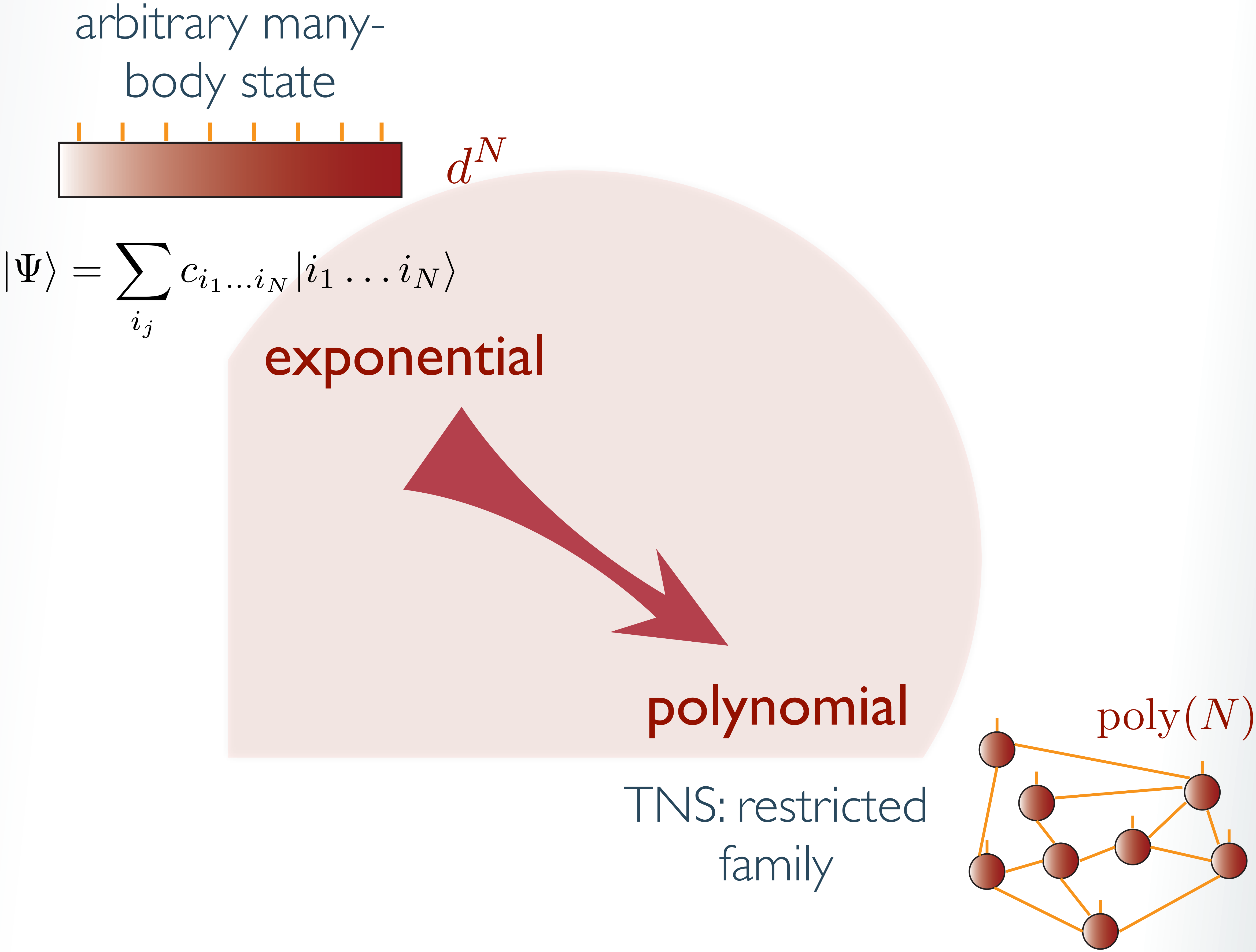
TNS: restricted family

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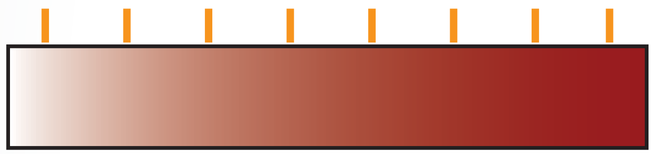

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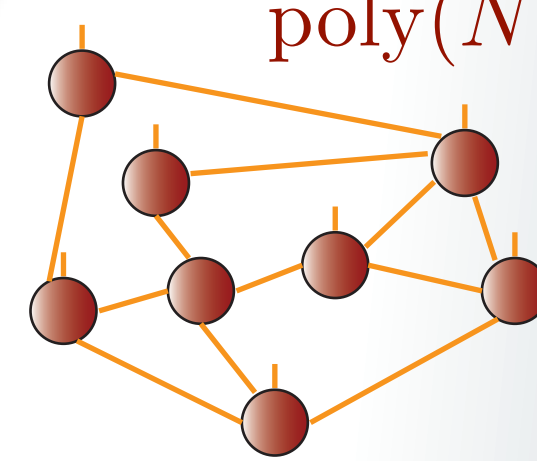


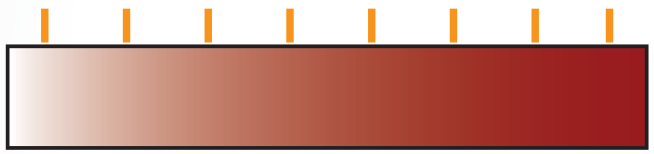
$\mathrm{poly}(N)$

good ansatz for ground states and thermal equilibrium: area law

entanglement hierarchy

efficient numerics

arbitrary many-body state



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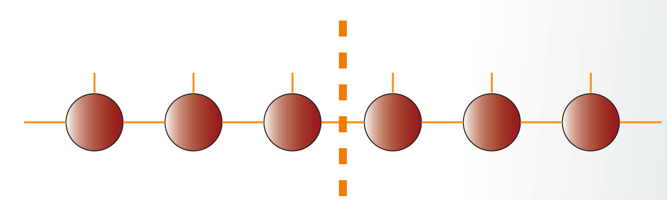
MPS

matrix product states



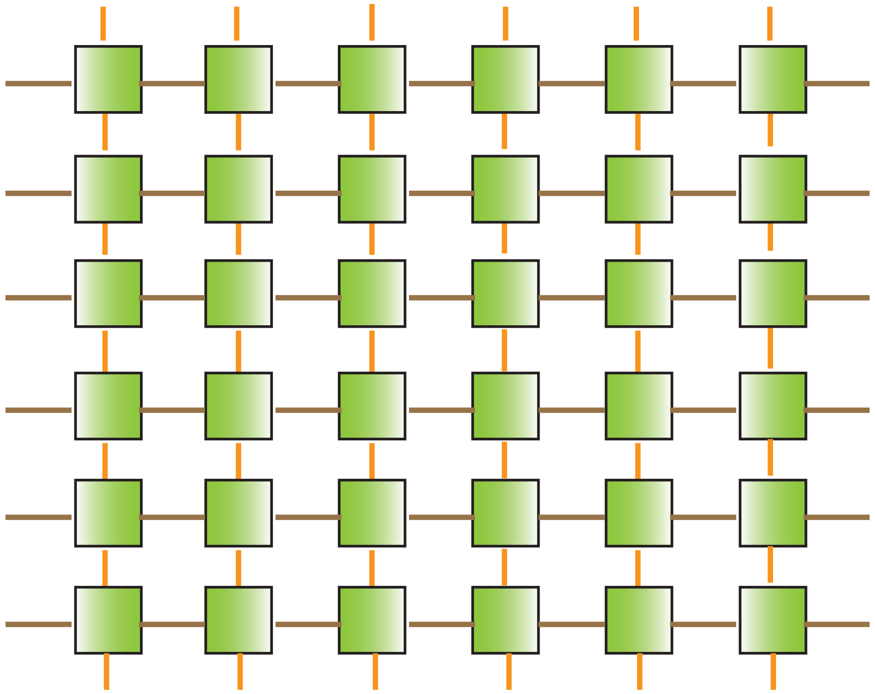
$S \leq \log(D)$

TNS: entanglement-based ansatzes for quantum many-body states

a side comment

tensor networks may also describe partition functions (observables)

need to contract a TN



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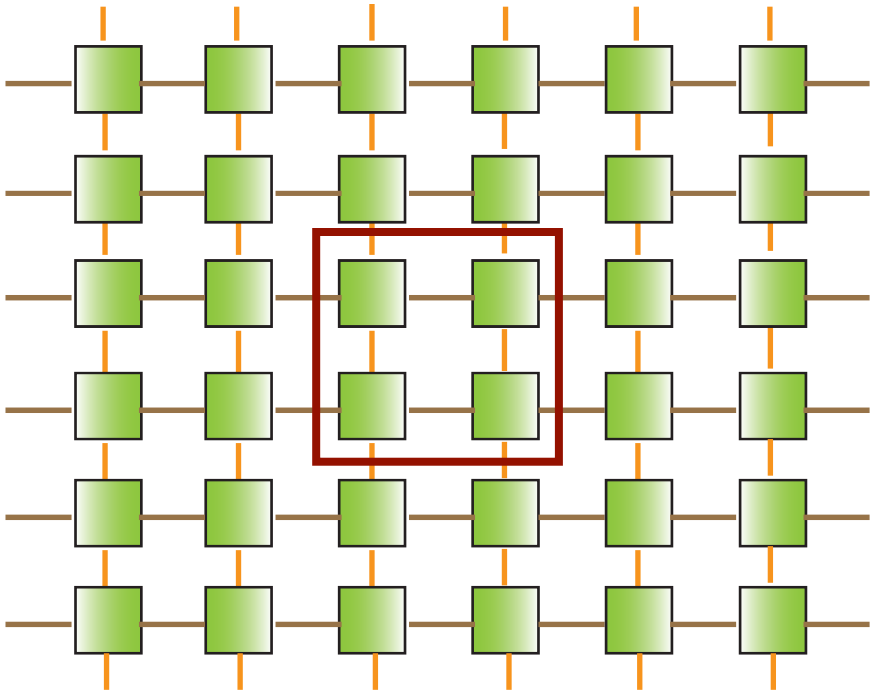

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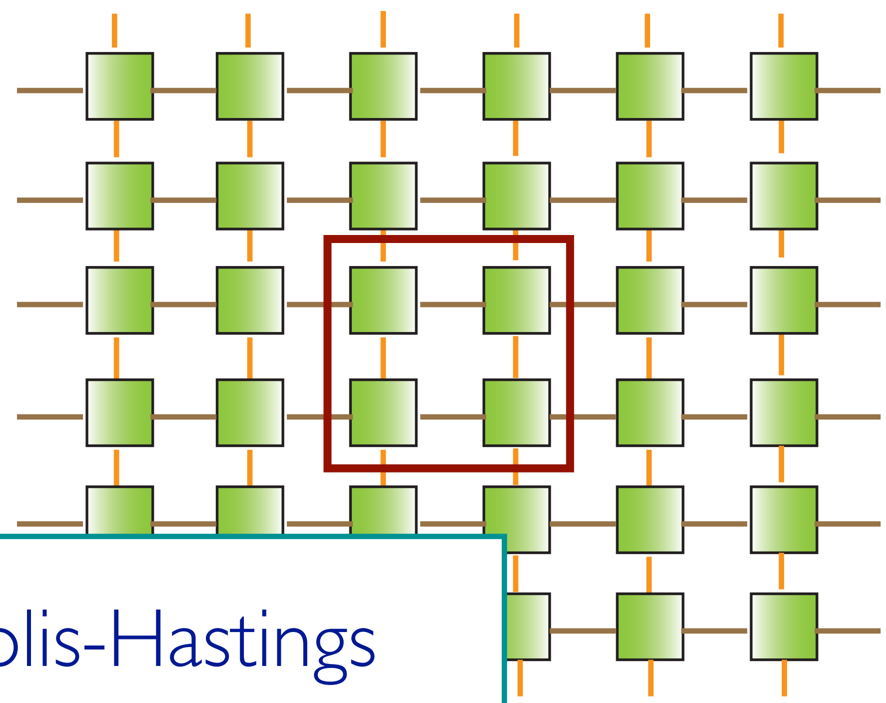
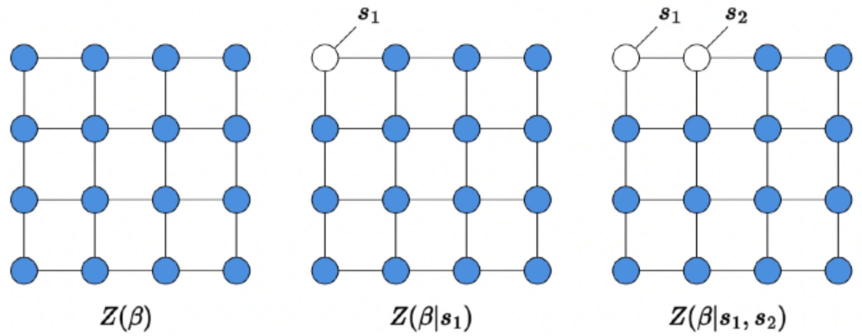


TRG approaches

TN assisted Metropolis-Hastings

collective updates



Frías-Pérez, Marien, Pérez-García, MCB, Iblisdir, SciPost Phys. 14, 123 (2023)

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as ansatz

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classify tensors (symmetries)

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TNS as (variational) ansätze for physical problems

efficient algorithms for GS, low excited states, thermal, dynamics

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entanglement: crucial ingredient to understand QMB systems

as (numerical) ansatz

Tensor Network States (TNS)

efficient numerical algorithms (small spatial dimensions) and good theoretical understanding

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new tools allow us to access some of these regimes a question we want to address…

how do quantum systems thermalize?

Thermalization of quantum systems

quantum system

$H \qquad |\Psi\rangle$

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quantum system

$$|\Psi\rangle \to U(t)|\Psi\rangle = e^{-iHt}|\Psi\rangle \quad \text{remains pure}$$

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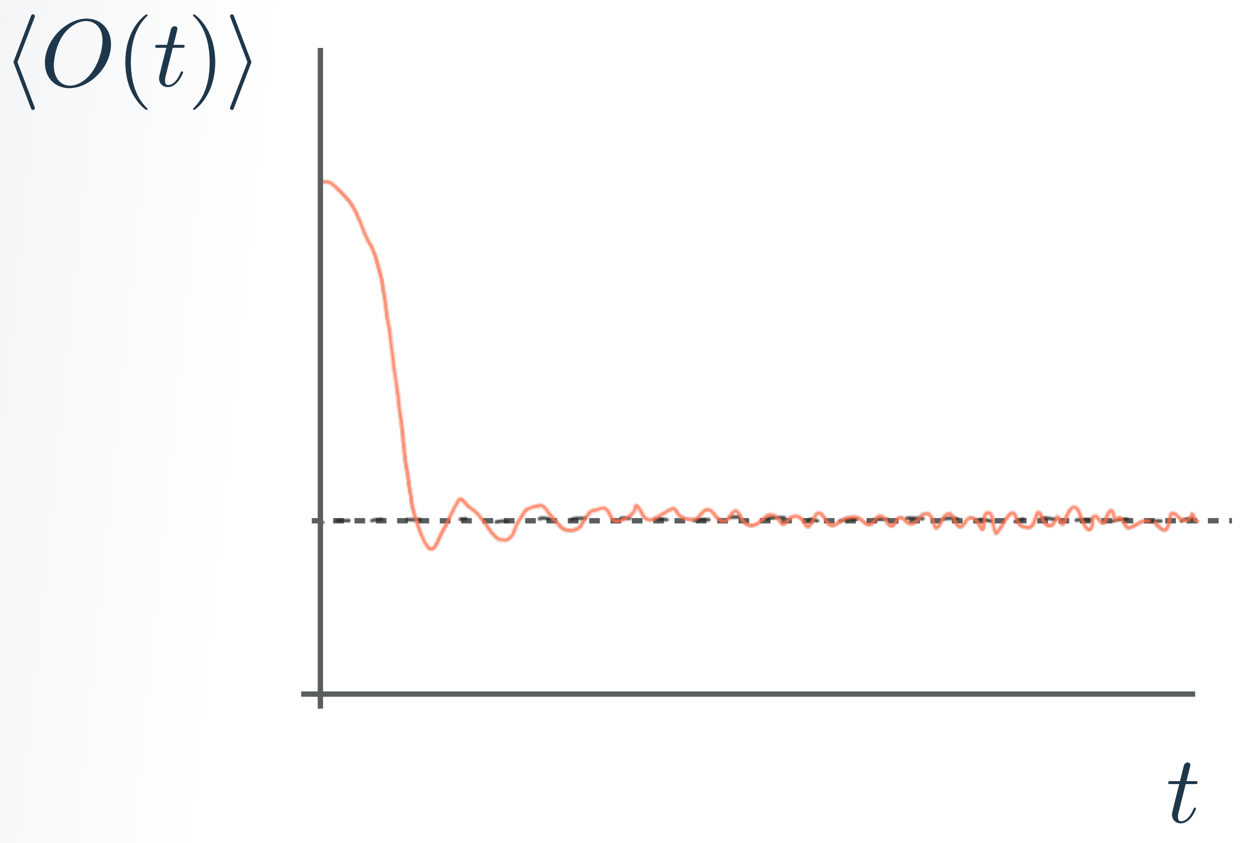

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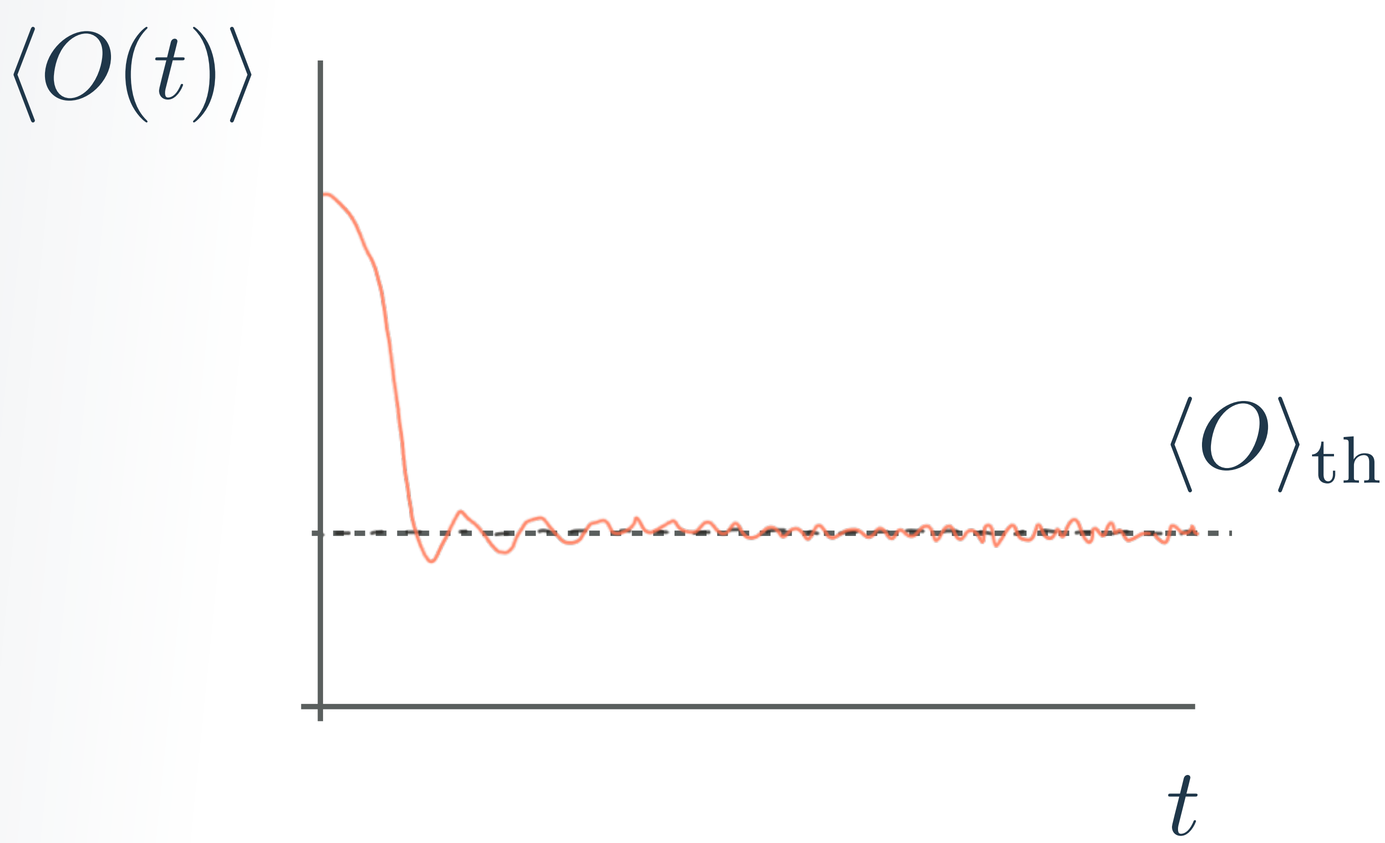

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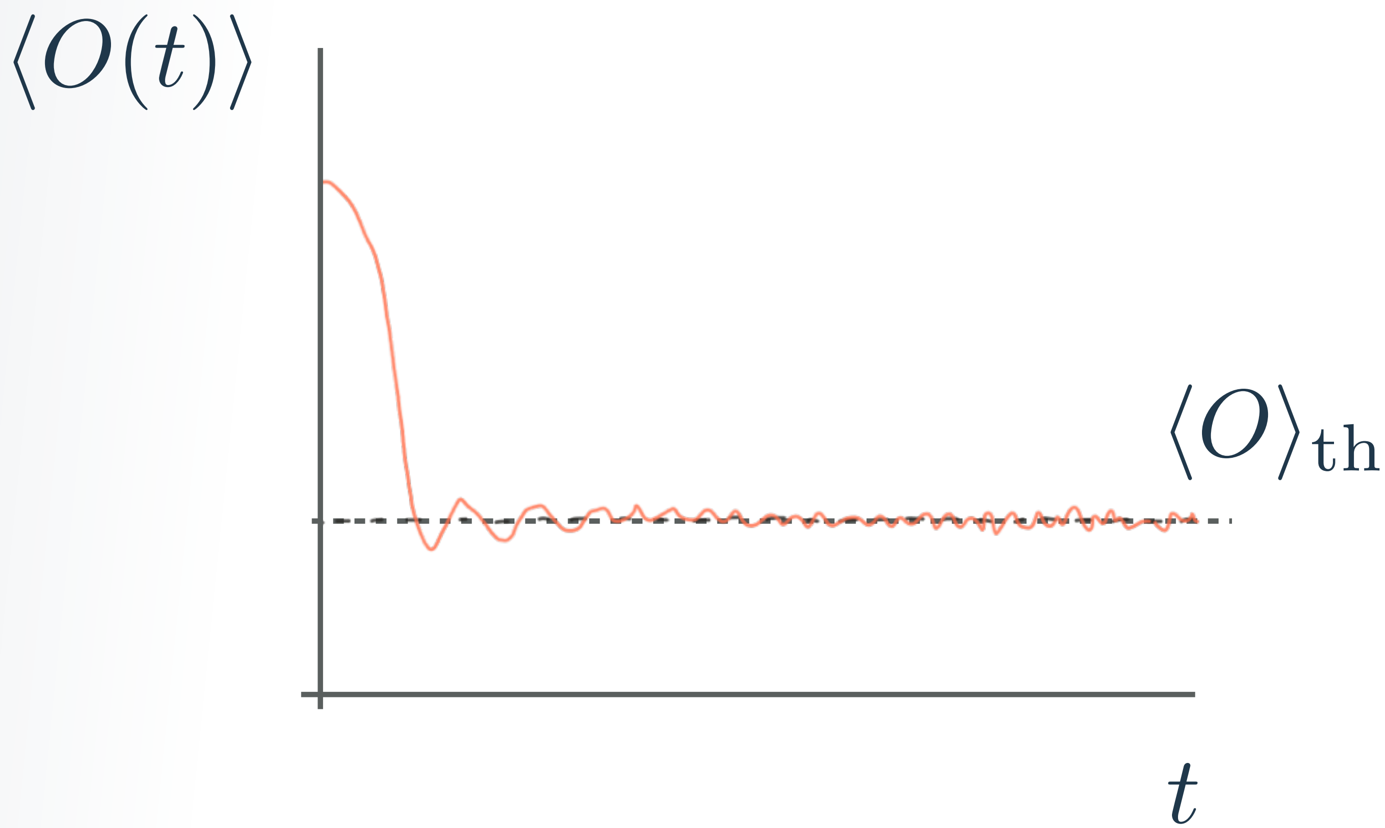

reach (remain close to) equilibrium value

predicted by thermodynamic ensemble (microcanonical)

Eigenstate Thermalization Hypothesis (ETH)

theoretical framework for quantum thermalization

review: D'Alessio et al, Adv Phys 65 (2016)

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ansatz for matrix elements of observables in energy eigenbasis

Srednicki, Deutsch 90s

$$O_{mn} = O(\bar{E})\delta_{mn} + e^{-\frac{S(\bar{E})}{2}} f_O(\bar{E},\omega) R_{mn}$$

$$\bar{E} = \frac{E_m + E_n}{2}$$

$$\omega = E_m - E_n$$

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implies (strong) thermalization for initial state with subextensive energy fluctuations

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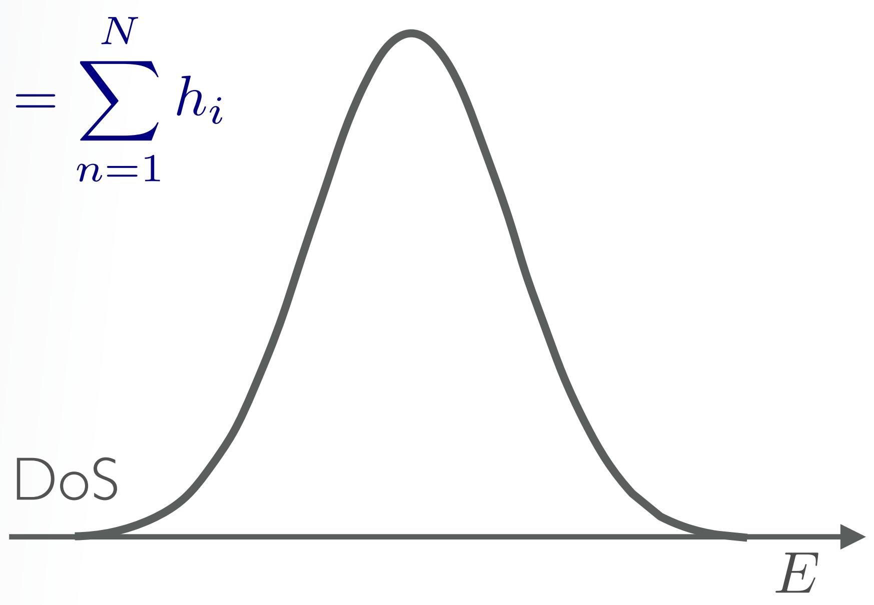

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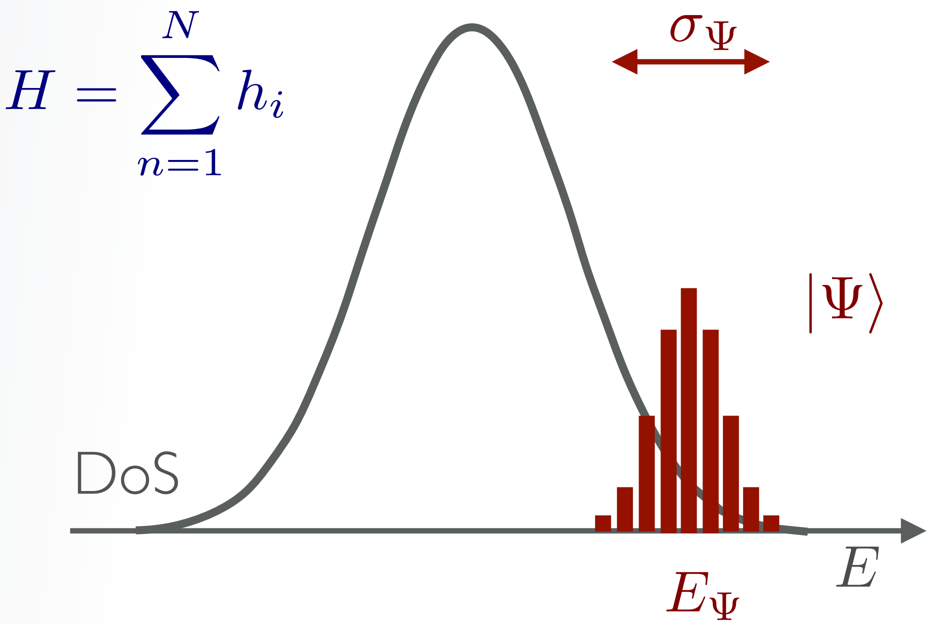

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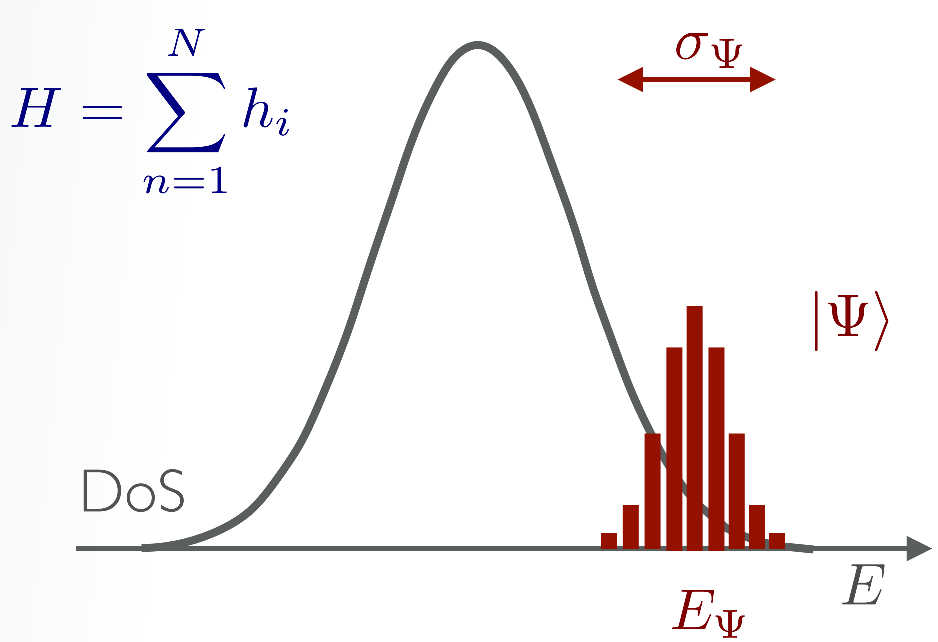

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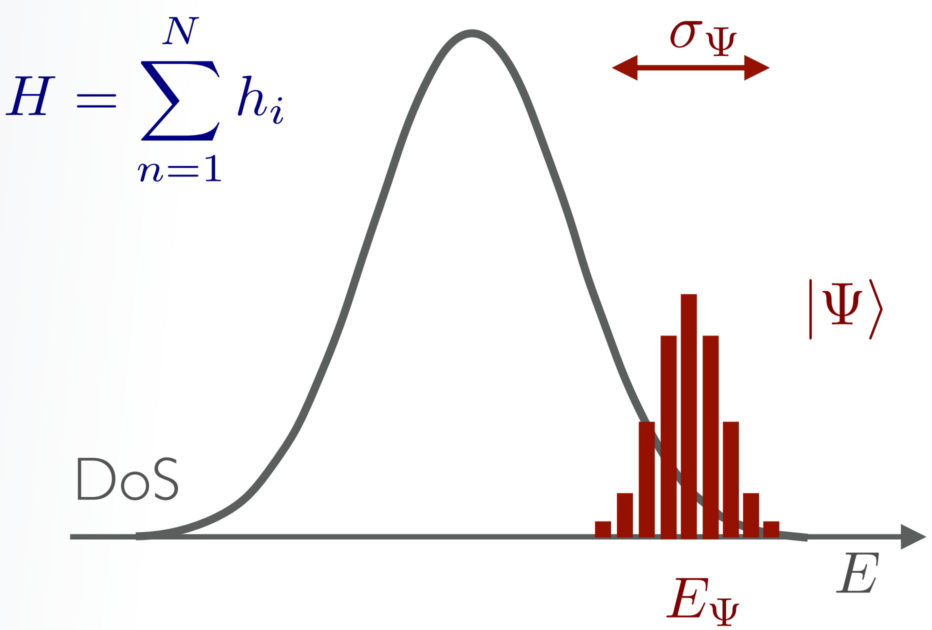

time average converges to microcanonical

fluctuations in time are exponentially small

Eigenstate Thermalization Hypothesis (ETH)

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problem: exponentially large in N $\Rightarrow$ Tensor Networks may be of help

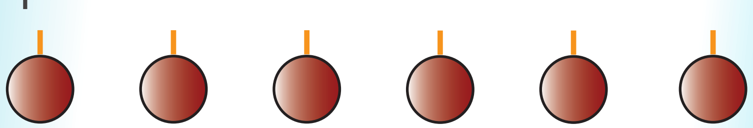
simulation of non-equilibrium dynamics with MPS

global quench in 1D

$t = 0$

$t = \infty$

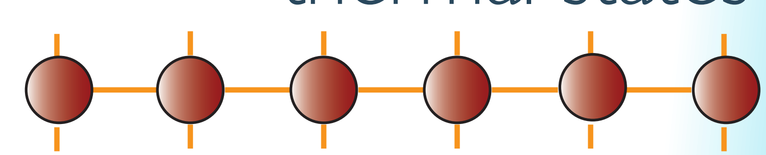
product state



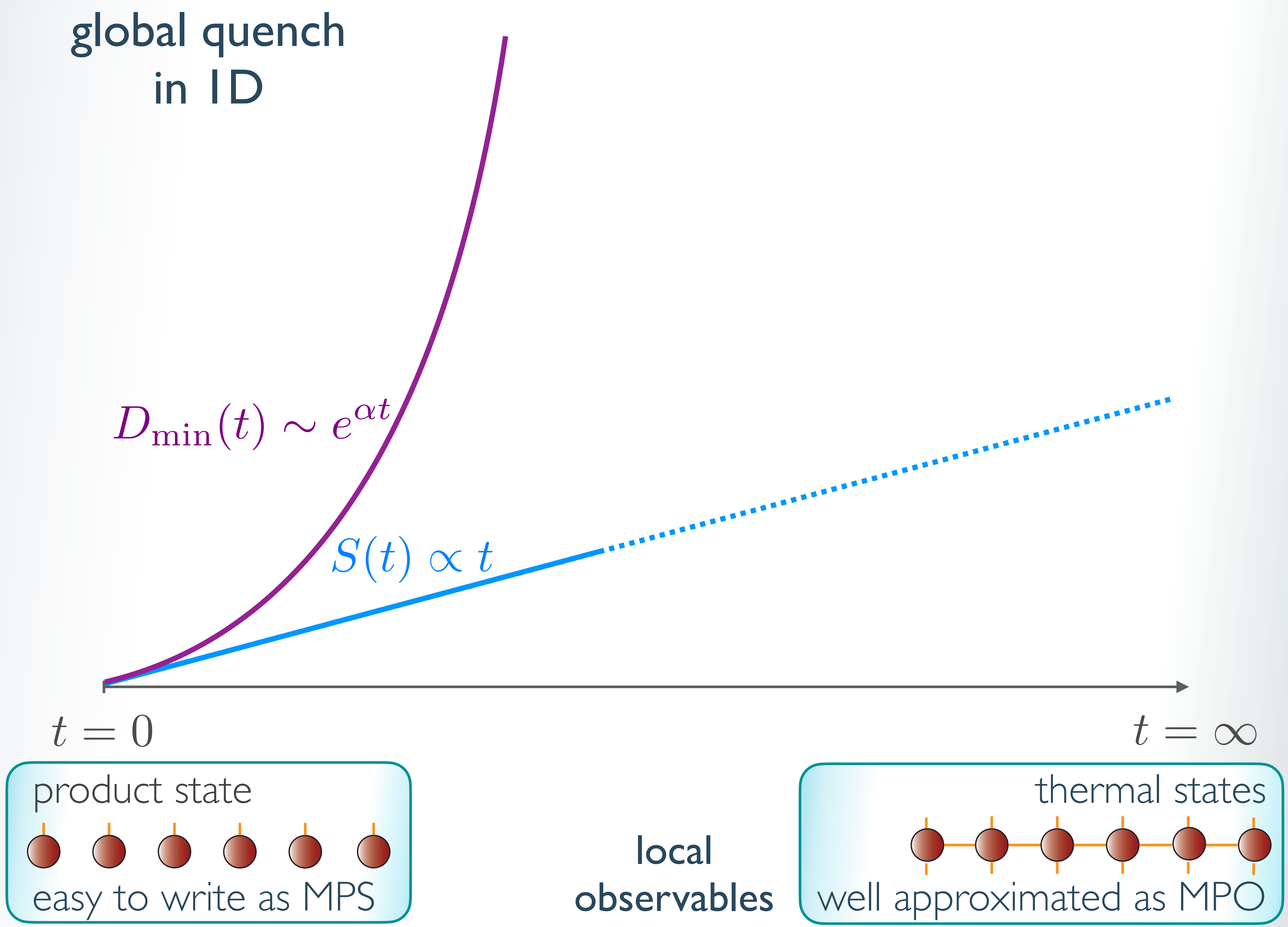
easy to write as MPS

local observables

thermal states



well approximated as MPO


global quench
in 1D
$D_{\min}(t) \sim e^{\alpha t}$
$S(t) \propto t$
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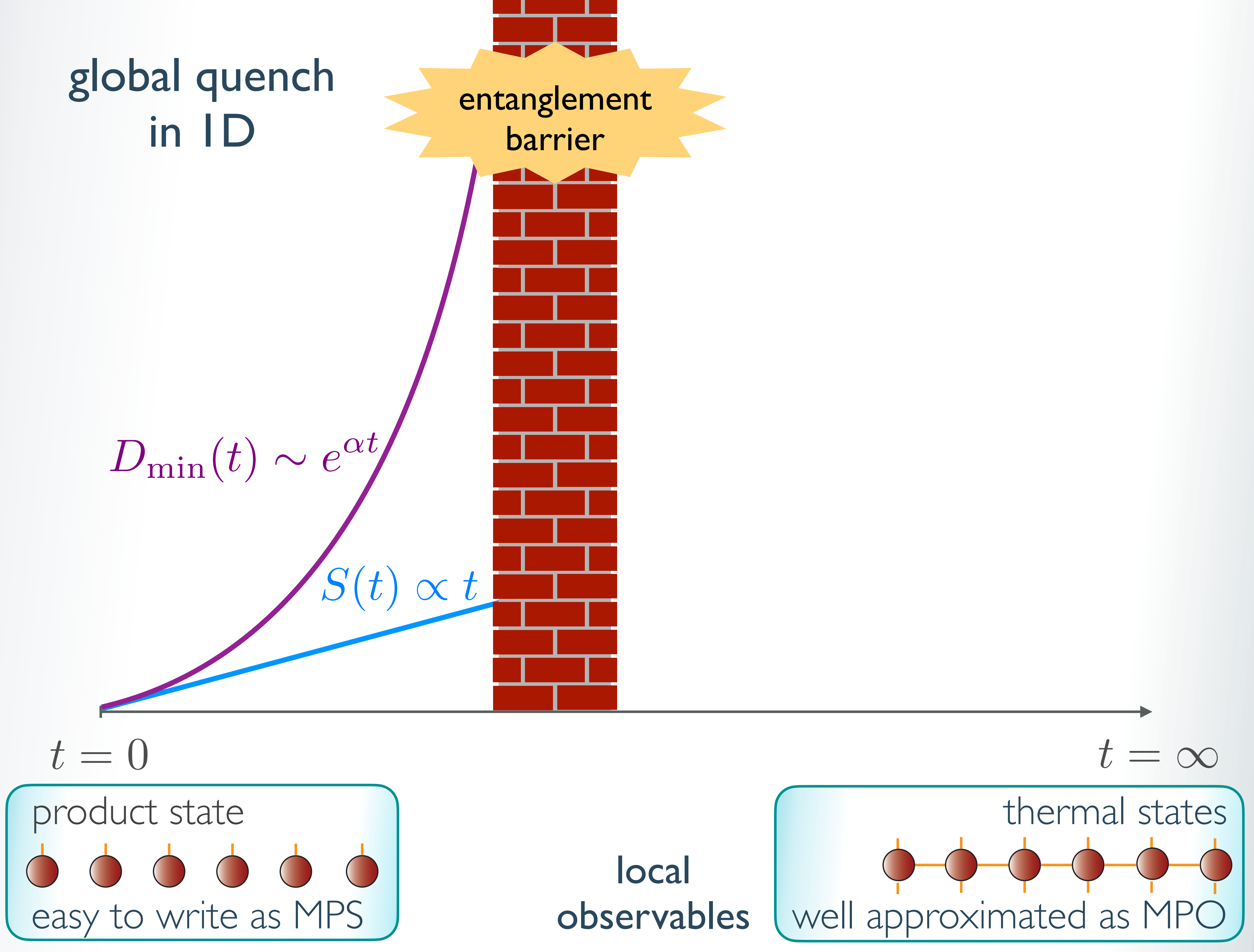
global quench
in 1D
entanglement
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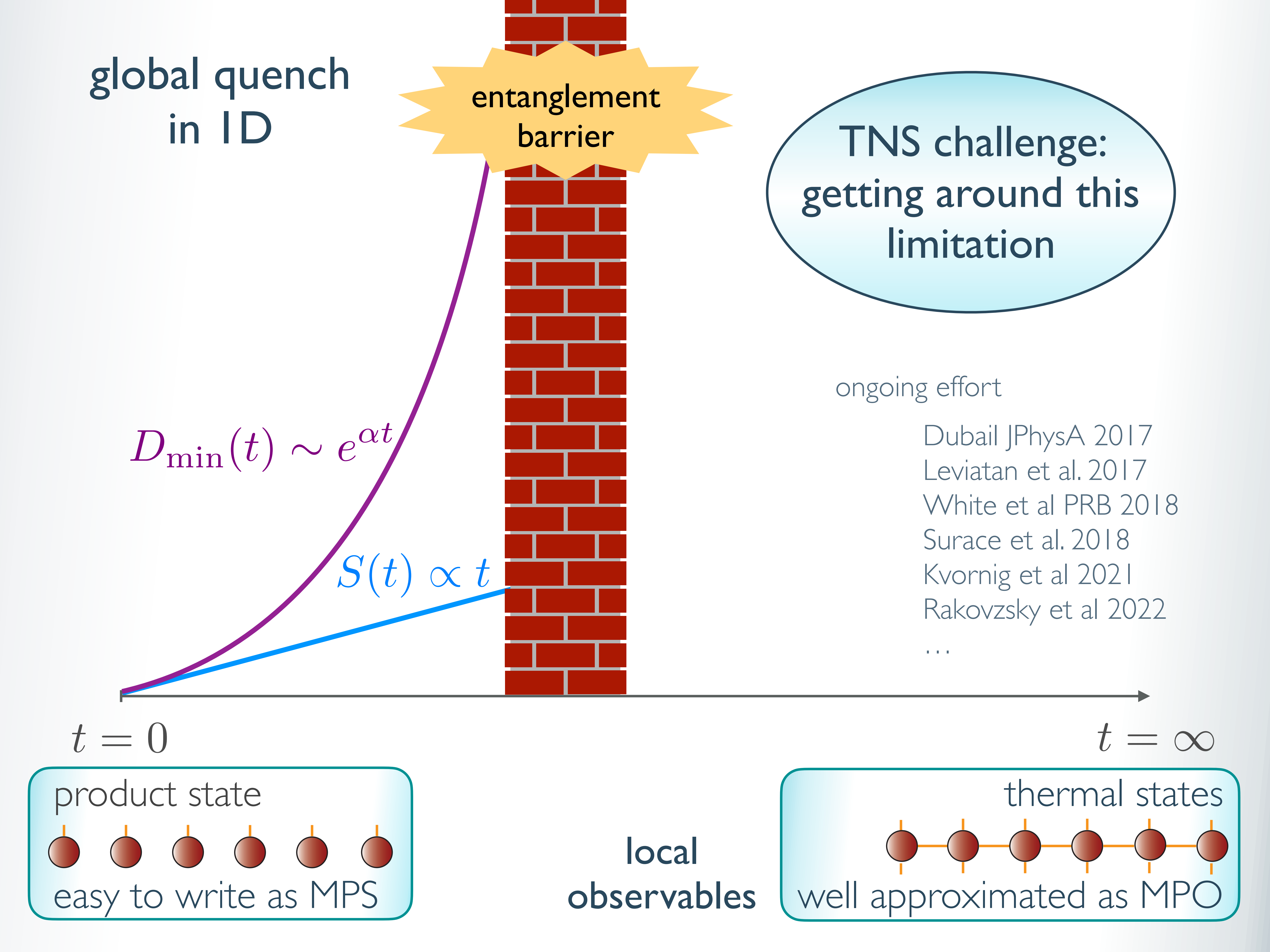
global quench
in 1D
entanglement
barrier
TNS challenge:
getting around this
limitation
ongoing effort
Dubail JPhysA 2017
Leviatan et al. 2017
White et al PRB 2018
Surace et al. 2018
Kvornig et al 2021
Rakovzsky et al 2022
...
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our approach: an alternative quantum/TNS tool

spectral (finite energy density) properties of the QMB Hamiltonian

MCB, Huse, Cirac, PRB 101, 144305 (2020)
Yang, Iblisdir, Cirac, MCB, PRL 124, 100602 (2020)
Papaefstathiou, Robaina, Cirac, MCB, PRD104, 014514 (2021)
Çakan, Cirac, MCB, PRB 103, 115113 (2021)
Lu, MCB, Cirac, PRX Quantum 2, 02032 (2021)
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Luo, Trivedi, MCB, Cirac, PRB 109, 134304 (2024)

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$$H = \sum_{n=1}^{N} h_i$$

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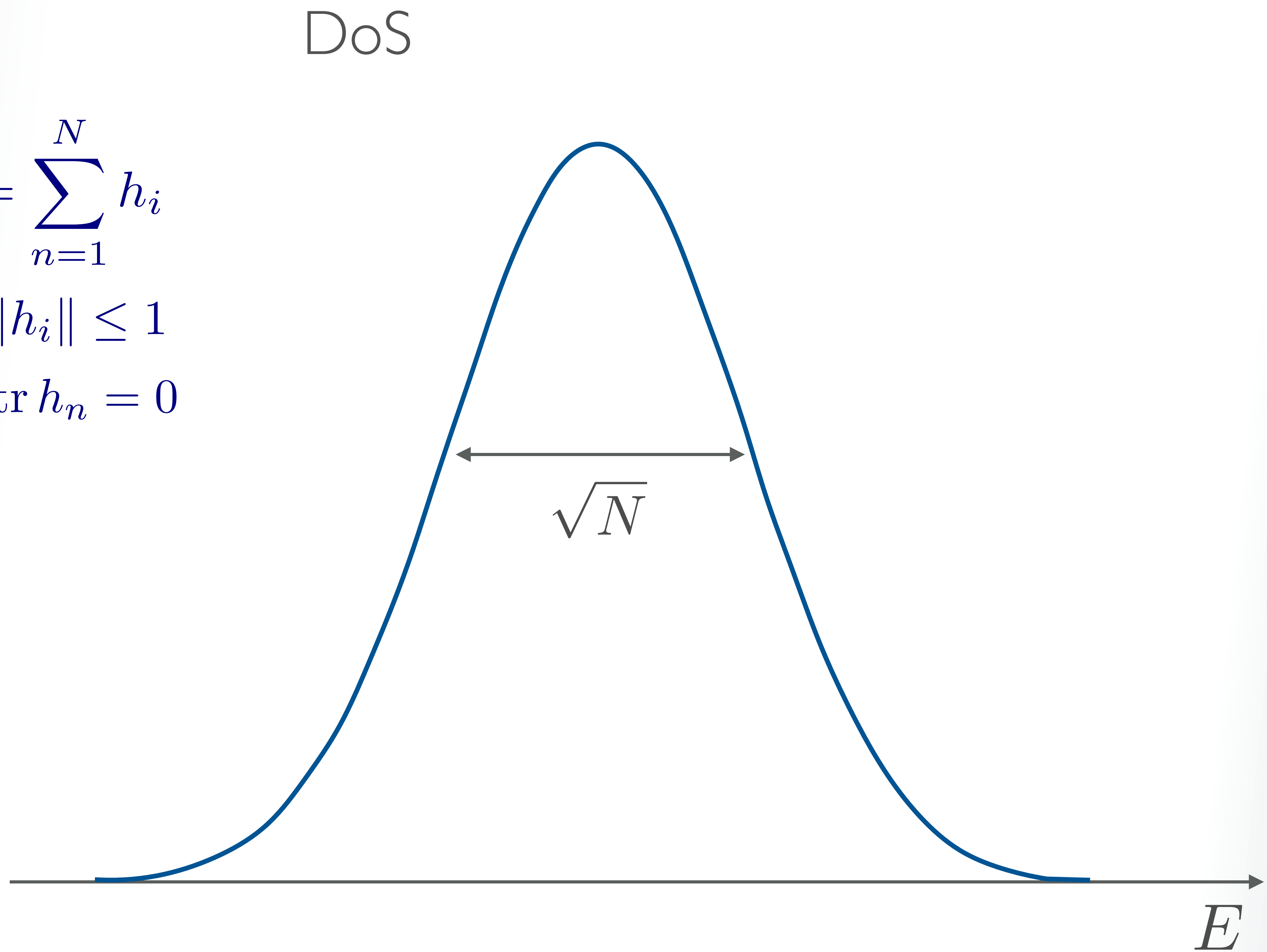

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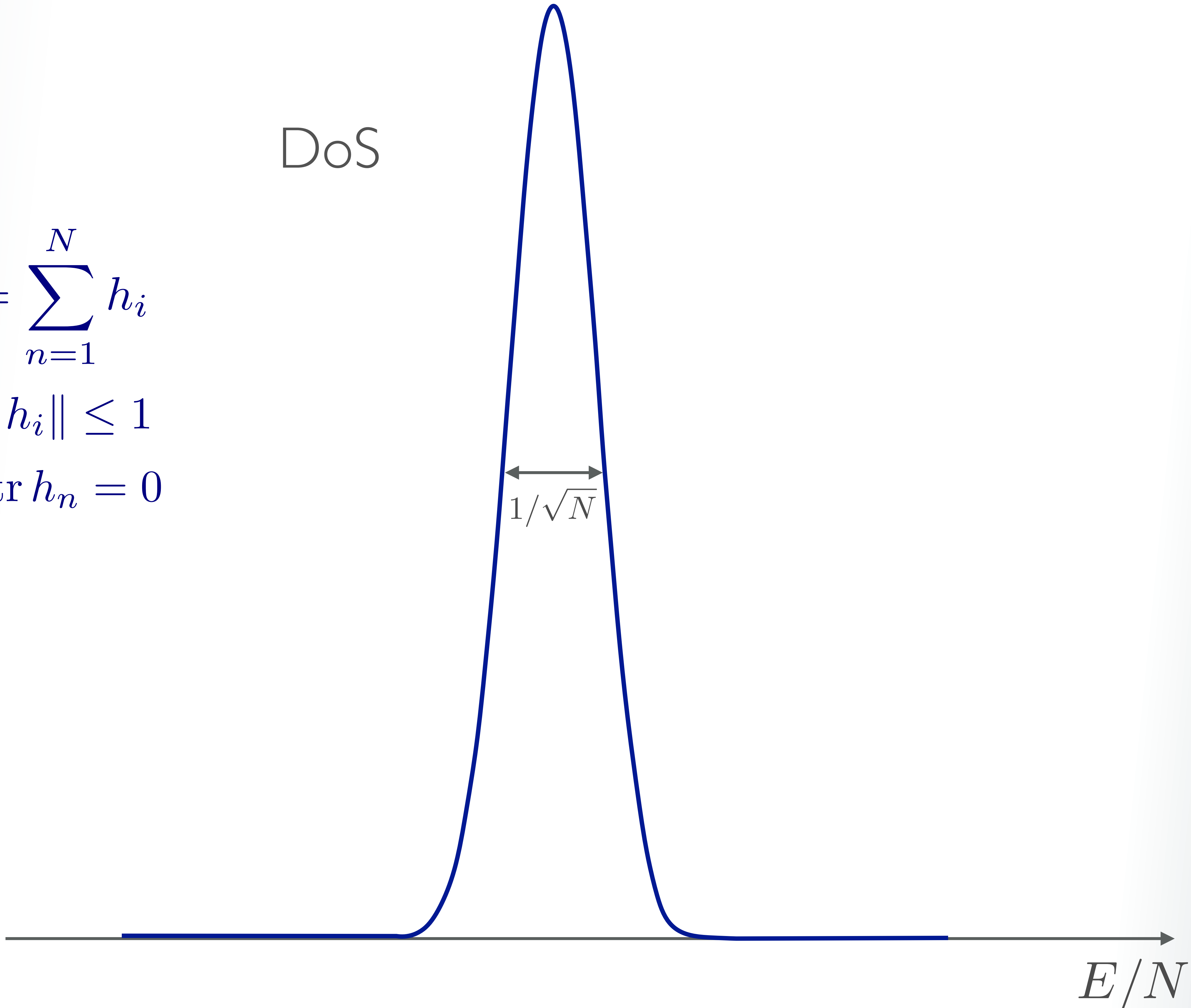

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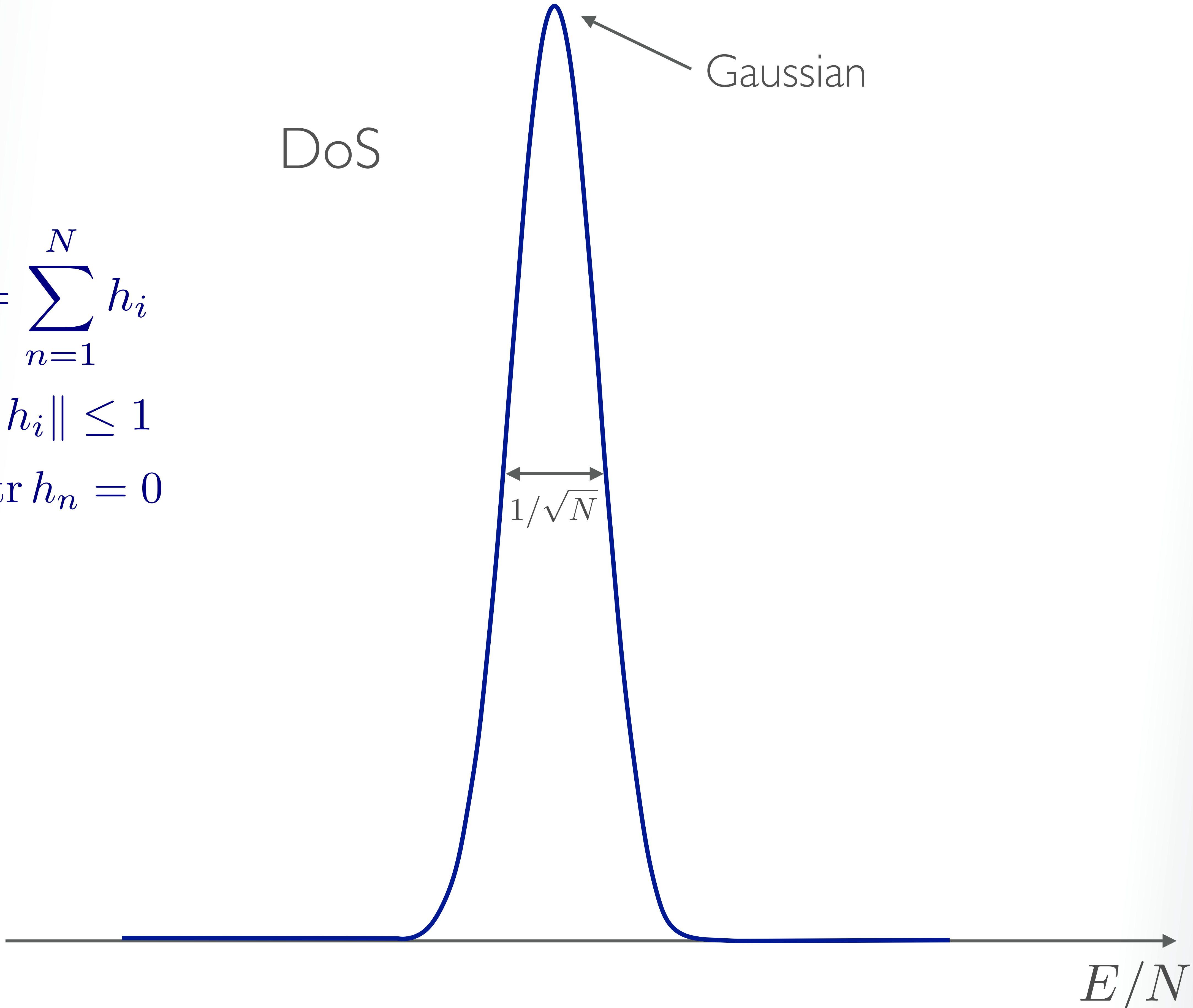

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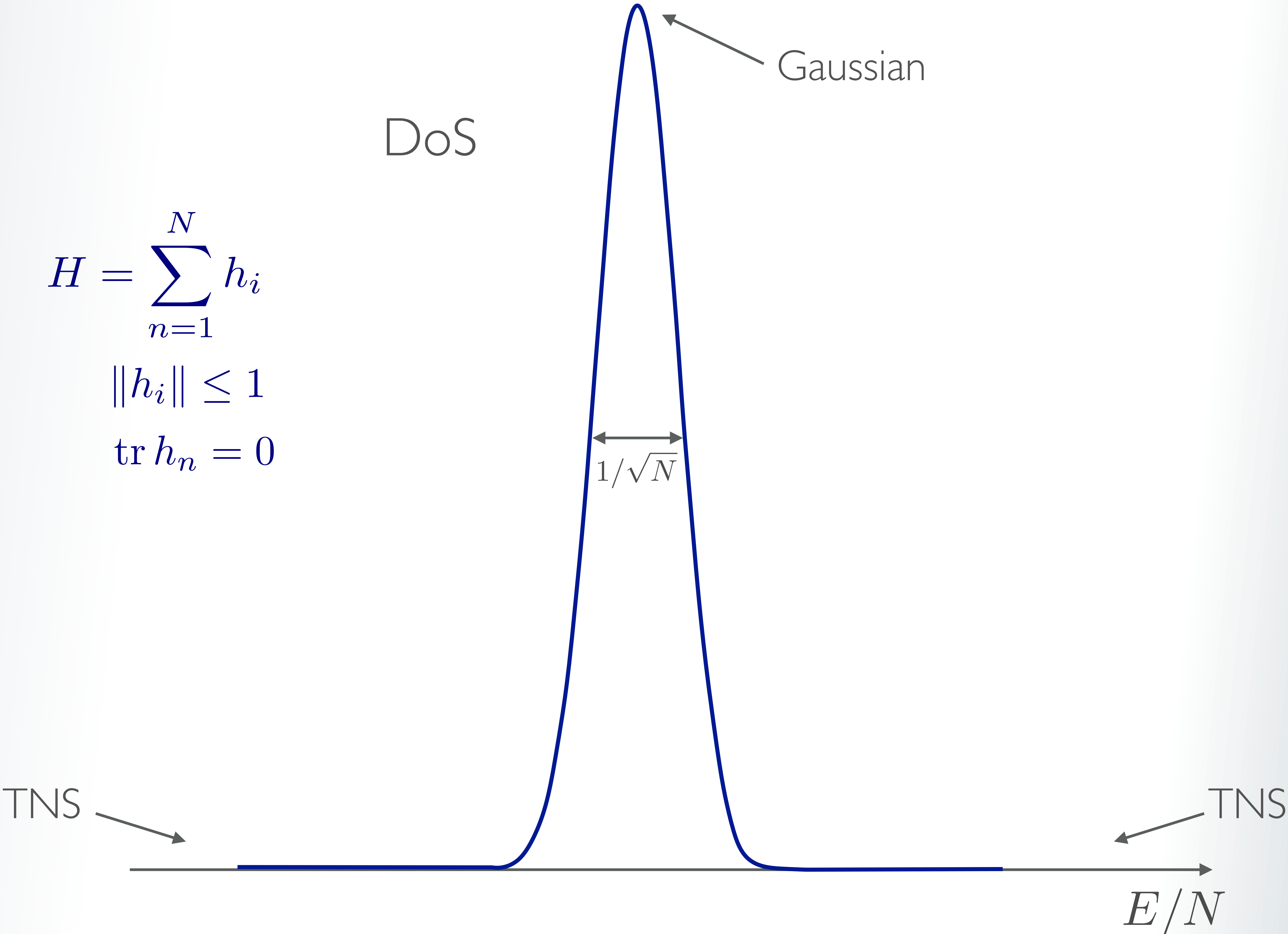

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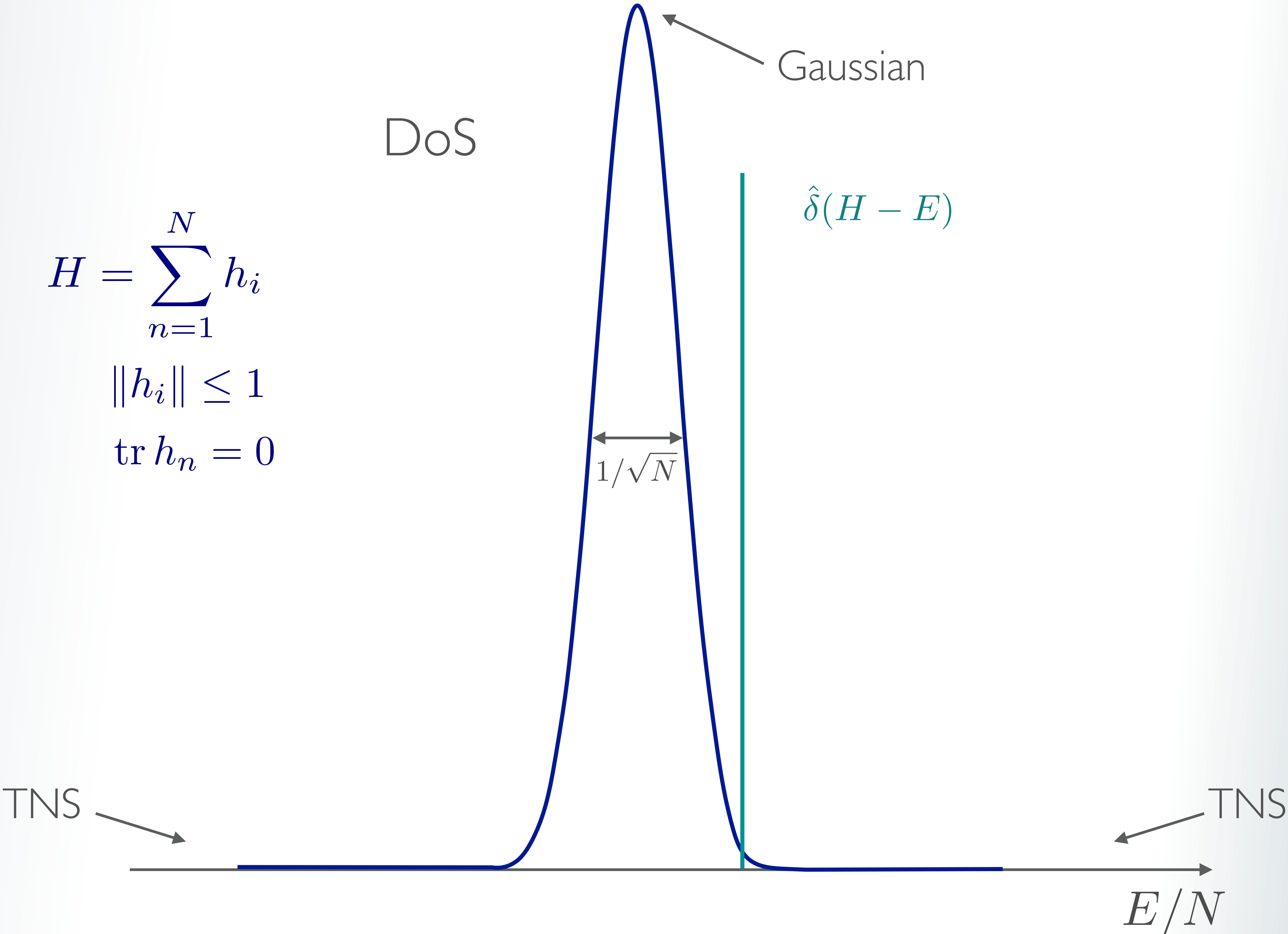

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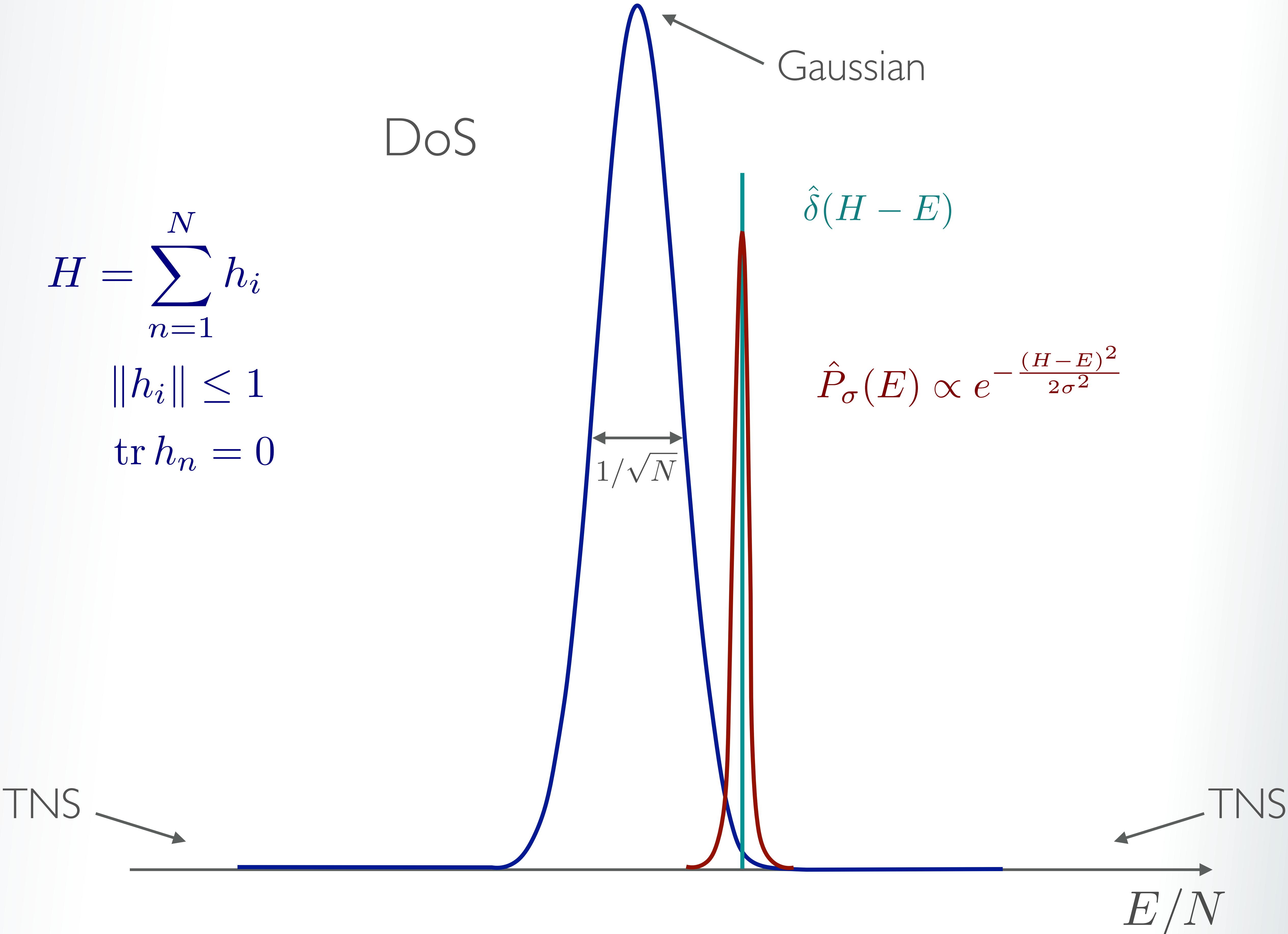

generalized density of states

$$g(E;O) = \sum_n \delta(E - E_n)\langle E_n|O|E_n\rangle$$

microcanonical average:
expectation value in eigenstates
with given energy

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unnormalised DOS

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unnormalised DOS

$$O = |\Psi\rangle\langle\Psi| \longrightarrow g(E;\Psi) = \sum_n \delta(E - E_n)|\langle E_n|\Psi\rangle|^2$$

local DOS

implementing the filter

Gaussian operator ⇒ not local

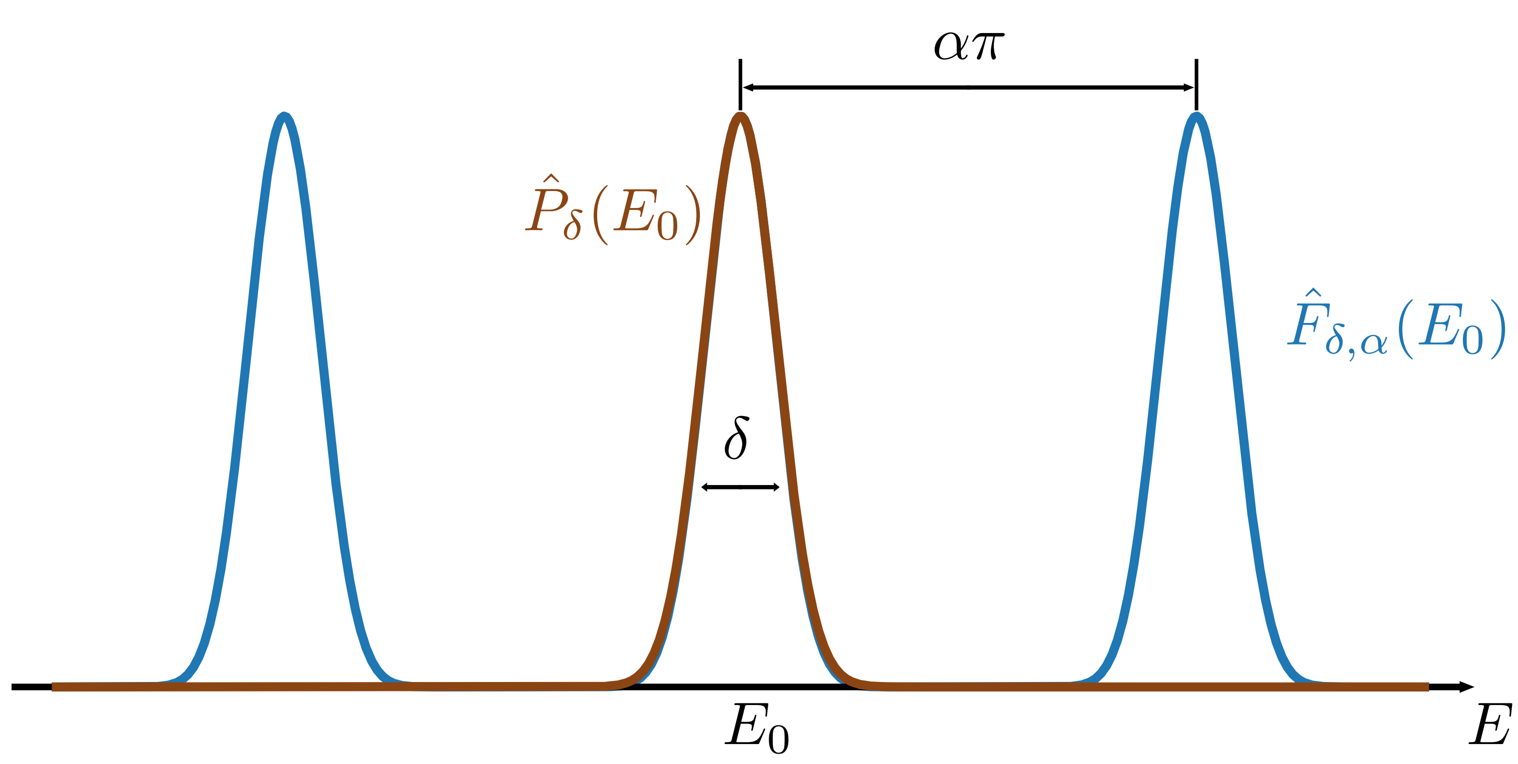
Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

implementing the filter

Gaussian operator ⇒ not local

⇒ cosine approximation

$$\cos^M(x) \approx e^{-Mx^2/2} \qquad x < \pi/2$$



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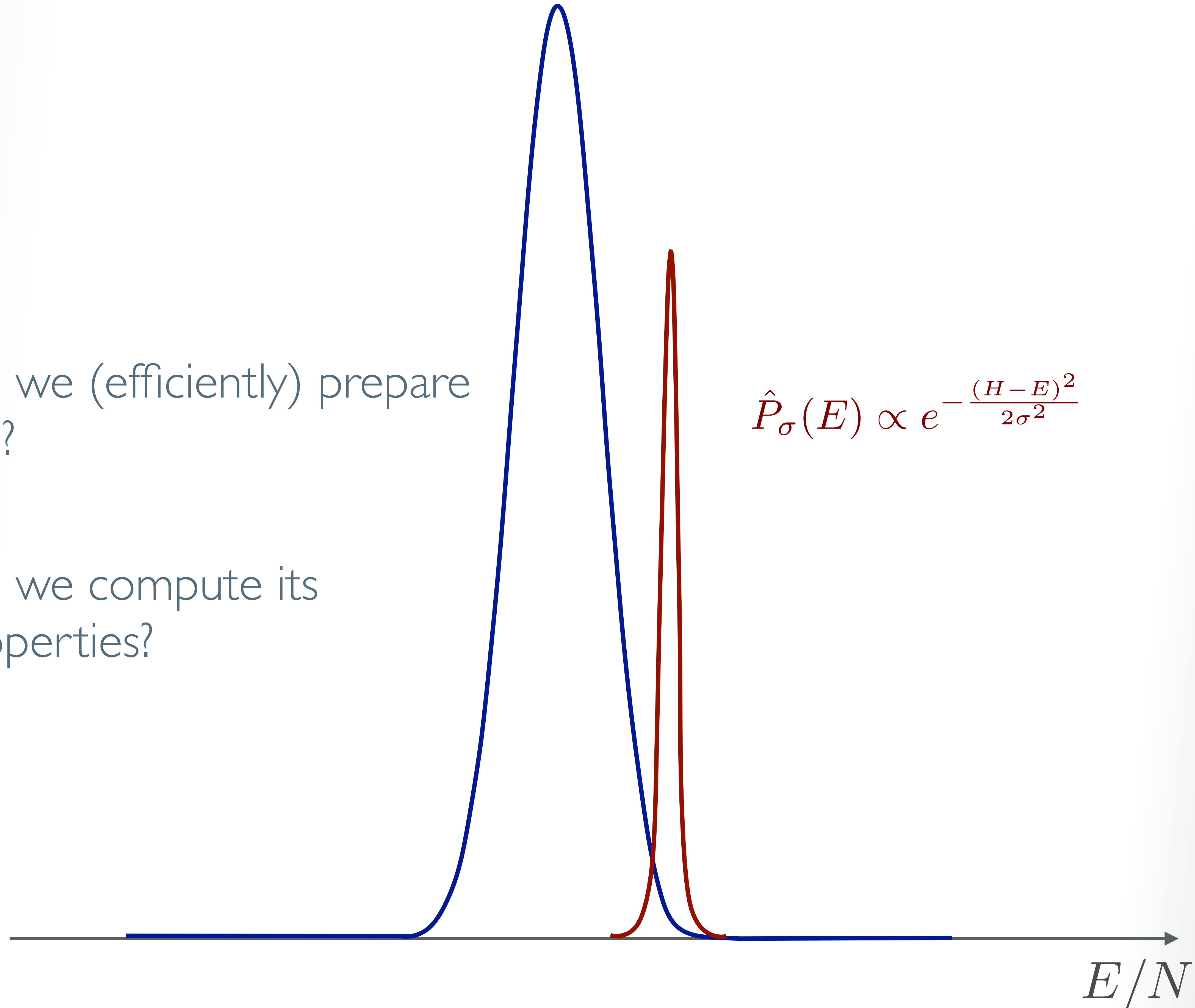
$$\exp\left(-\frac{H^2}{2\delta^2}\right) \approx \sum_{m=-x\alpha/\delta}^{x\alpha/\delta} c_m e^{i2mH/\alpha}$$

Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

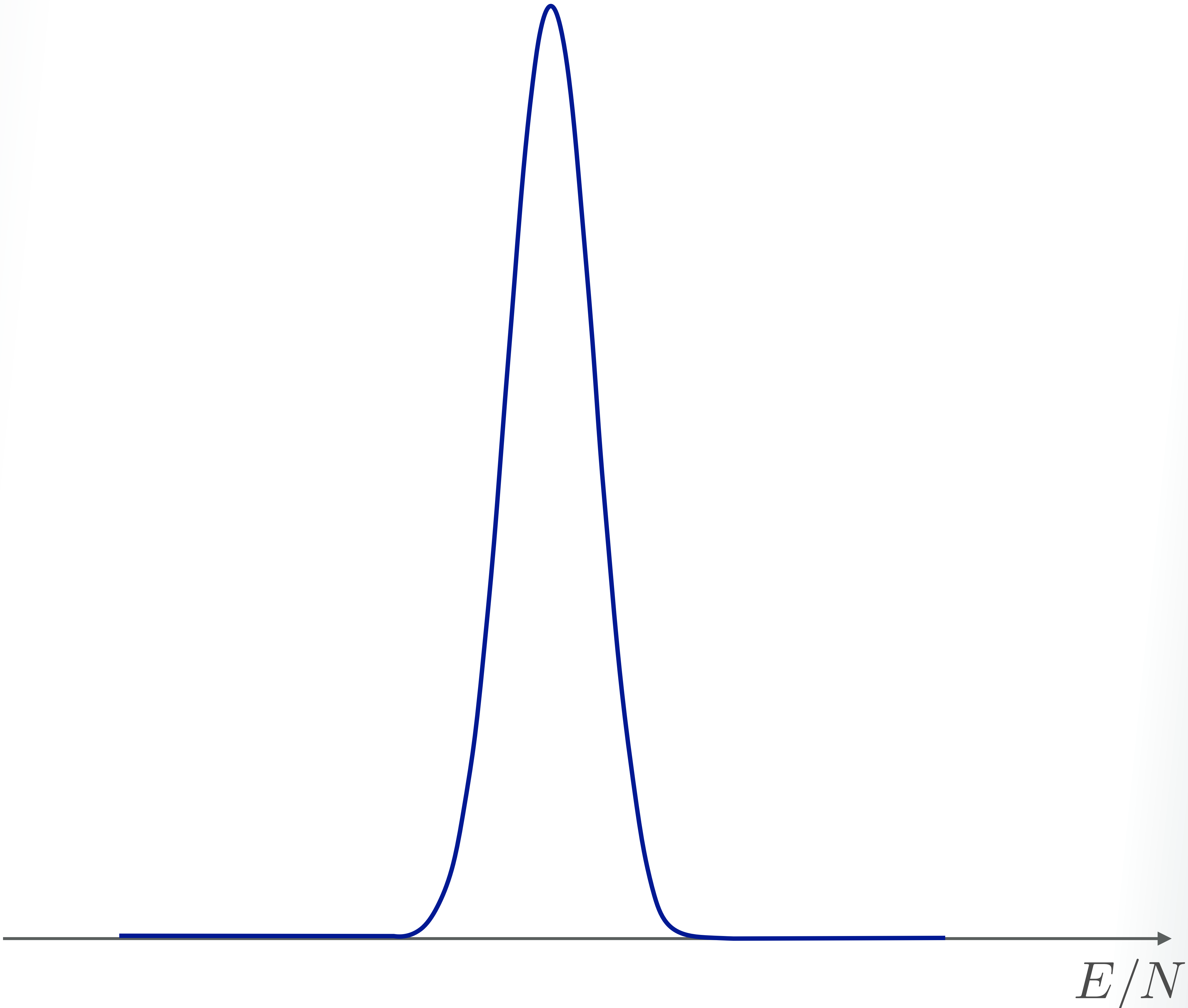
This talk

can we (efficiently) prepare this?

can we compute its properties?



Can we prepare a filtered state?



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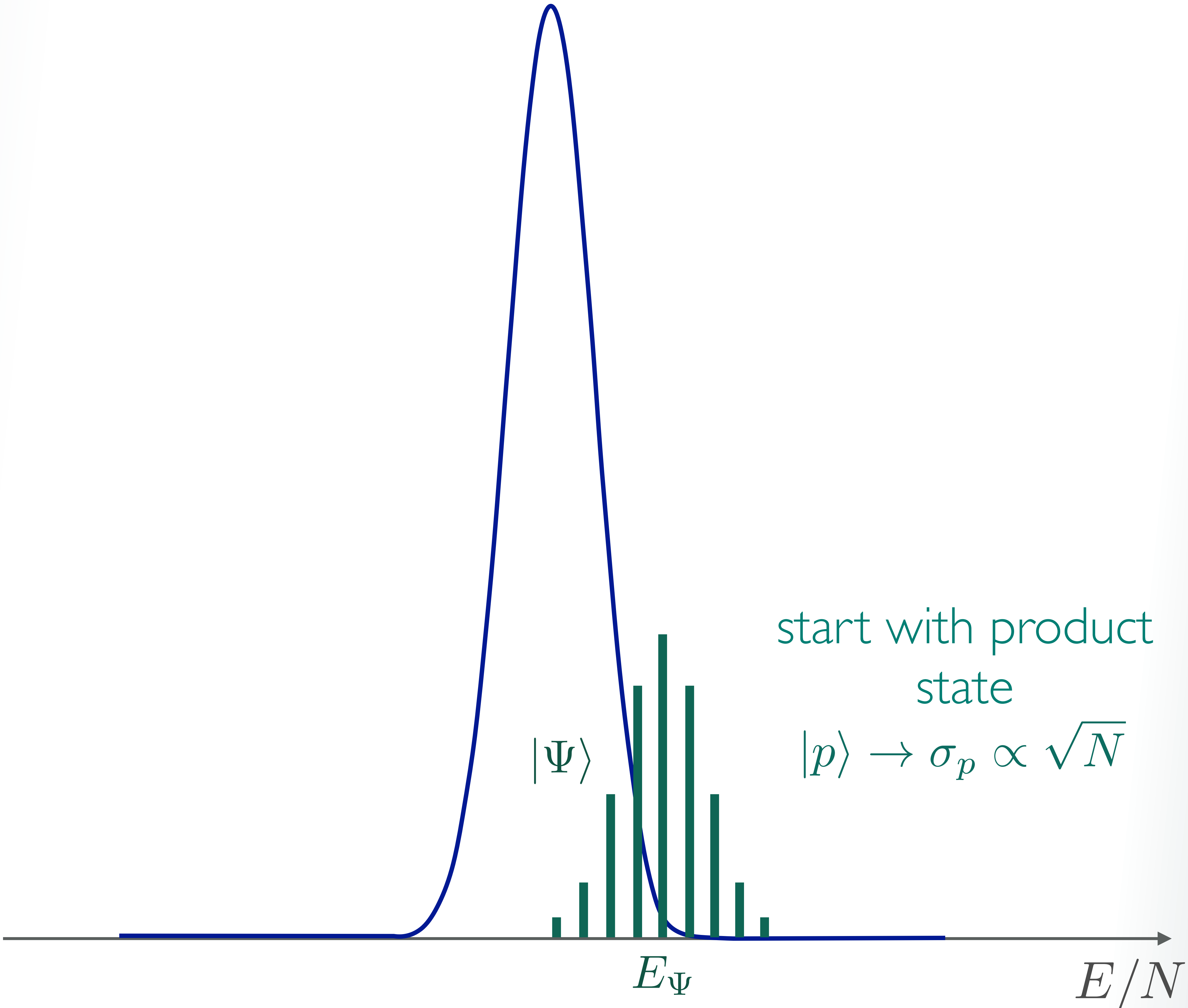
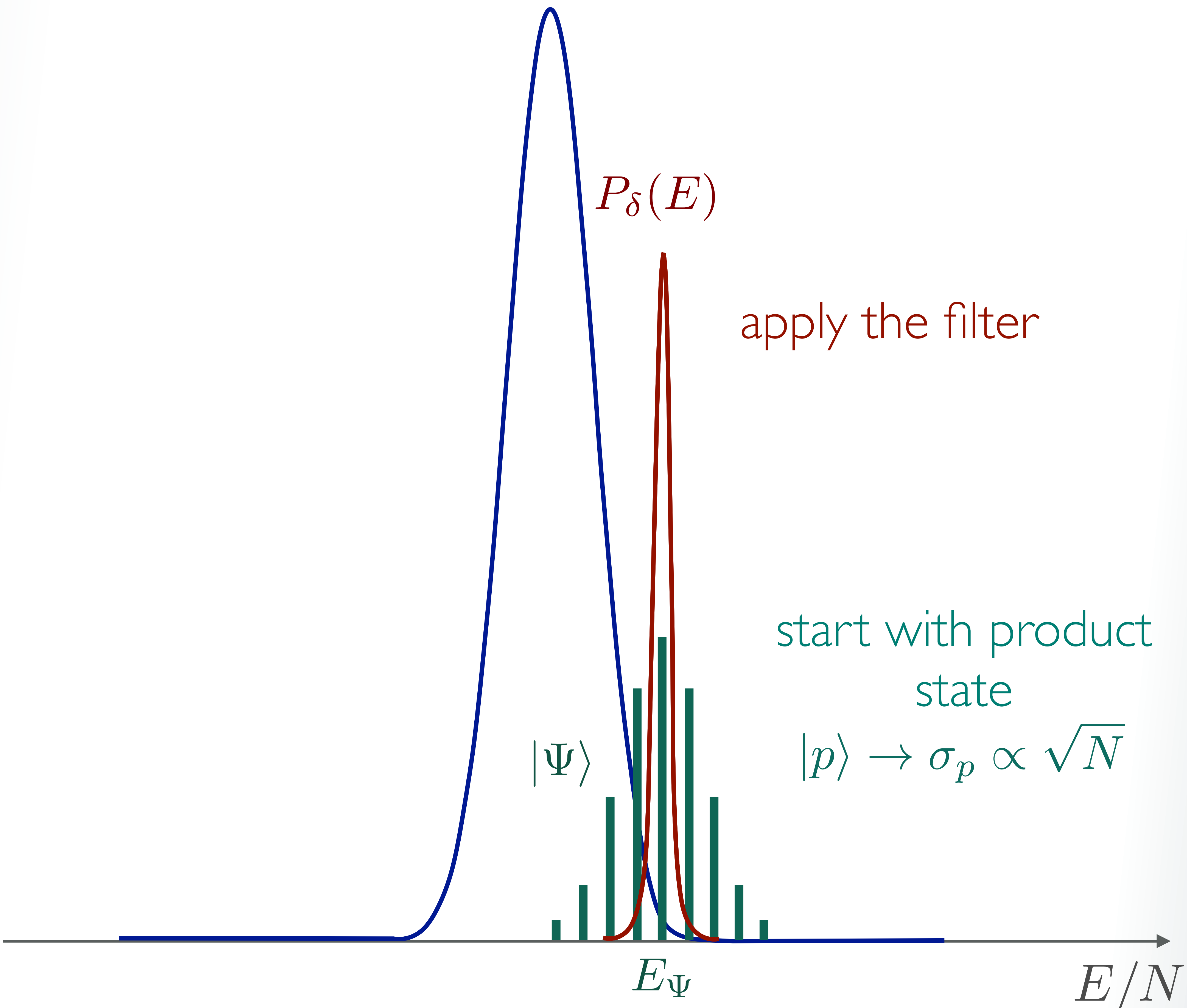


start with product state

$|p\rangle \to \sigma_p \propto \sqrt{N}$

Can we prepare a filtered state?



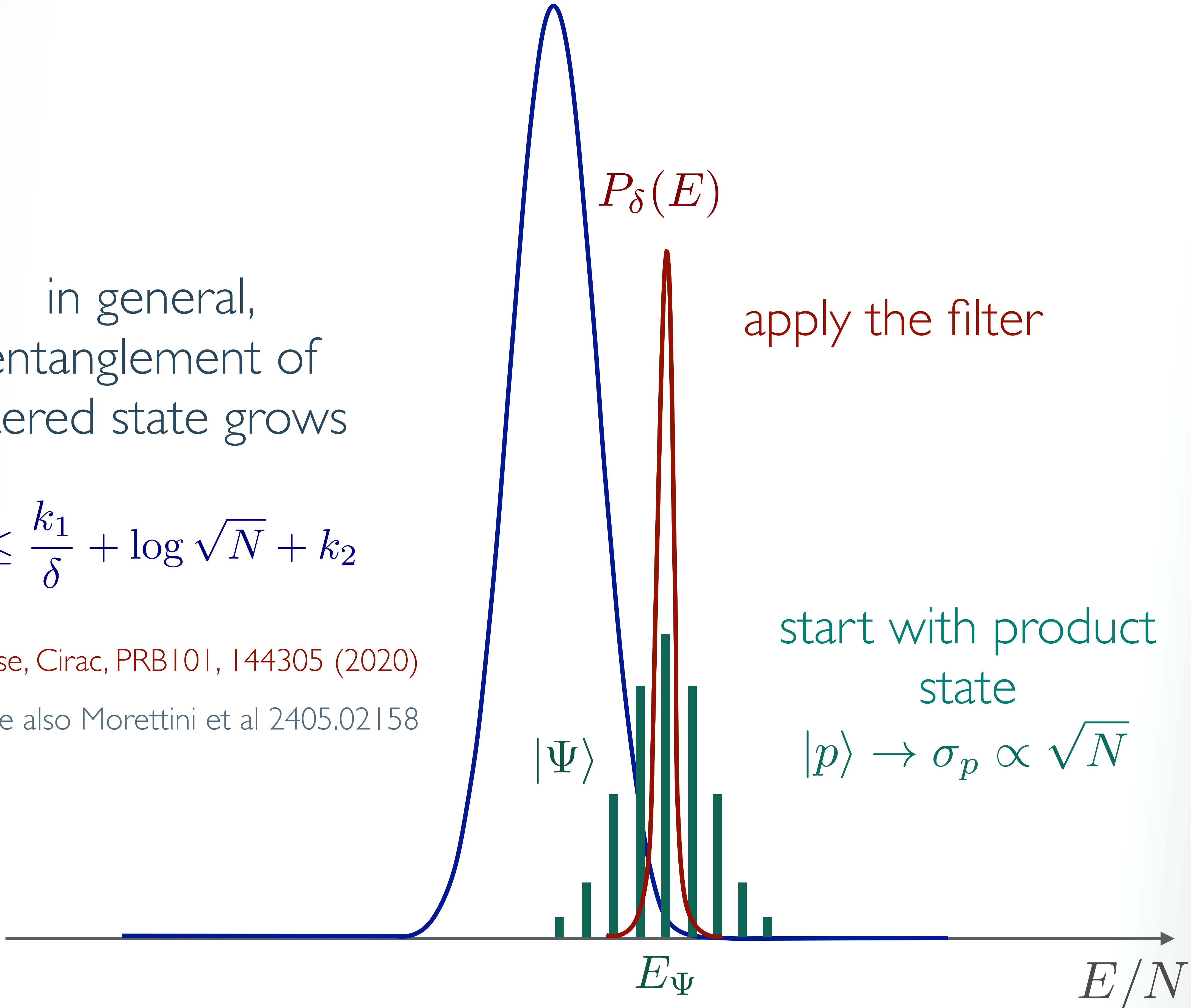
Can we prepare a filtered state?

in general, entanglement of filtered state grows

$$S \leq \frac{k_1}{\delta} + \log\sqrt{N} + k_2$$

MCB, Huse, Cirac, PRB101, 144305 (2020)

see also Morettini et al 2405.02158



apply the filter

start with product state

$|p\rangle \to \sigma_p \propto \sqrt{N}$

reducing the energy variance costs entanglement

IDEA:

$$\exp\left[-\frac{(H-E)^2}{2\delta^2}\right]|p\rangle \approx \sum_{m=-R}^{R} c_m e^{-i2mE/\alpha} e^{i2mH/\alpha}|p\rangle$$

PRB 101, 144305 (2020)

reducing the energy variance costs entanglement

IDEA:

1. reduce the number of terms (overlap)

Hartmann et al., Lett. Math. Phys. 2004

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2. each term bounded $S \Rightarrow D$

van Acoleyen et al. PRL 2013

PRB 101, 144305 (2020)

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3. sum has bounded $D \Rightarrow S$

$$D \leq C\sqrt{N}\left(D_0^{1/\delta} - 1\right)$$

$$S \leq \frac{k_1}{\delta} + \log\sqrt{N} + k_2$$

PRB 101, 144305 (2020)

reducing the energy variance costs entanglement

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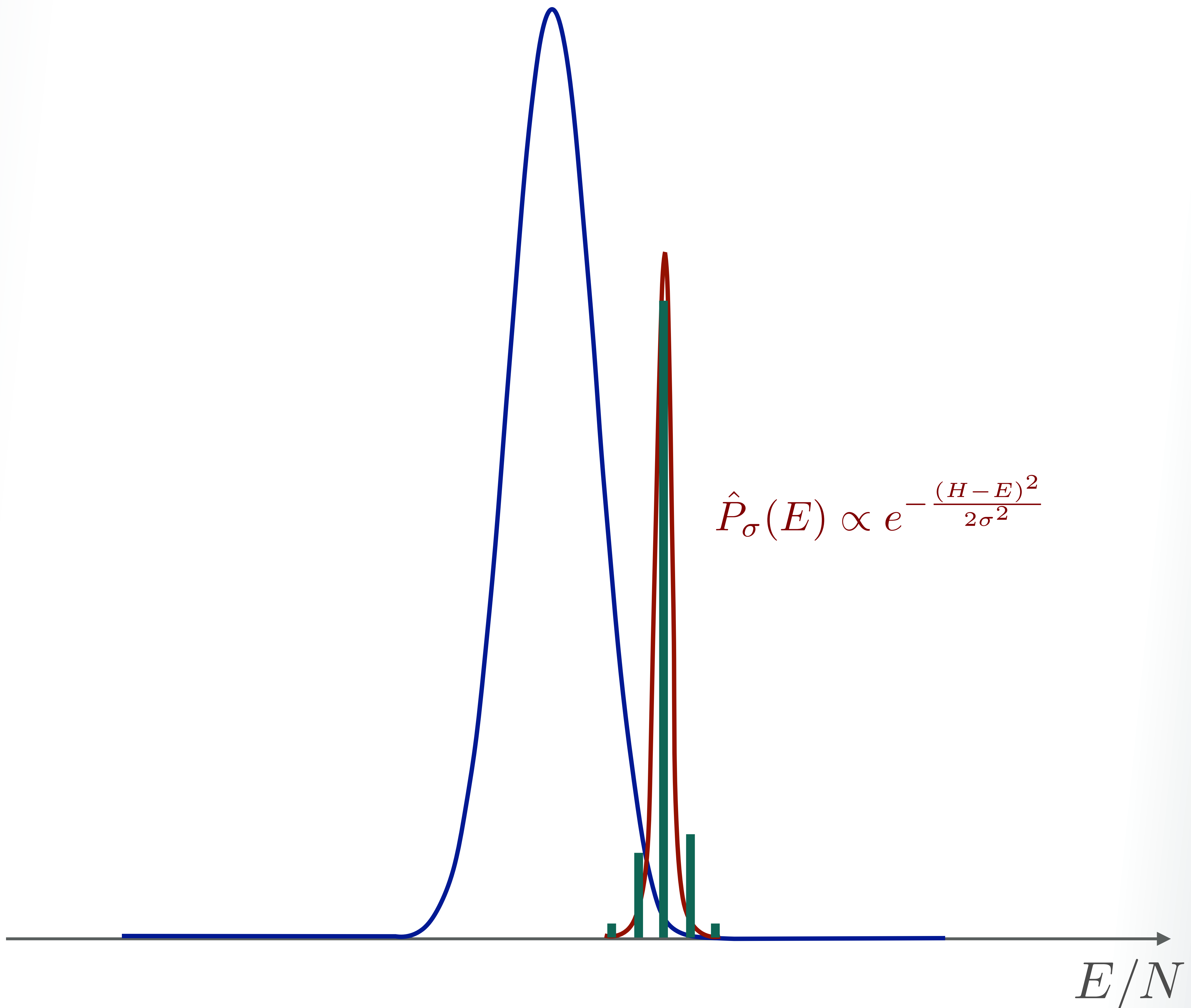
MPS could reach

$\delta^{-1} \sim O(\log N)$

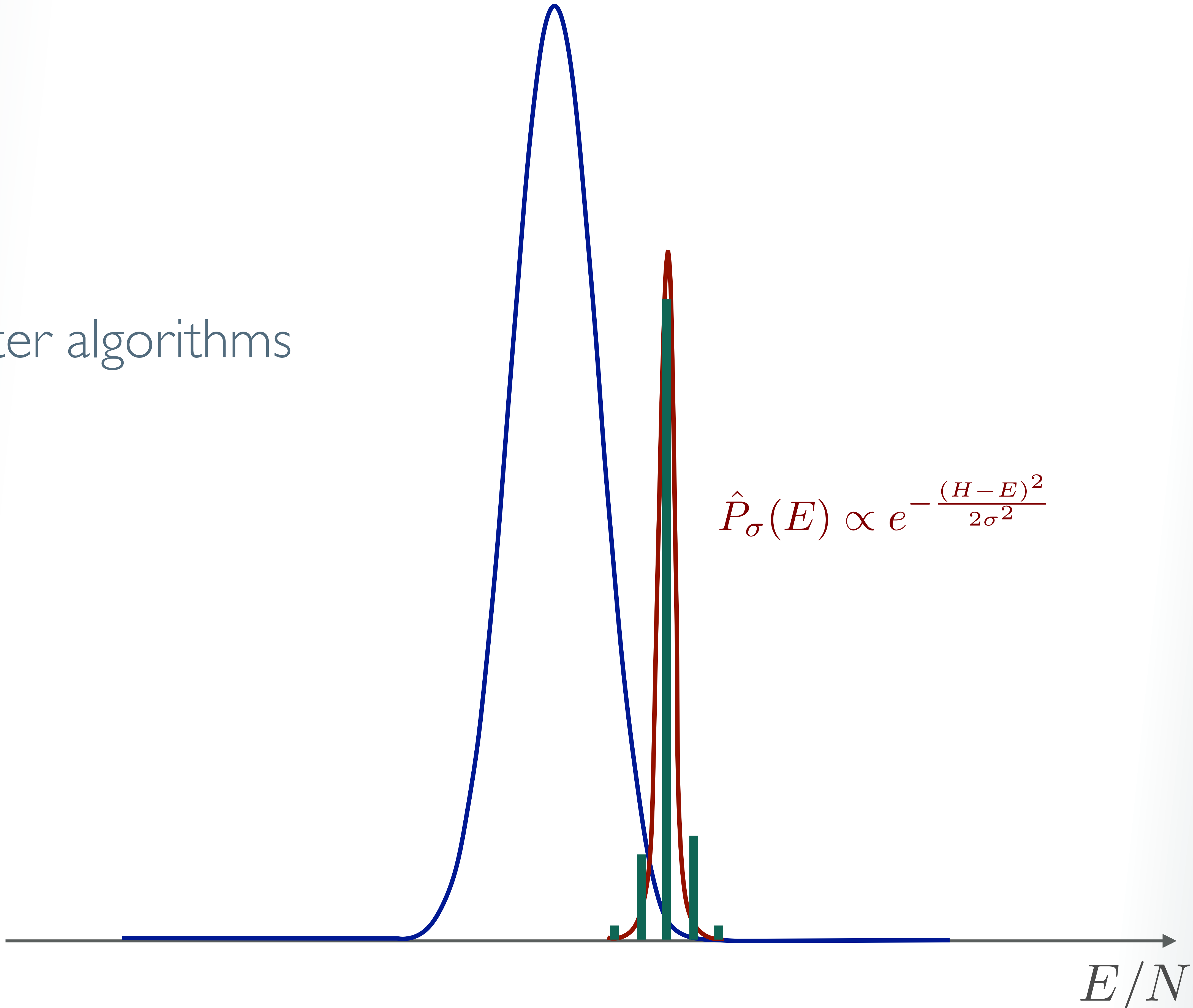
PRB 101, 144305 (2020)

Can we compute the properties of this state?



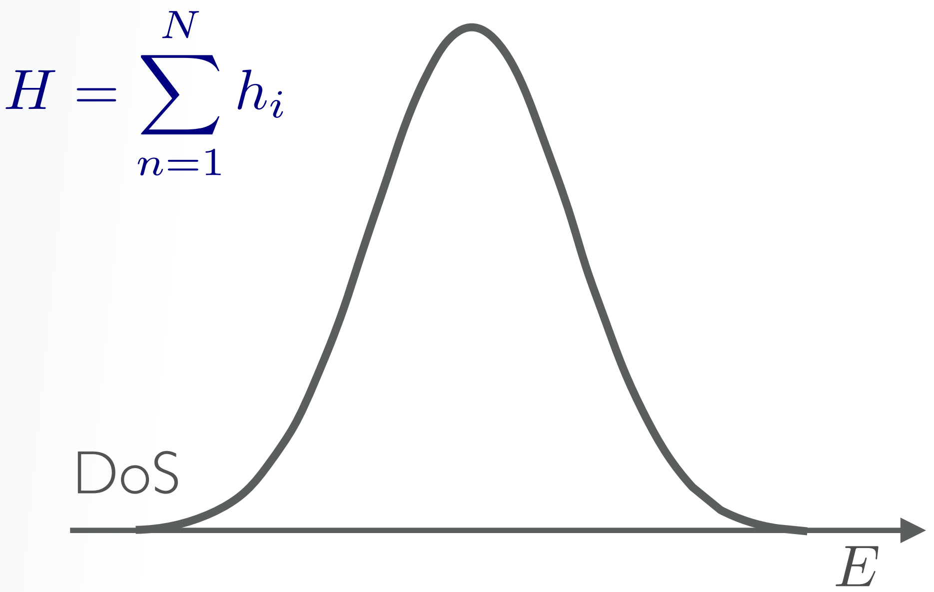
Can we compute the properties of this state?

filter algorithms



energy filter

1 filtering a state



Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

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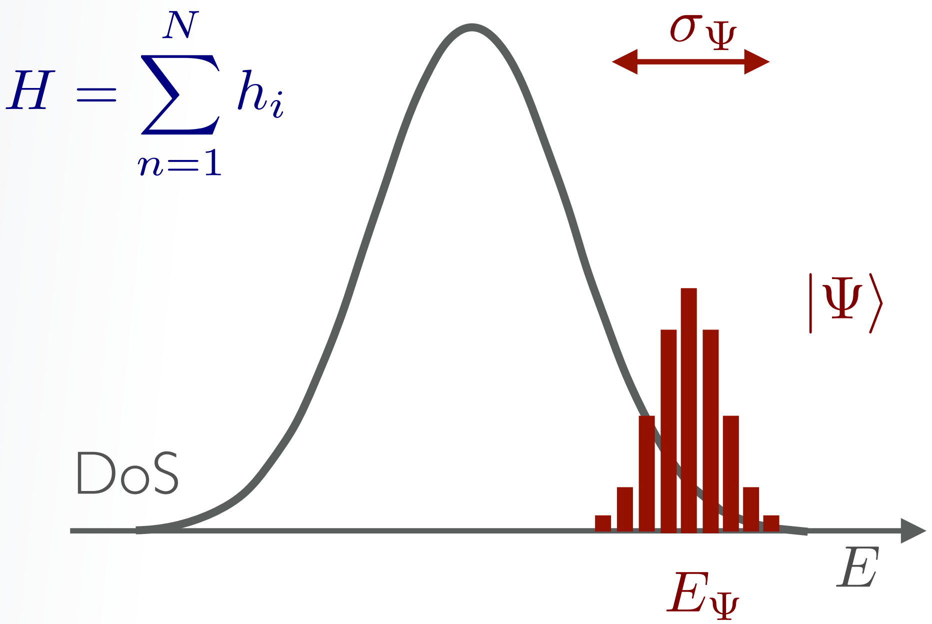

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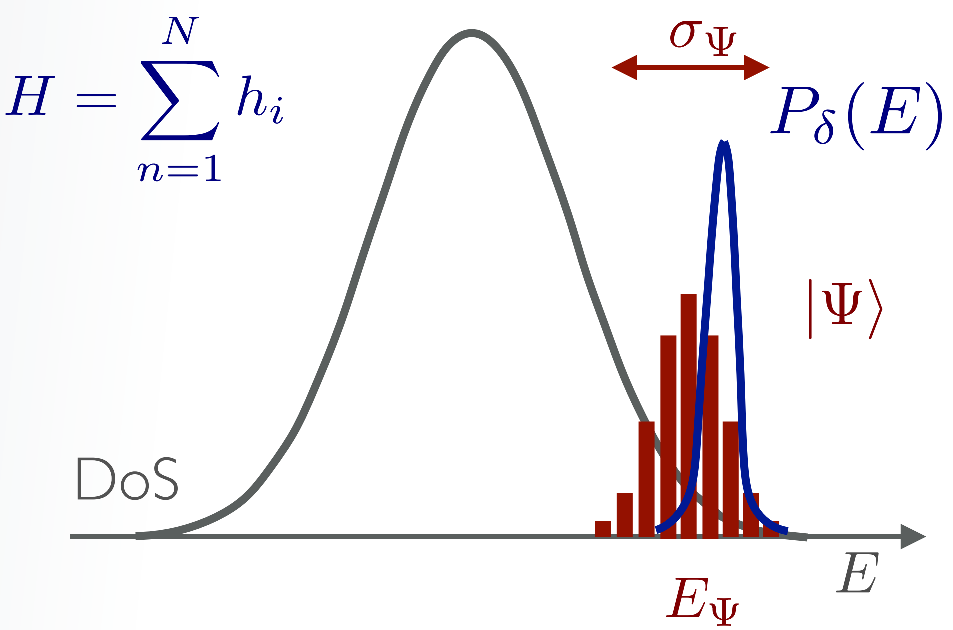

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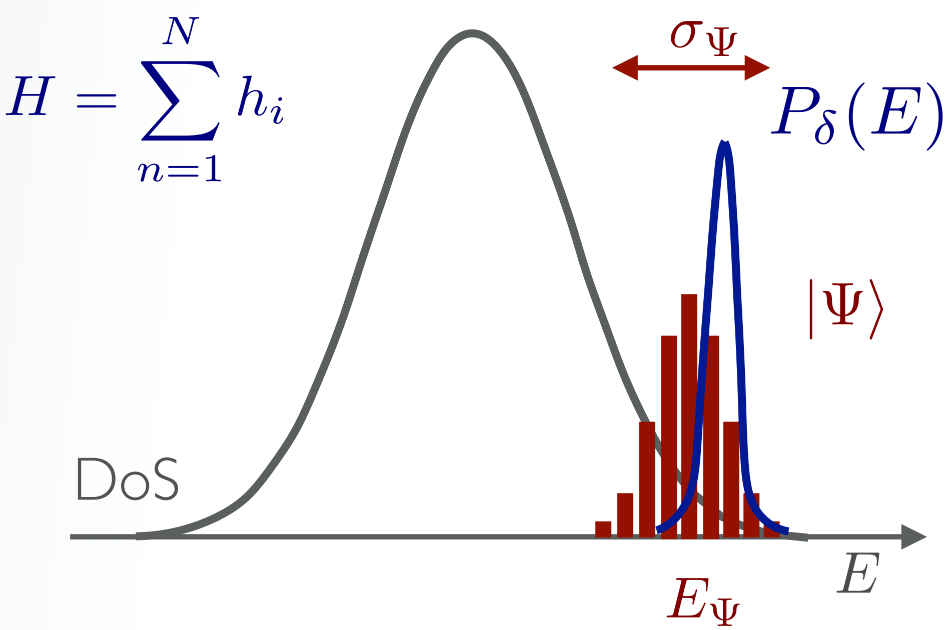
energy filter

1 filtering a state

decrease energy variance ⇒ microcanonical

$$\langle P_\delta(E)\Psi|O|P_\delta(E)\Psi\rangle \Rightarrow O(E)$$

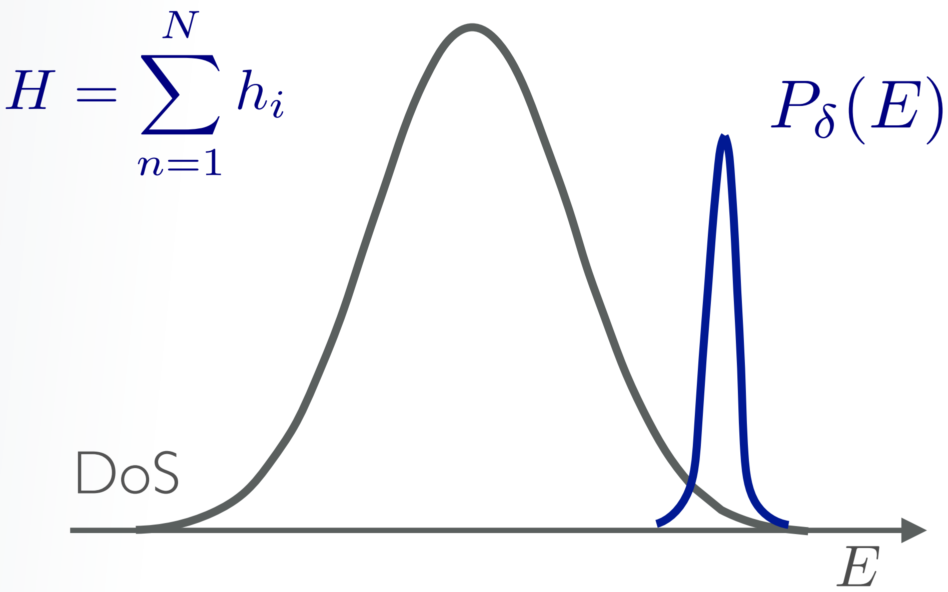
$$\langle\Psi|P_\delta(E)|\Psi\rangle \quad \Rightarrow \text{LDOS}$$



Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

energy filter

2 filter as ensemble



Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

energy filter

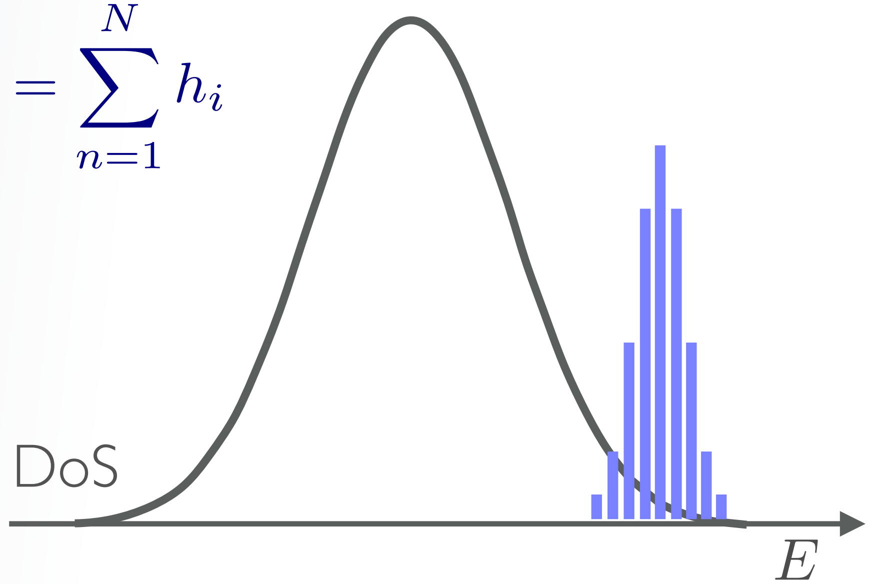
2 filter as ensemble

diagonal in energy eigenbasis ⇒ microcanonical

$$\frac{\mathrm{tr}\left(OP_\delta(E)\right)}{\mathrm{tr}P_\delta(E)} \Rightarrow O(E)$$

$$\mathrm{tr}P_\delta(E) \Rightarrow \text{DOS}$$

$$H = \sum_{n=1}^{N} h_i$$



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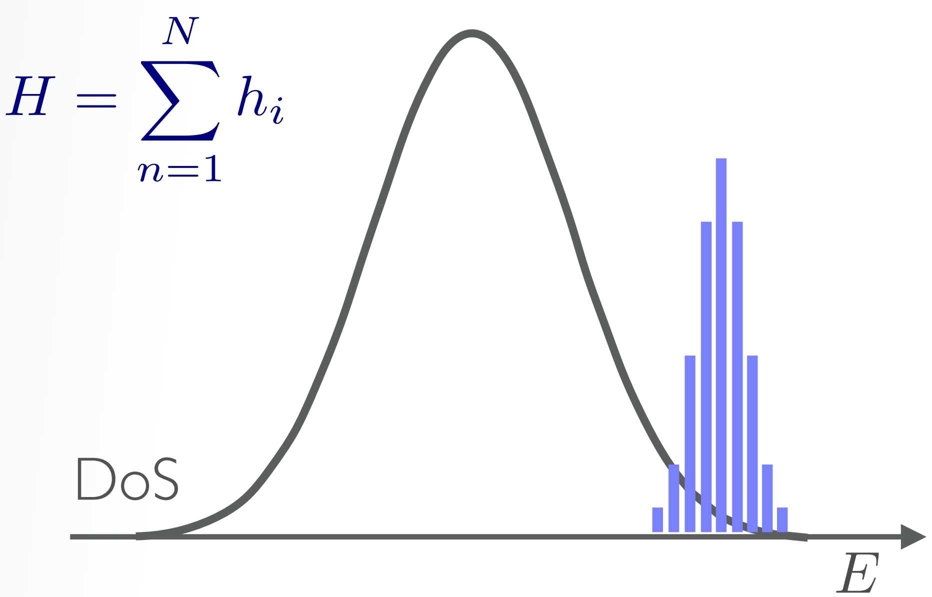

equivalent to diagonal ensemble of a certain pure state

Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

energy filter

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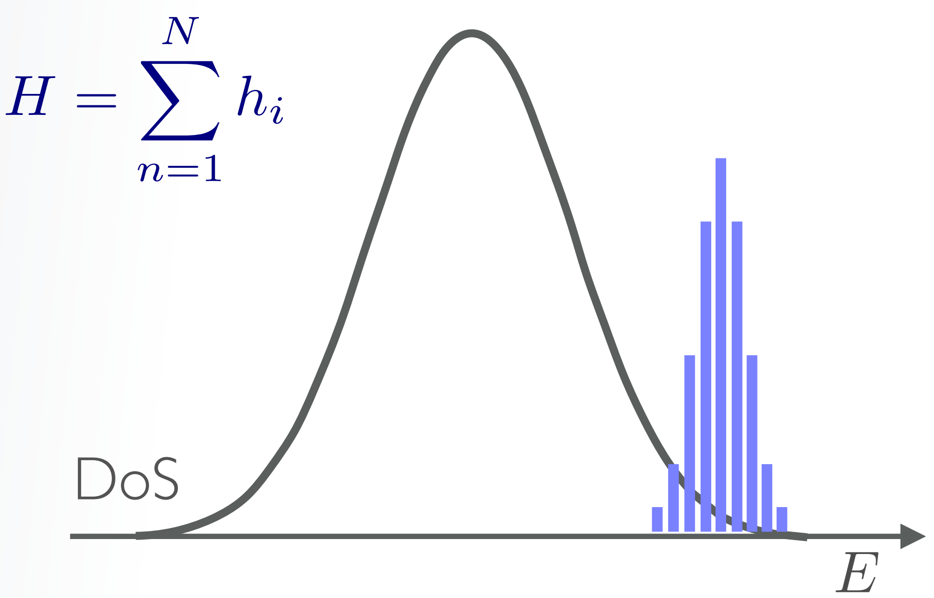

equivalent to diagonal ensemble of a certain pure state

reached only after long time evolution

Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

computing observables

Gaussian filter ⇒ approximated by series of evolutions

$$\exp\left[-\frac{(H-E)^2}{2\delta^2}\right] \approx \sum_{m=-R}^{R} c_m e^{-i2mE/\alpha} e^{i2mH/\alpha}$$

Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

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largest time $t_{\max} = \frac{2x}{\delta}$

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quantum inspired classical method

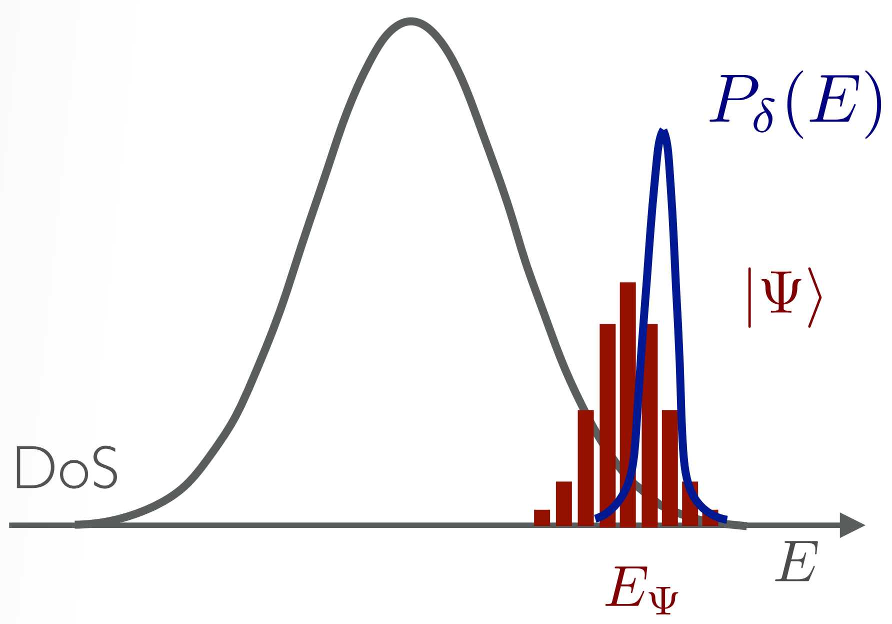
Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

computing observables

e.g. (broadened) local density of states

$$D_{\delta,\Psi}(E) = \langle\Psi|P_\delta(E)|\Psi\rangle$$

$$P_\delta(E) = \sum_{m=-R}^{R} c_m e^{-i(H-E)t_m} \qquad R = xN/\delta \qquad t_m = 2m/N$$



Lu et al. PRX Quantum 2, 02032 (2021)

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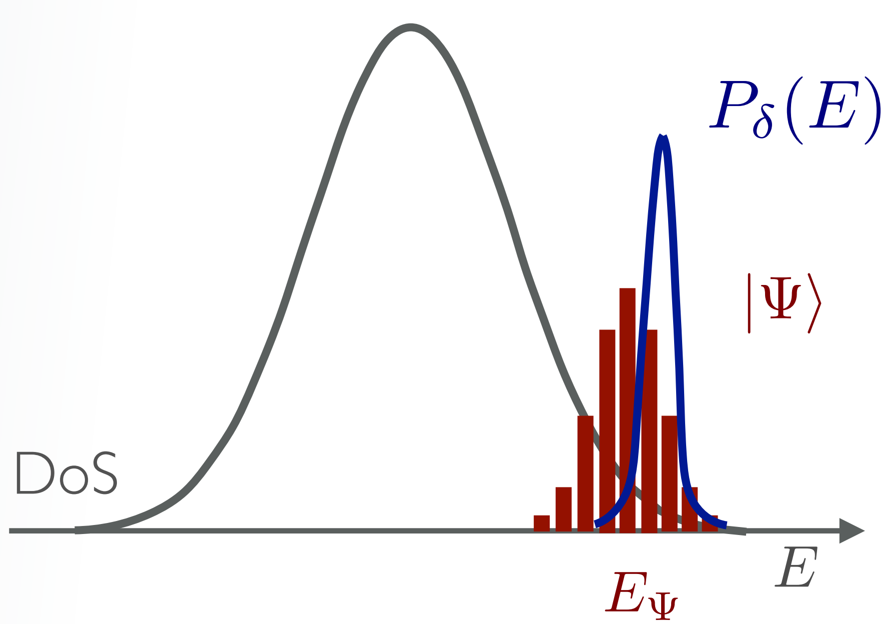
$$t_m = 2m/N$$

$$D_{\delta,\psi}(E) = \sum_{m=-R}^{R} c_m a_\psi(t_m) e^{iEt_m}$$

$$\langle\Psi|e^{-iHt_m}|\Psi\rangle$$



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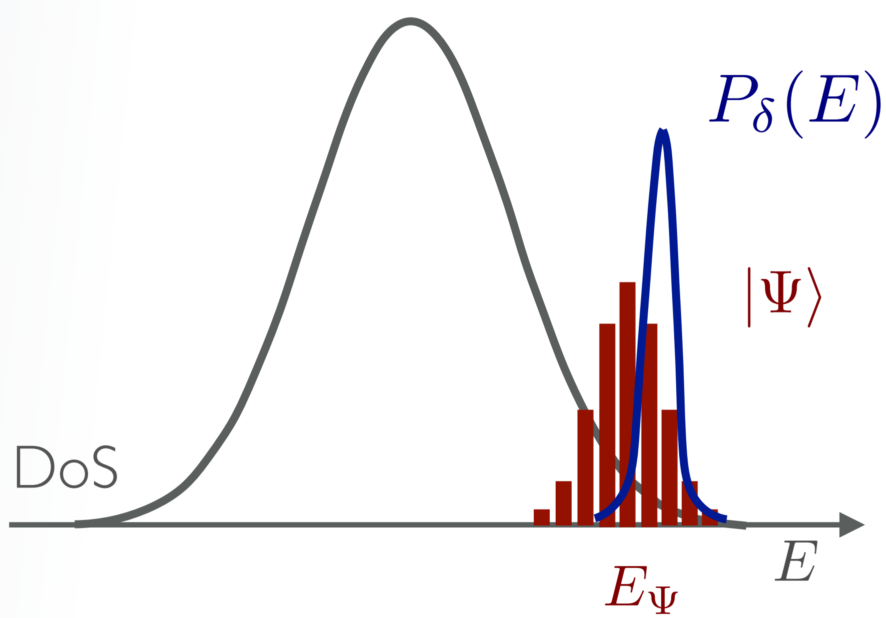


Q simulator: prepare state, evolve, measure

$$t_{\max} \propto \frac{1}{\delta}$$

Lu et al. PRX Quantum 2, 02032 (2021)

computing observables

can compute observables:

$$\tilde{A}_{\delta,\Psi}(E) = \frac{\langle\Psi|P_\delta(E) A P_\delta(E)|\Psi\rangle}{\langle\Psi|P_\delta(E)^2|\Psi\rangle}$$

potential problem: denominator too small

shown to be large enough in vicinity of E_Ψ

Lu et al. PRX Quantum 2, 02032 (2021)

computing observables

can compute observables:

$$\tilde{A}_{\delta,\Psi}(E) = \frac{\langle\Psi|P_\delta(E)AP_\delta(E)|\Psi\rangle}{\langle\Psi|P_\delta(E)^2|\Psi\rangle}$$

potential problem: denominator too small

shown to be large enough in vicinity of E_Ψ

better convergence

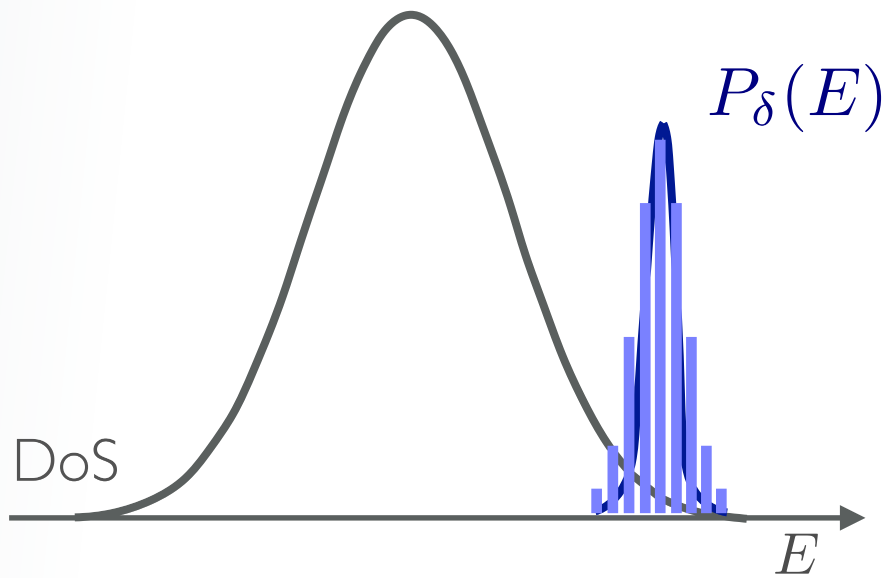
$$A_\delta(E) = \frac{\mathrm{tr}[AP_\delta(E)]}{\mathrm{tr}[P_\delta(E)]}$$

Lu et al. PRX Quantum 2, 02032 (2021)

computing observables

expectation values in filter ensemble

$$A_\delta(E) = \frac{\mathrm{tr}[A P_\delta(E)]}{\mathrm{tr}[P_\delta(E)]}$$

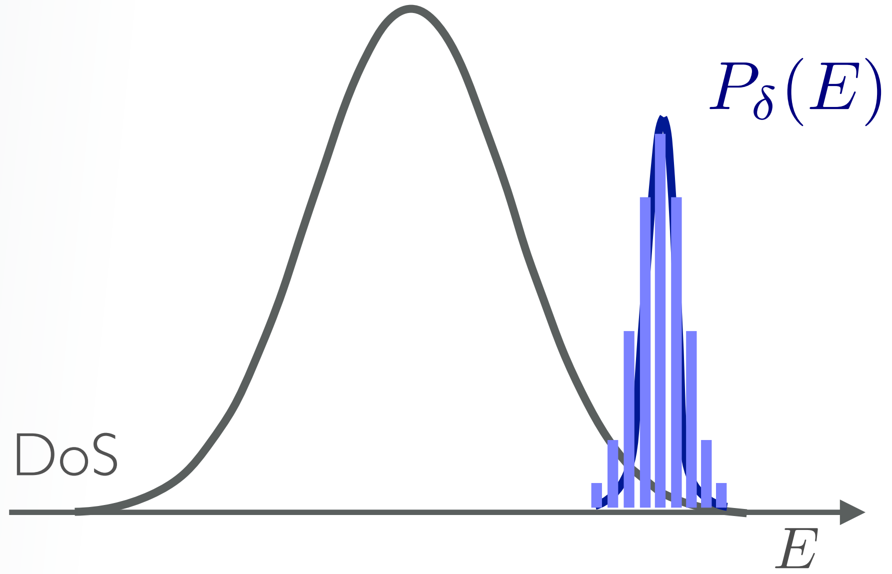


Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

algorithm

can be computed using Monte Carlo sampling

$$A_\delta(E) = \frac{\sum_\Psi \langle\Psi|AP_\delta(E)|\Psi\rangle}{\sum_{\Psi'} \langle\Psi'|P_\delta(E)|\Psi'\rangle}$$



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importance sampling (classical)

Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

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computed by filter algorithm

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Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

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computed by filter algorithm

importance sampling (classical)

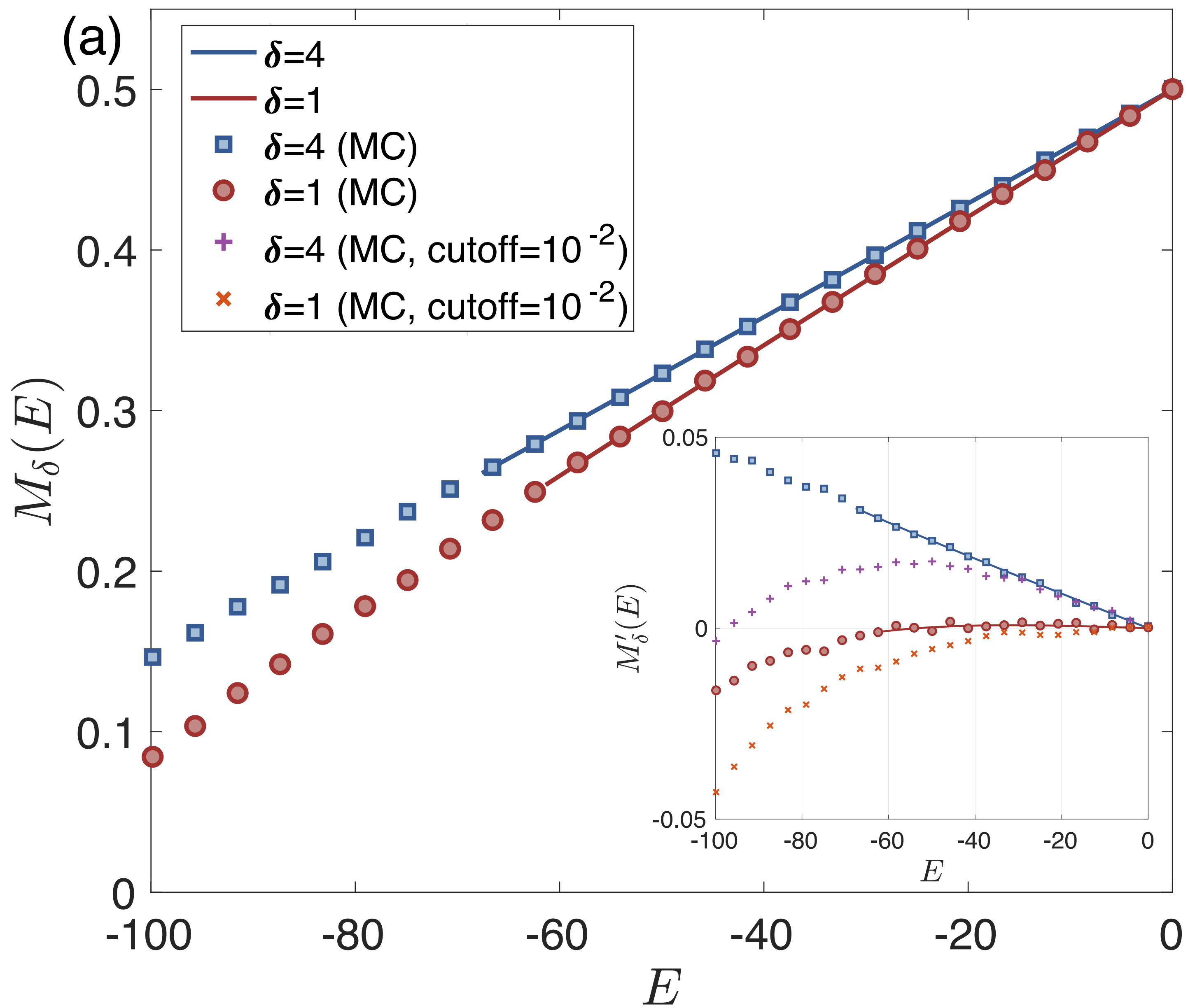
simulating classically with TNS we can reach $\delta \sim 1/\log N$

Lu et al. PRX Q2, 02032 (2021); Yang et al PRB 106, 024307 (2022)

hybrid strategy for microcanonical quantities

Ising model, N=100

$$M = \frac{1}{2N}\sum_{n=1}^{N}(\sigma_{n,z}+1)$$



Lu et al. PRX Quantum 2, 02032 (2021)

weak ETH probe: diagonal part

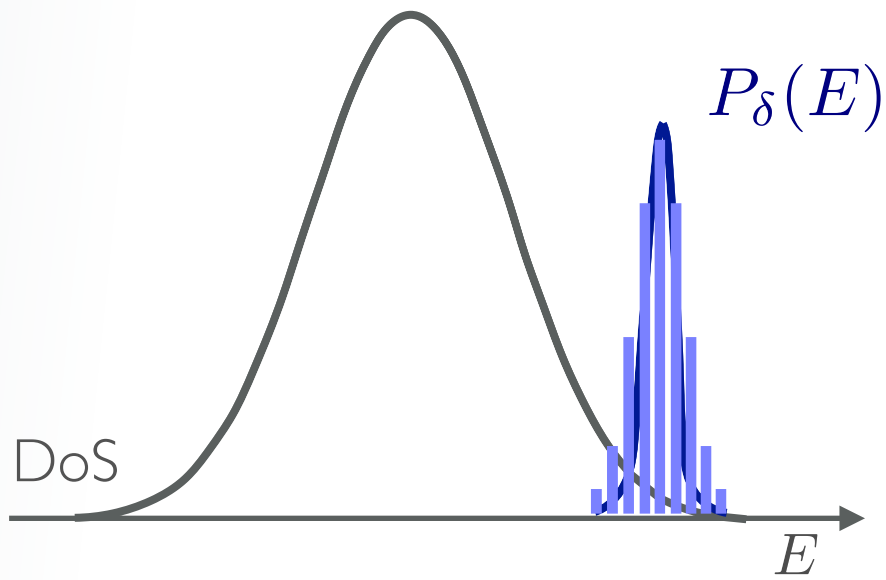
weak ETH probe: diagonal part

$$O_{\alpha\beta} = O(\bar{E})\delta_{\alpha\beta} + e^{-\frac{S(\bar{E})}{2}} f_O(\bar{E},\omega) R_{\alpha\beta}$$

converge to thermal for large systems

TNS simulation

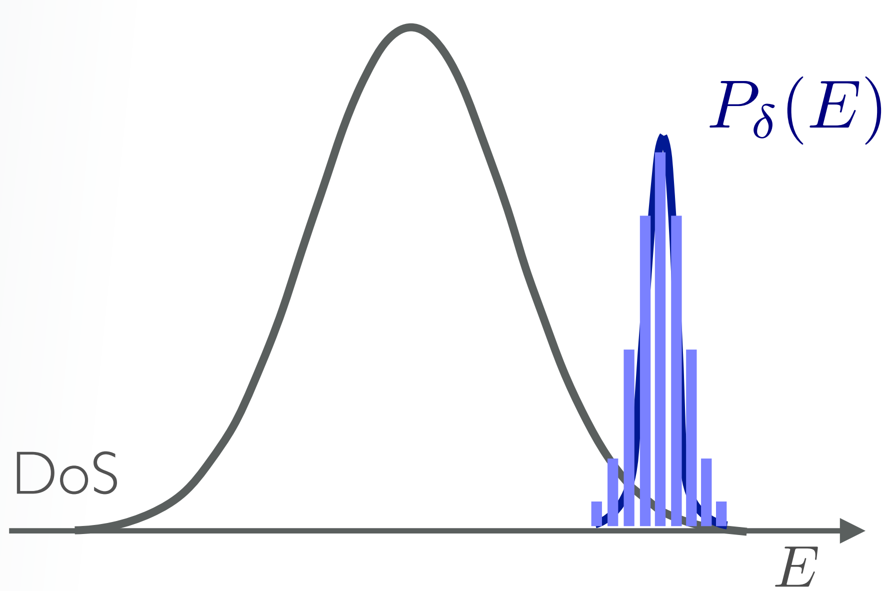
$$A_\delta(E) = \frac{\mathrm{tr}[AP_\delta(E)]}{\mathrm{tr}[P_\delta(E)]}$$



TNS simulation

$$A_\delta(E) = \frac{\mathrm{tr}[AP_\delta(E)]}{\mathrm{tr}[P_\delta(E)]}$$

ETH $\Rightarrow$ $$A_{nn} \sim A(E_n) + \delta \frac{dA}{dE}$$



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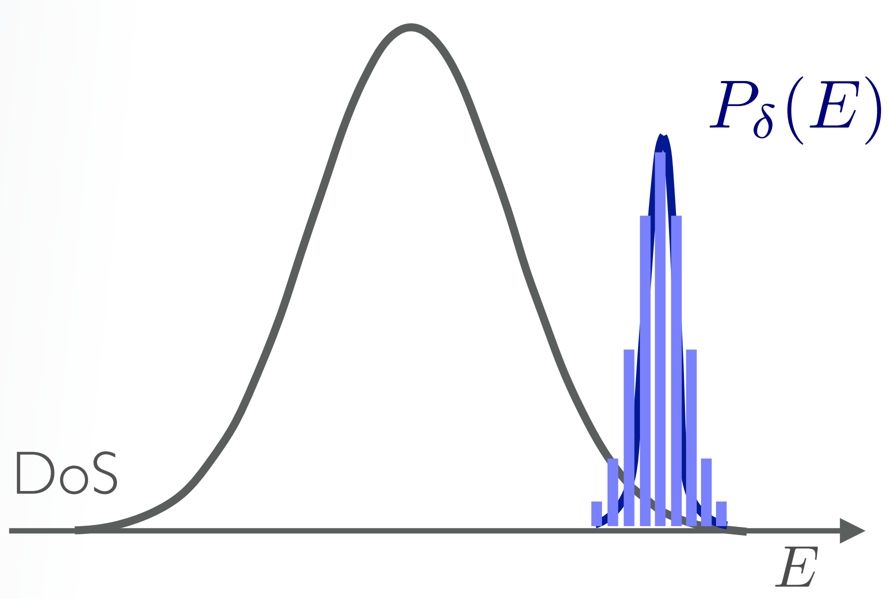


for intensive quantities

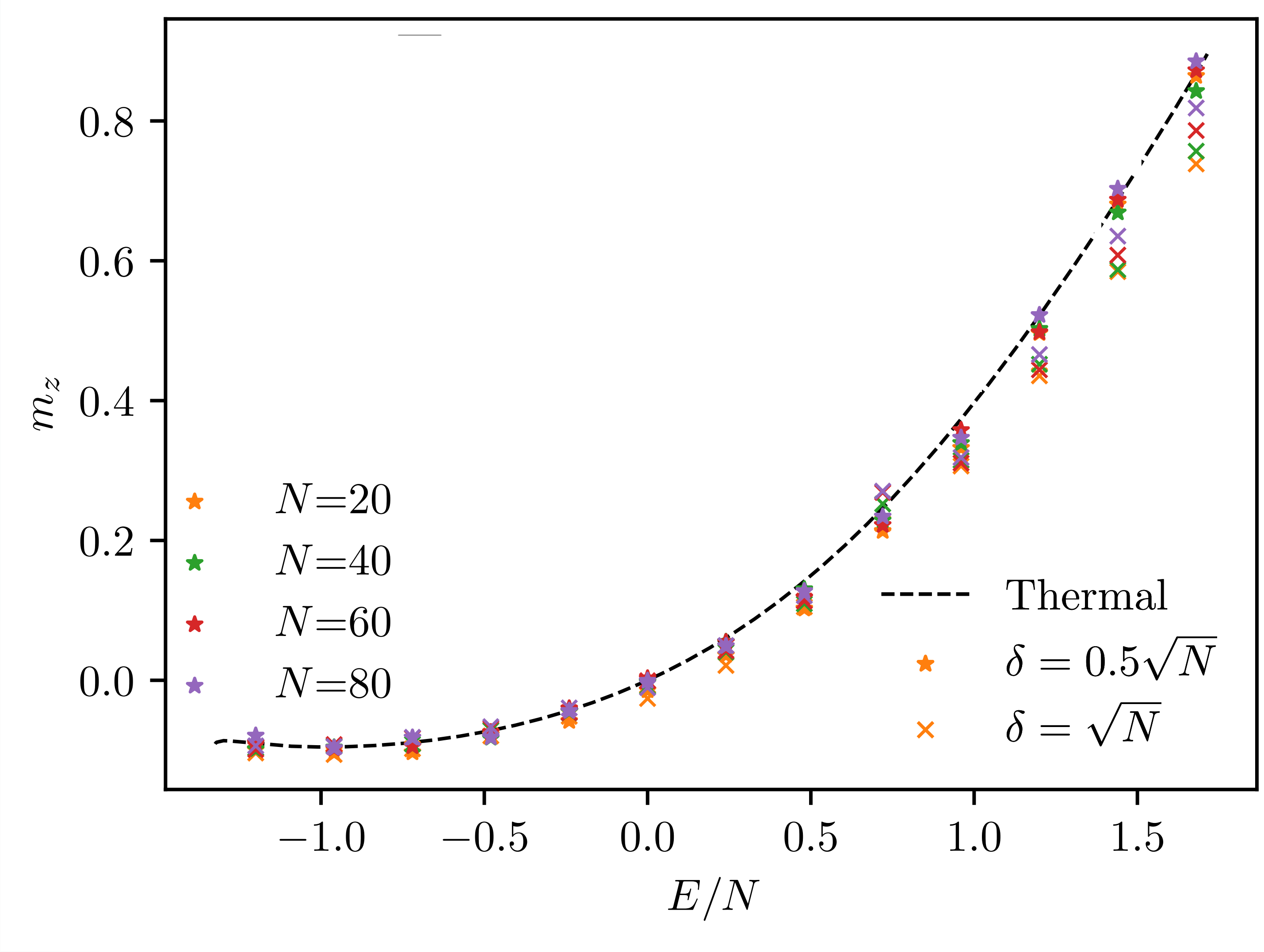
$\delta/N \to 0$ as $N \to \infty$

is enough for convergence to microcanonical test on non-integrable Ising chain

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

TNS simulation

non-integrable quantum Ising chain



microcanonical properties

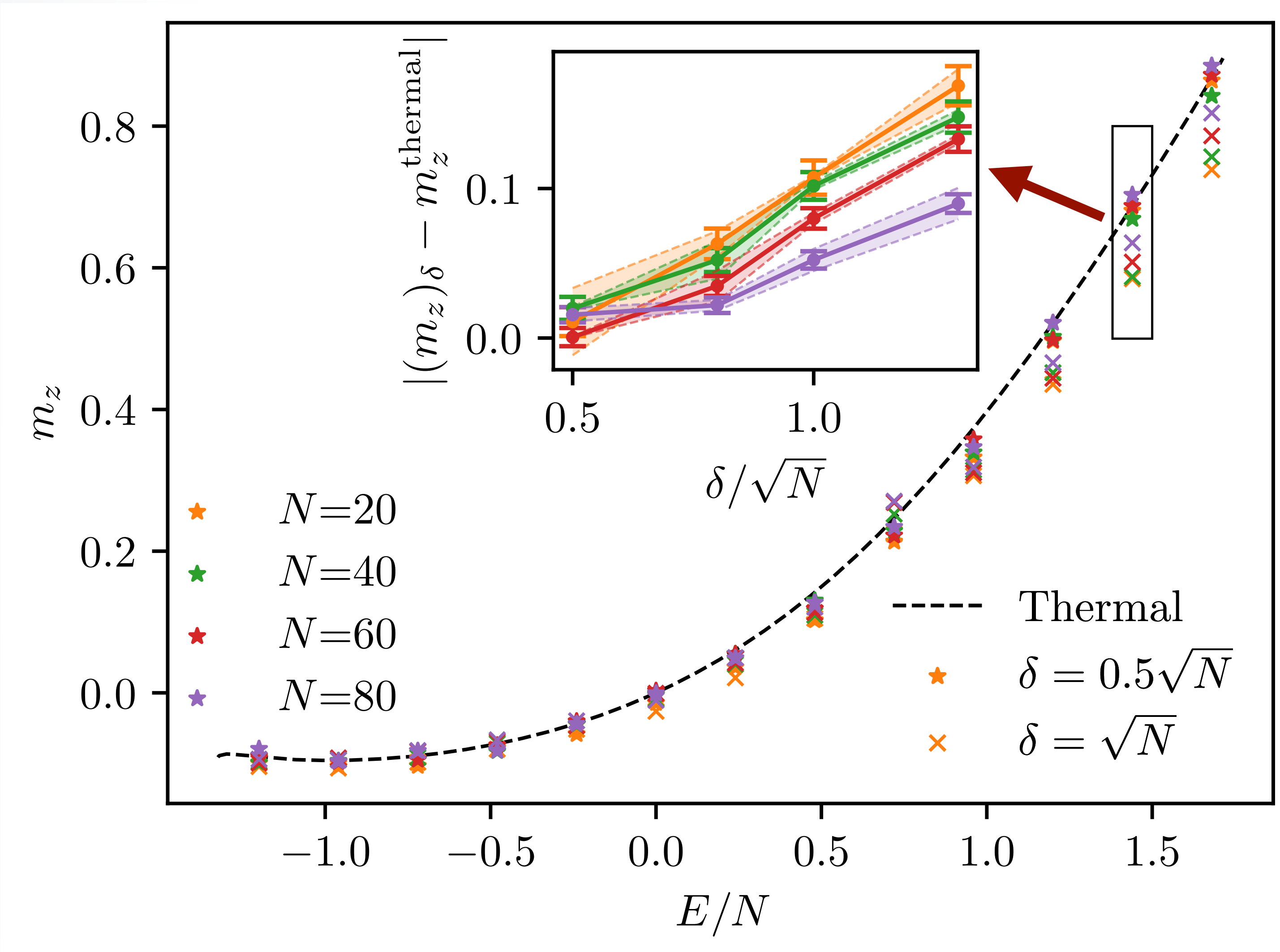
average magnetization

MPO + sampling over product states

Yang et al PRB 106, 024307 (2022)

TNS simulation

non-integrable quantum Ising chain



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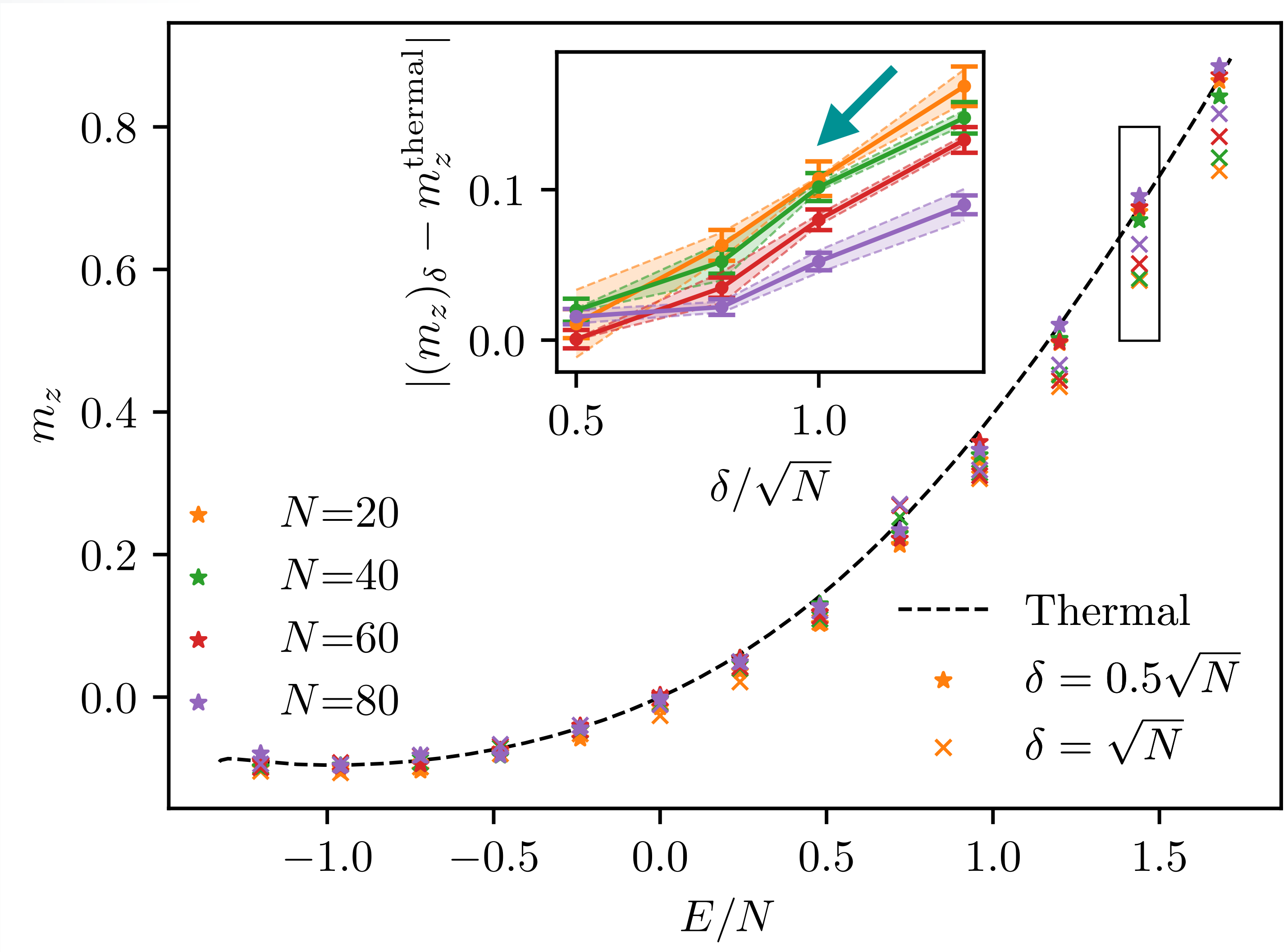

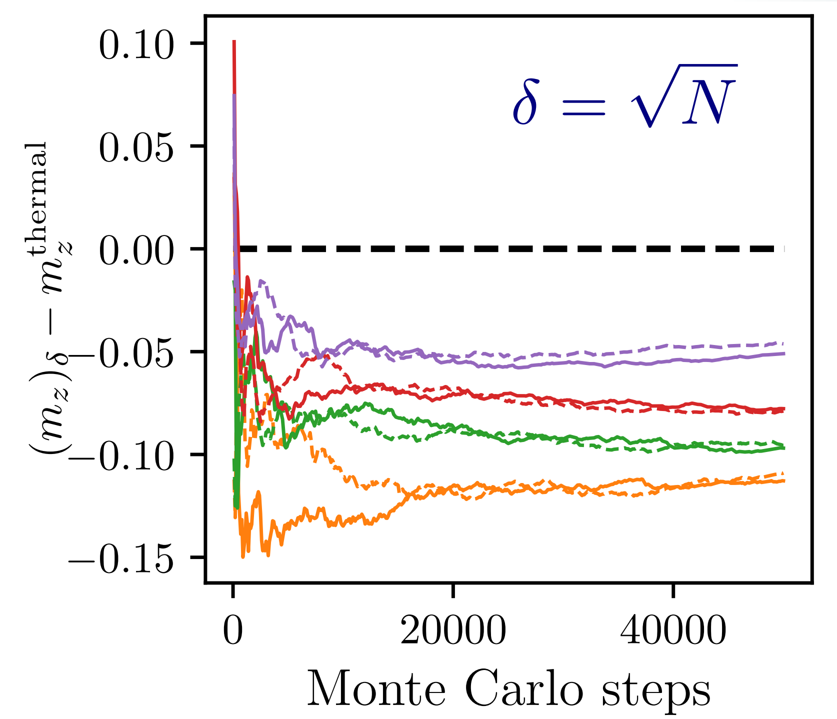

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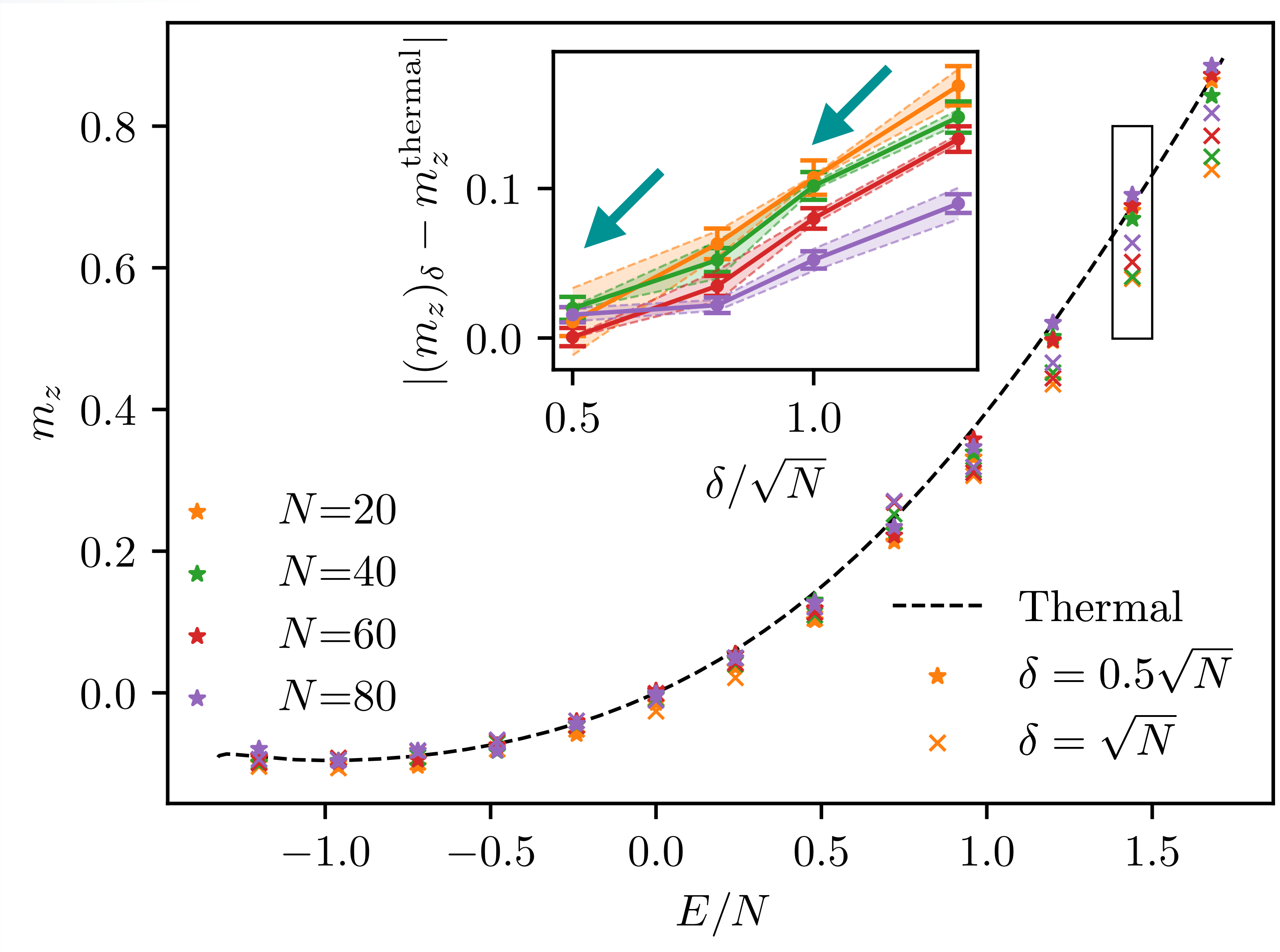

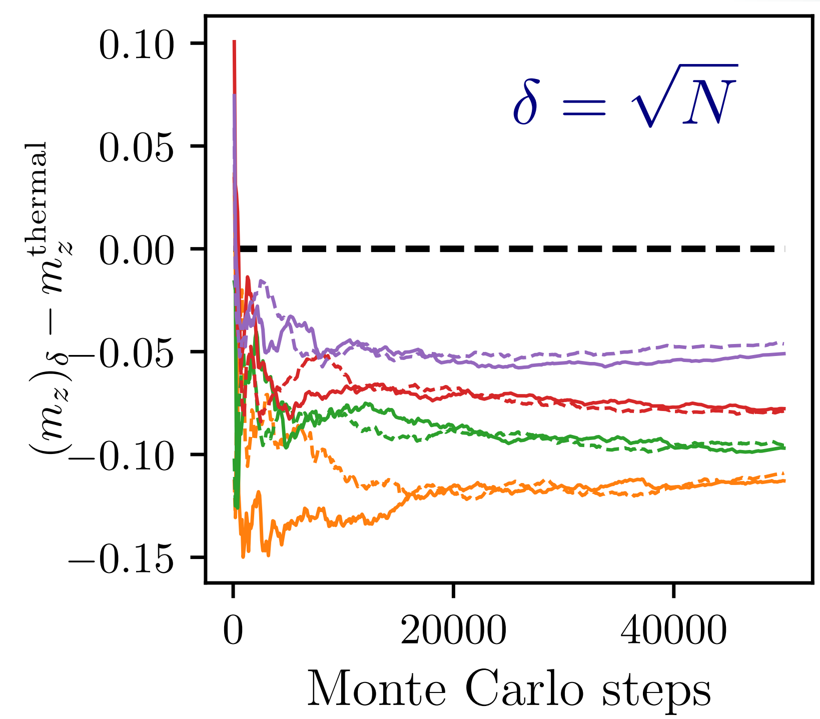

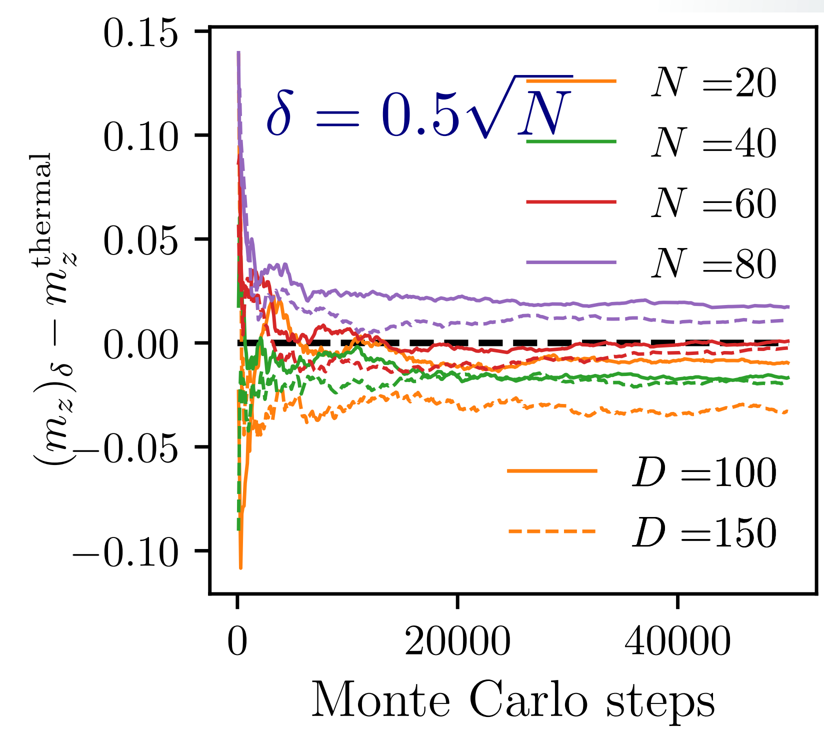

microcanonical properties

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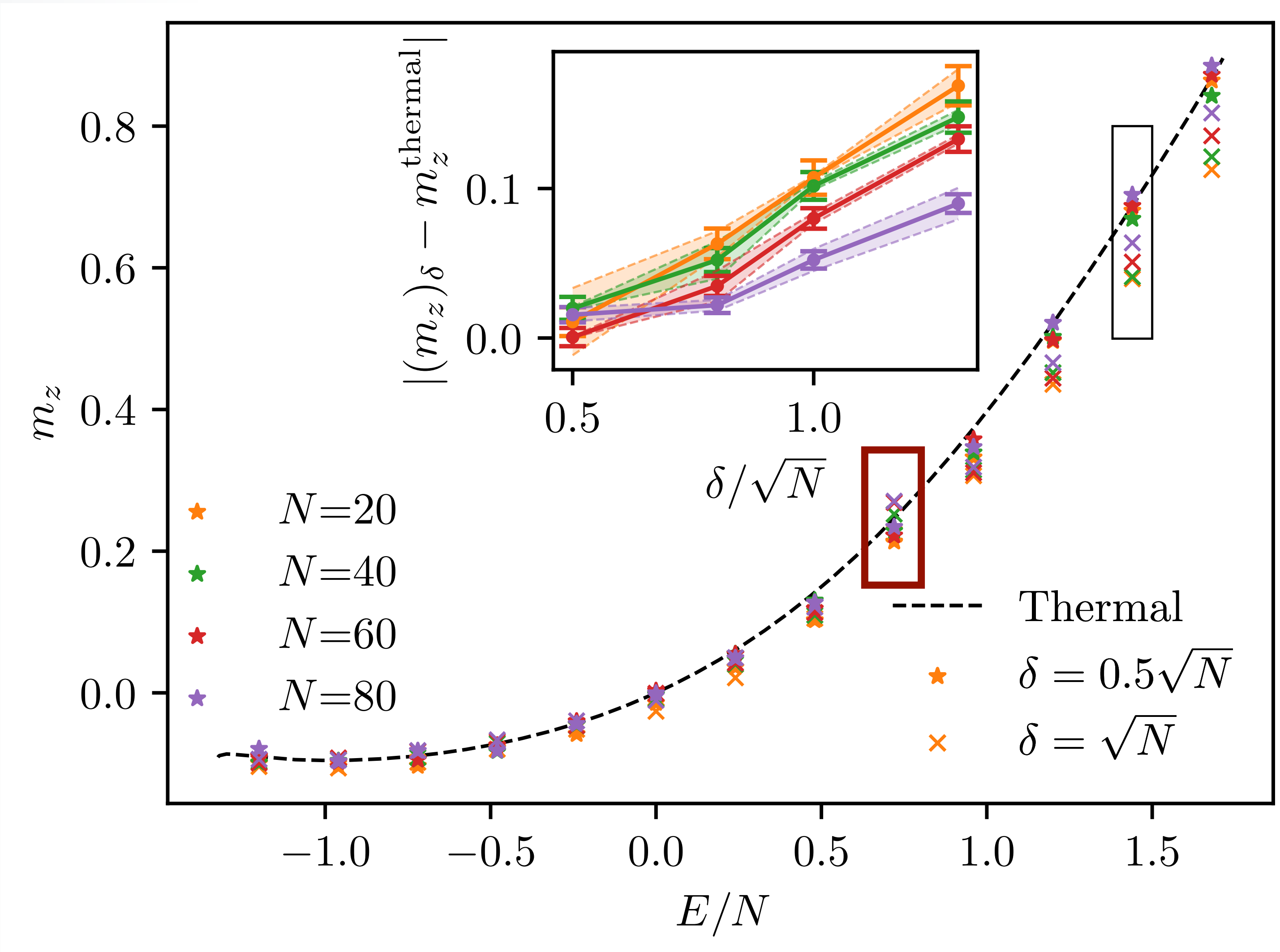
Yang et al PRB 106, 024307 (2022)

TNS simulation

non-integrable Ising model



microcanonical properties

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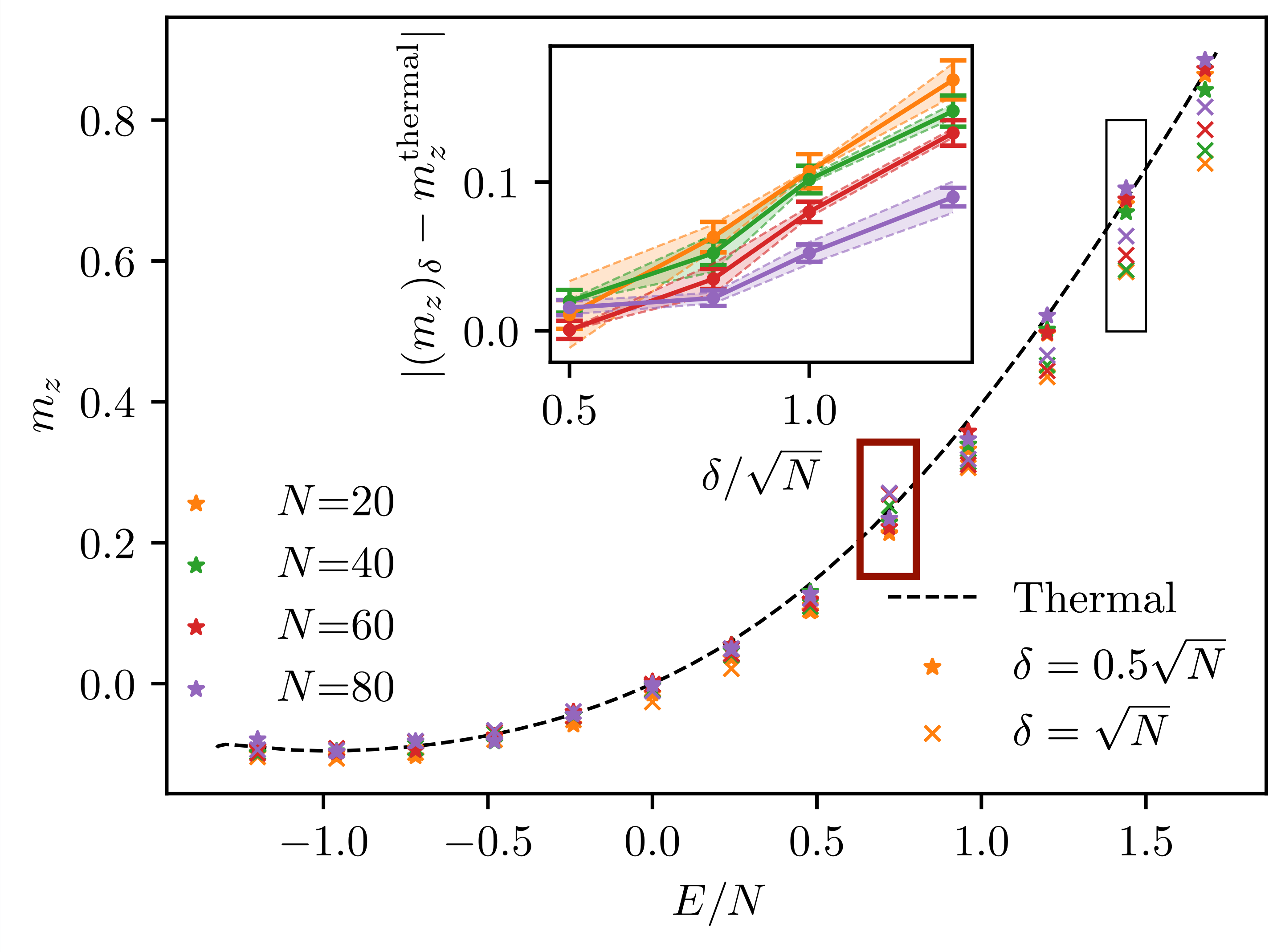
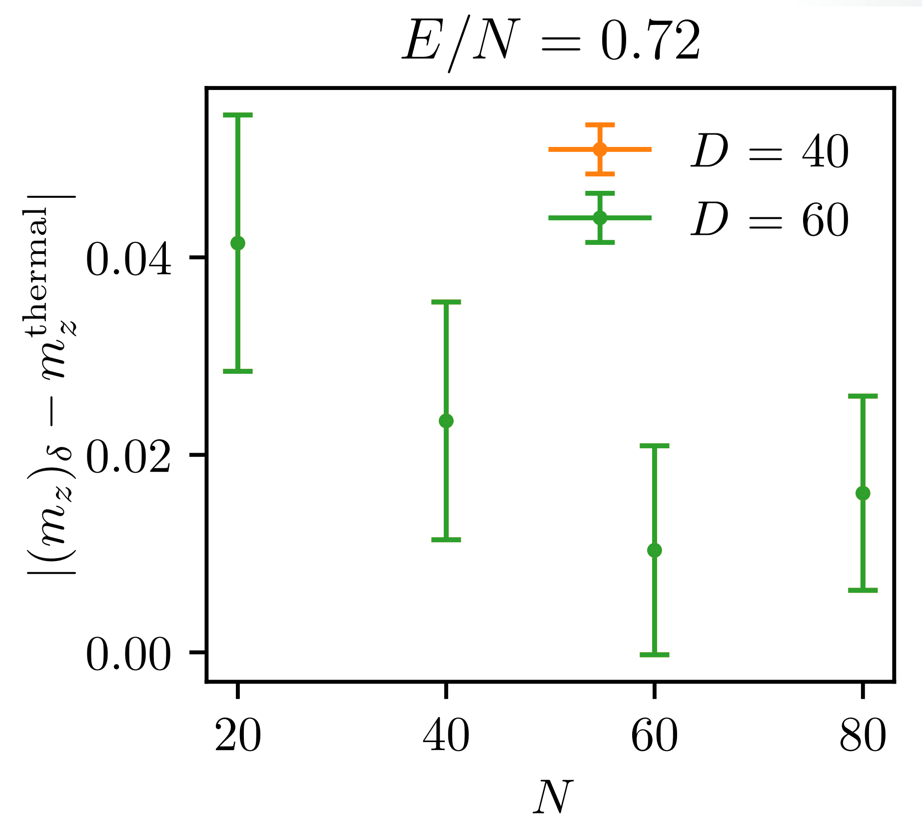


also sampling over product states and evolve MPS



microcanonical properties

average magnetization

Yang et al PRB 106, 024307 (2022)

more challenging: off-diagonal part of ETH more challenging: off-diagonal part of ETH

$$O_{\alpha\beta} = O(\bar{E})\delta_{\alpha\beta} + e^{-\frac{S(\bar{E})}{2}} f_O(\bar{E}, \omega) R_{\alpha\beta}$$

structure function

Luitz, Bar Lev, PRL2016; Mondaini, Rigol 2017; Brenes et al PRL2020, PRB 2020…; Schönle et al PRB2021; Essler, de Klerk, 2307.12410; ….

filter ensemble as ETH probe

function $f_O(\bar{E}, \omega)$ related to two-time correlators

Luo et al PRB 109, 134304 (2024)

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$$C_O(t) = \mathrm{tr}\left(\rho_E O(t) O(0)\right)$$

$$S_O(\omega) = \sum_{\alpha\beta} \rho_{\alpha\alpha} |O_{\alpha\beta}|^2 \delta(\omega - E_\beta + E_\alpha)$$

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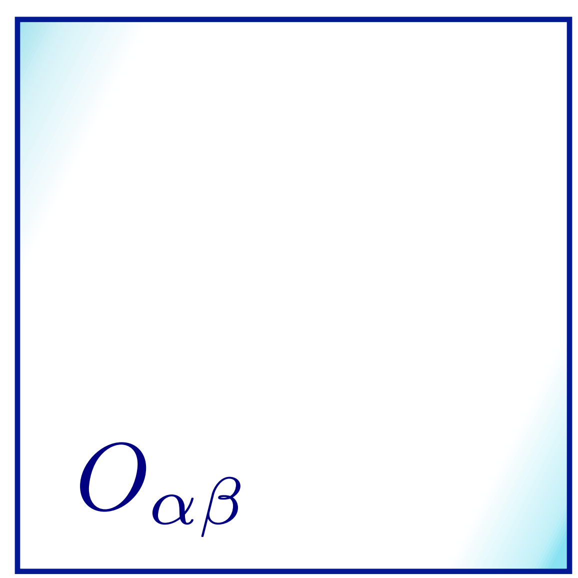

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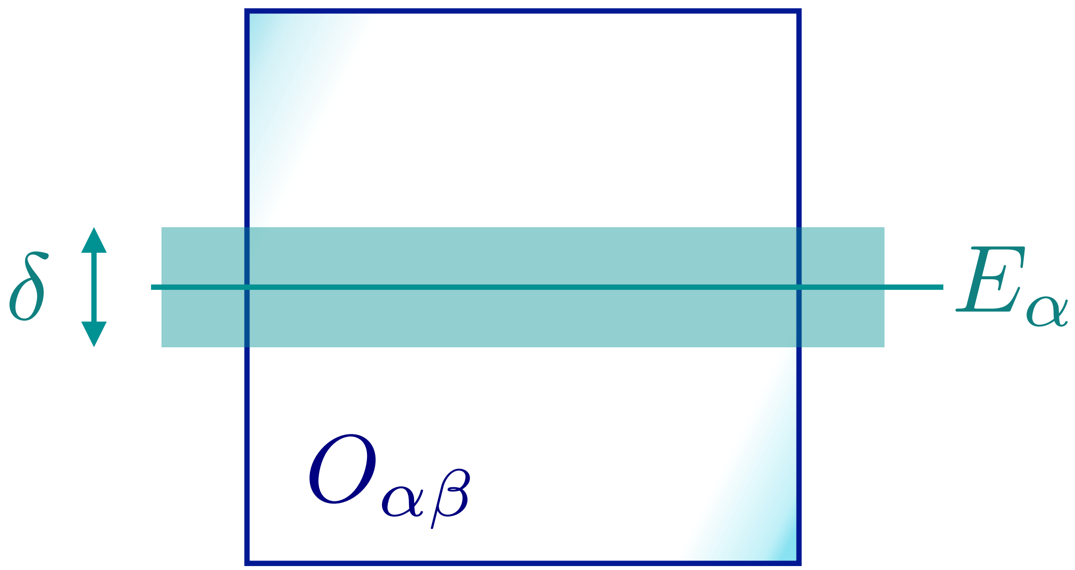

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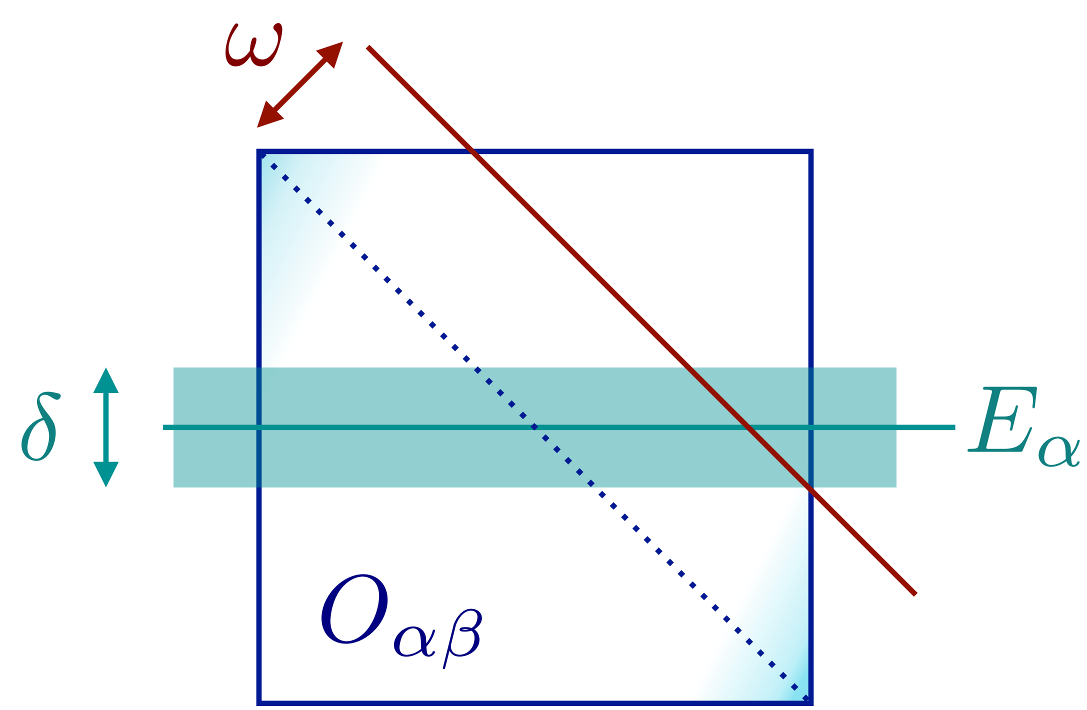

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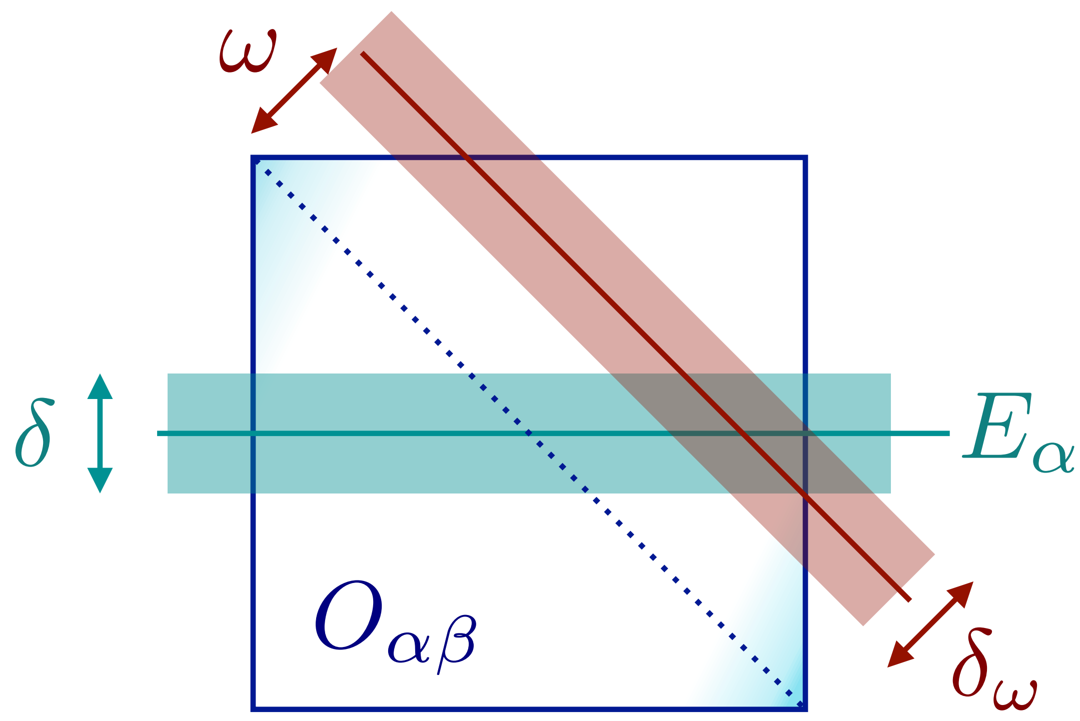

$P_{\delta_\omega}(\omega)$

filter in energy difference (commutator)

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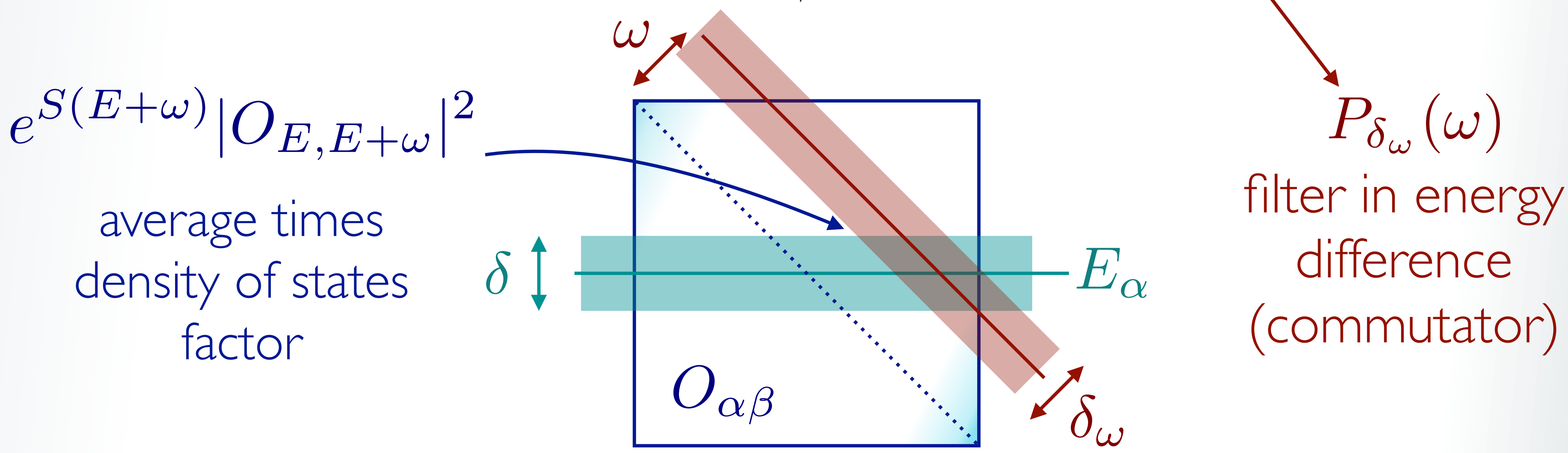

Luo et al PRB 109, 134304 (2024)

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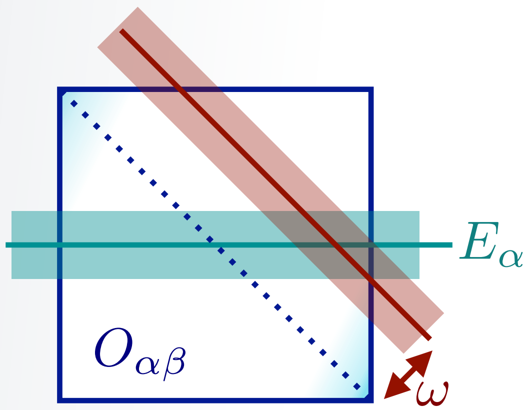


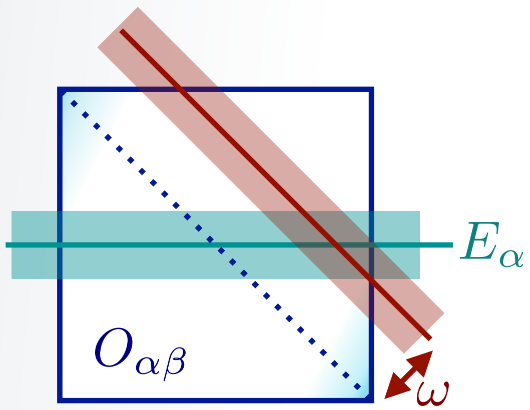
broadened spectral function of filter ensemble

$$S_O^\rho(\omega) \approx e^{S(E+\omega)} |O_{E,E+\omega}|^2$$

see also Pappalardi, Foini, Kurchan, 2304.10948

Luo et al PRB 109, 134304 (2024)

filter ensemble as ETH probe



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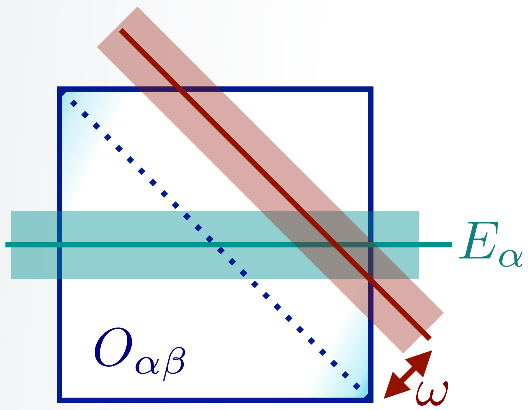
using ETH

Luo et al PRB 109, 134304 (2024)

filter ensemble as ETH probe



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using ETH

entropy factor extracted from DoS calculation or eliminated from $S_O^\rho(-\omega)$

Luo et al PRB 109, 134304 (2024)

filter ensemble as ETH probe

errors from two filters with independent widths

filter ensemble

$$S_O^{P_\delta}(\omega) = e^{\frac{S(E+\omega)-S(E)}{2}} |f_O(E+\omega/2,\omega)|^2 \left[1 + O\left(\frac{\delta^2}{N^2}\right)\right]$$

filter ensemble as ETH probe

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filter in energy difference

$$S'^{P_\delta}_O(\omega) \sim S_O^{P_\delta}(\omega) + \frac{1}{2}\delta_\omega^2 \partial_\omega^2 S_O^{P_\delta}$$

numerical results

model: quantum Ising chain

$$H = -J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z$$

Luo et al PRB 109, 134304 (2024)

numerical results

model: quantum Ising chain

$$H = -J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - J_2 \sum_{i=1}^{N-2} \sigma_i^z \sigma_{i+2}^z - \sum_{i=1}^{N} (g + r_i) \sigma_i^x$$

Luo et al PRB 109, 134304 (2024)

numerical results

model: quantum Ising chain

integrable

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Luo et al PRB 109, 134304 (2024)

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model: quantum Ising chain

integrable

non-integrable

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Luo et al PRB 109, 134304 (2024)

numerical results

model: quantum Ising chain

integrable

non-integrable

disordered

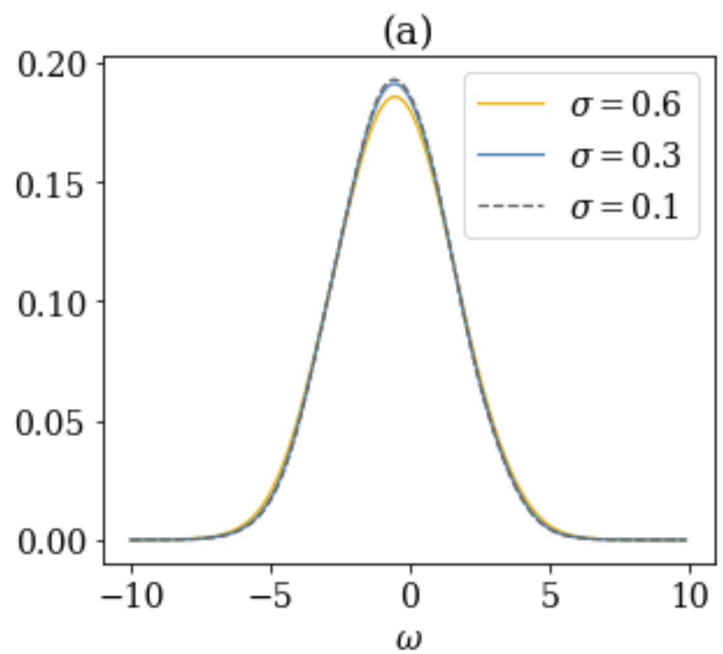
$$H = -J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - J_2 \sum_{i=1}^{N-2} \sigma_i^z \sigma_{i+2}^z - \sum_{i=1}^{N} (g + r_i) \sigma_i^x$$

Luo et al PRB 109, 134304 (2024)

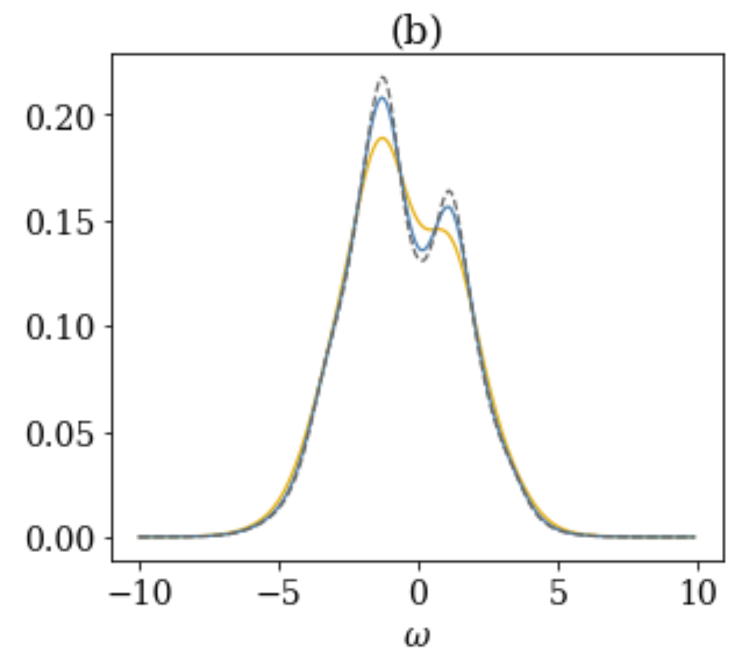
broadened spectral function

$N = 40$
$E/N = 0.5$

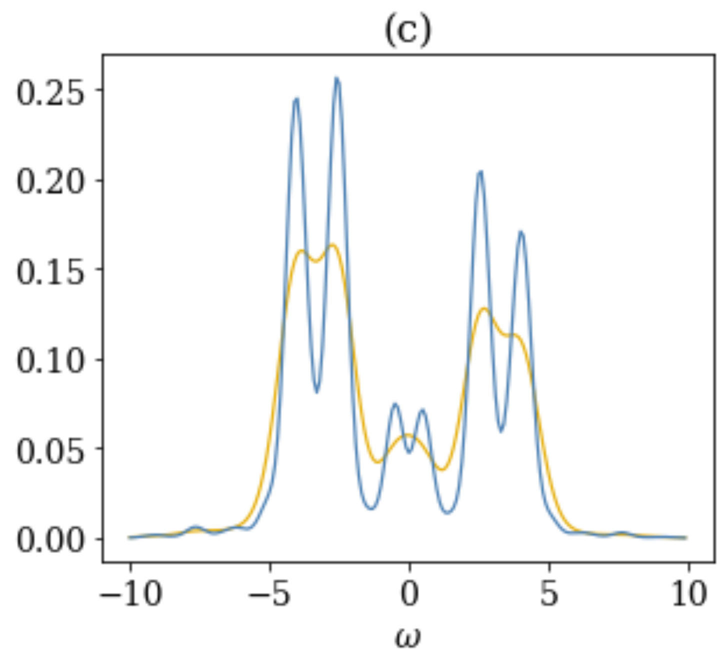
integrable



non-integrable



disordered



sufficiently narrow filters

Luo et al PRB 109, 134304 (2024)

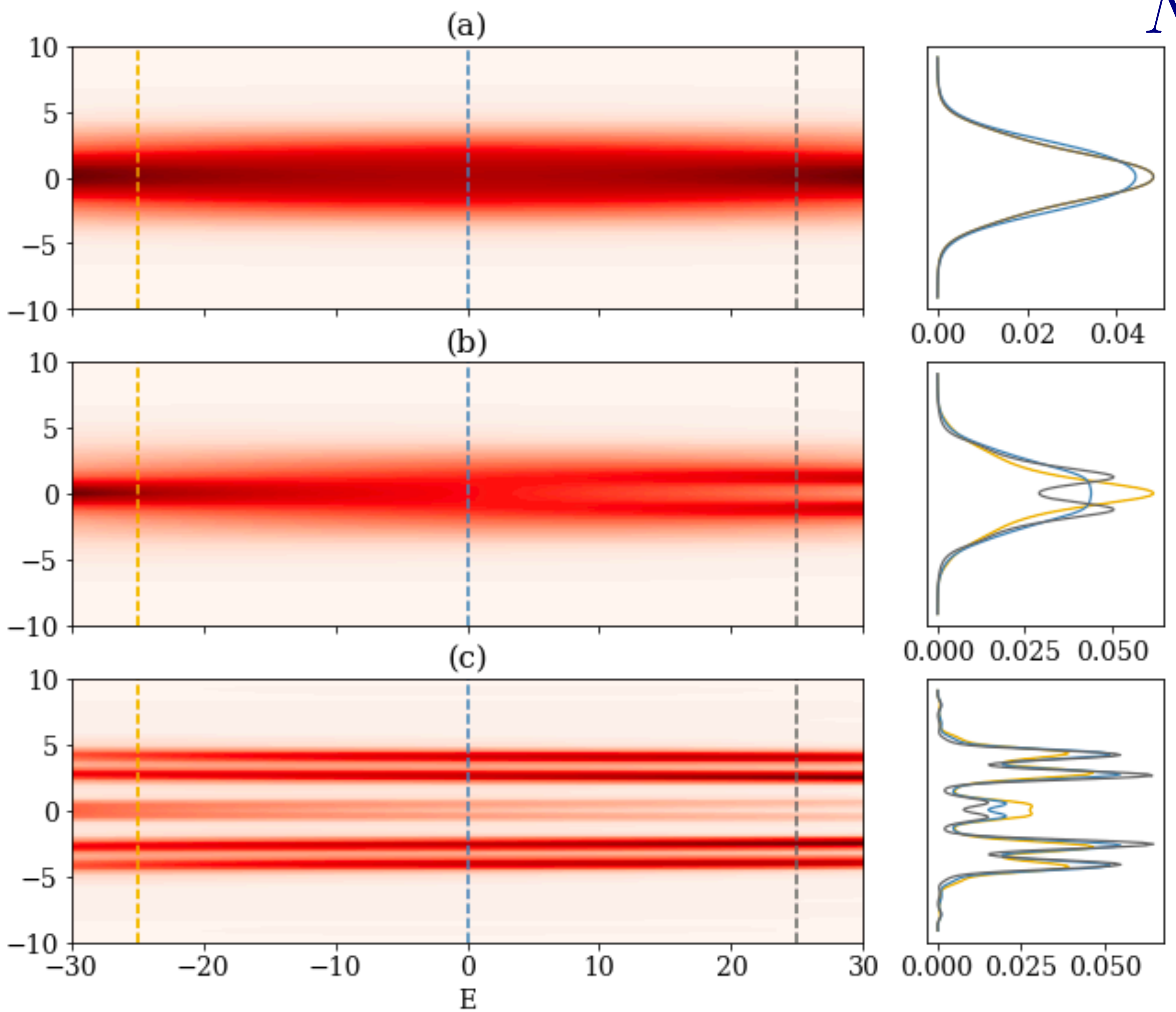
mapping out the function $|f_O(E,\omega)|^2$

$N = 40$

integrable

non-integrable

disordered



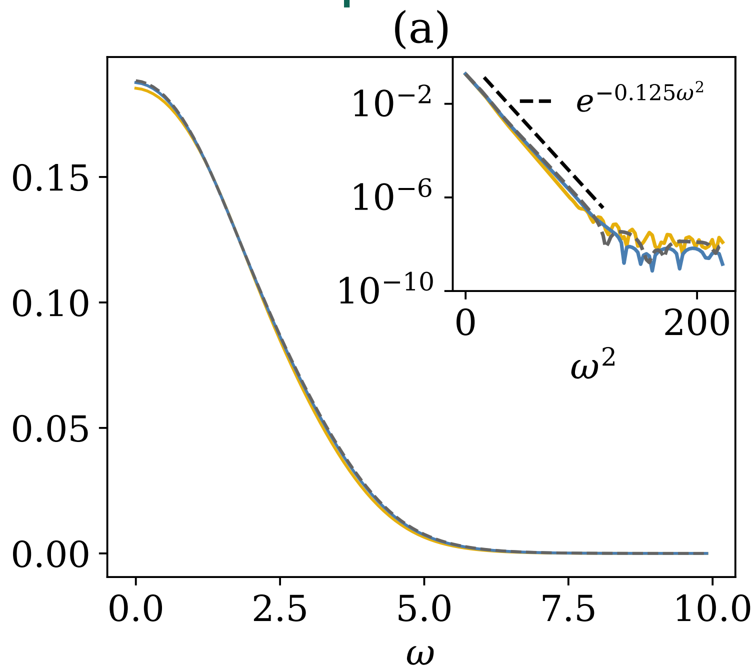
Luo et al PRB 109, 134304 (2024)

ω-dependence of $|f_O(E,\omega)|^2$

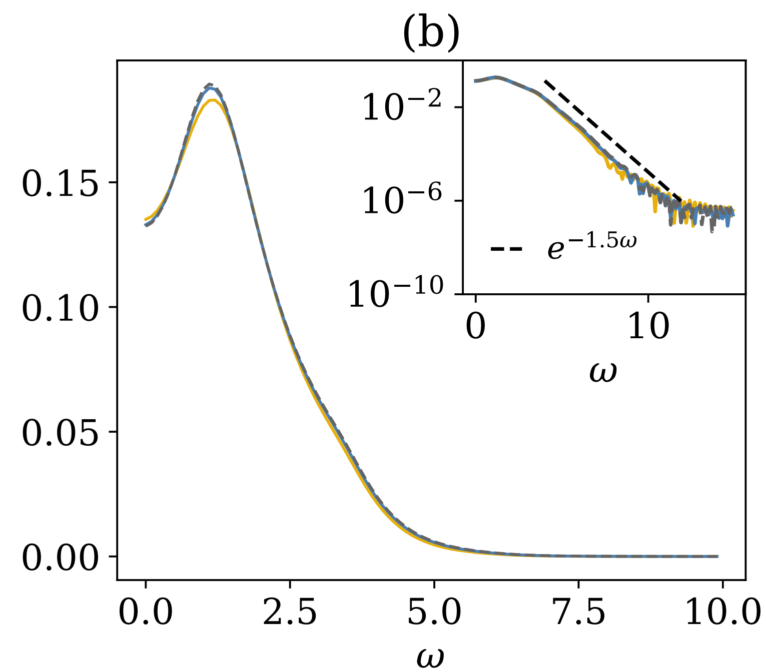
$N = 20 - 60$

$E/N = 0.5$

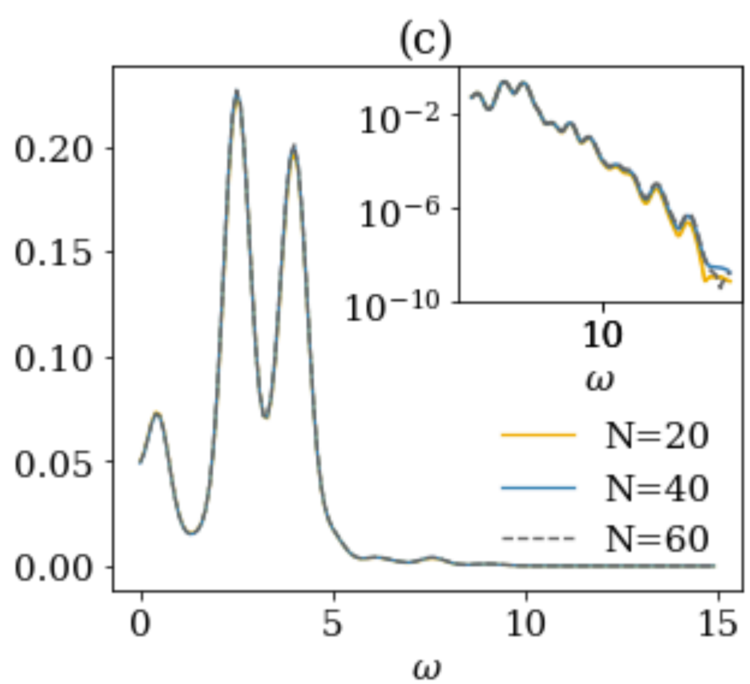
integrable



non-integrable



disordered



converged in size
asymptotic behaviour

Luo et al PRB 109, 134304 (2024)

other results with TNS + filter method

diagonal ensemble

Ising non-integrable

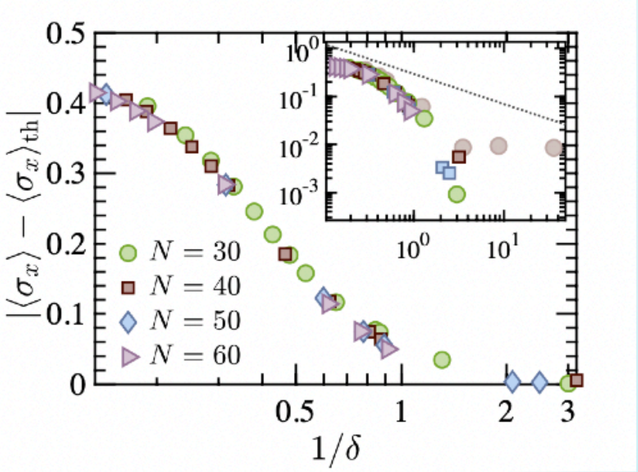
$$H_{\text{Ising}} = J\sum_i \sigma_z^{[i]}\sigma_z^{[i+1]} + g\sum_i \sigma_x^{[i]} + h\sum_i \sigma_z^{[i]}$$

$$J = 1,\ g = -1.05,\ h = 0.5$$

product initial states

$$|Z+\rangle := |0\rangle^{\otimes N}$$

local observable



approach thermal as filter narrows

entropy in diagonal ensemble
grows ~linearly with N

Çakan et al., PRB103, 115113 (2021)

other results with TNS + filter method

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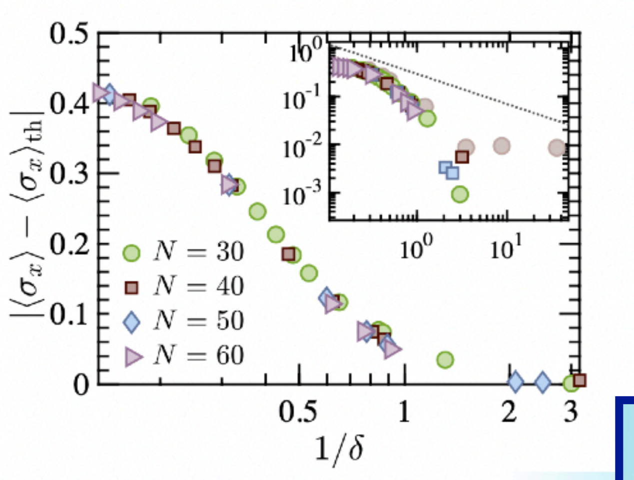

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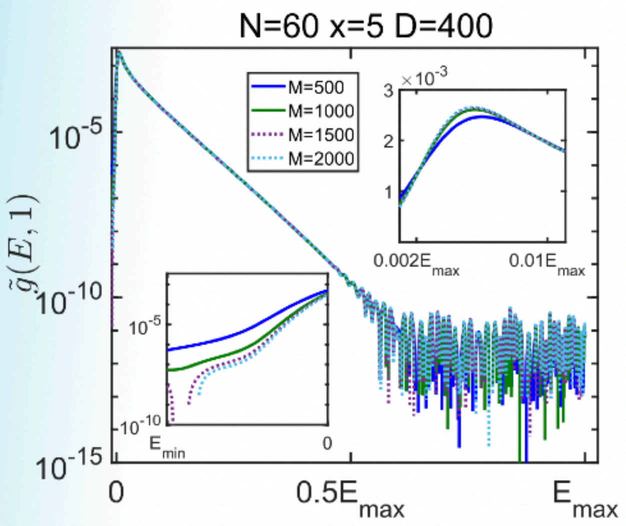
Çakan et al., PRB103, 115113 (2021)

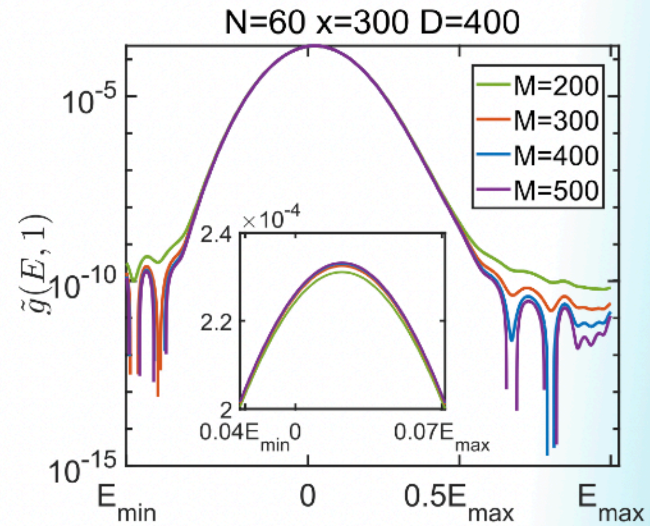
DoS of Schwinger model

large lattice spacing



asymmetric shape

small lattice spacing



near Gaussian shape

I. Papaefstathiou et al., PRD104, 014514 (2021)

To conclude

MCQST

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DFG TRR 360

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energy filters & TNS can provide other (classical / quantum) tools to get dynamical properties

MCQST

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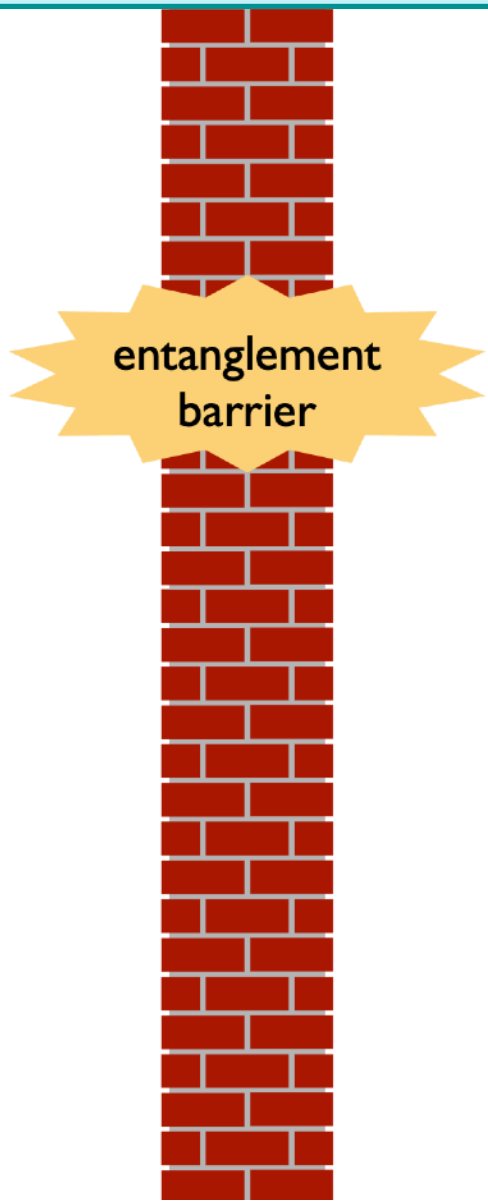

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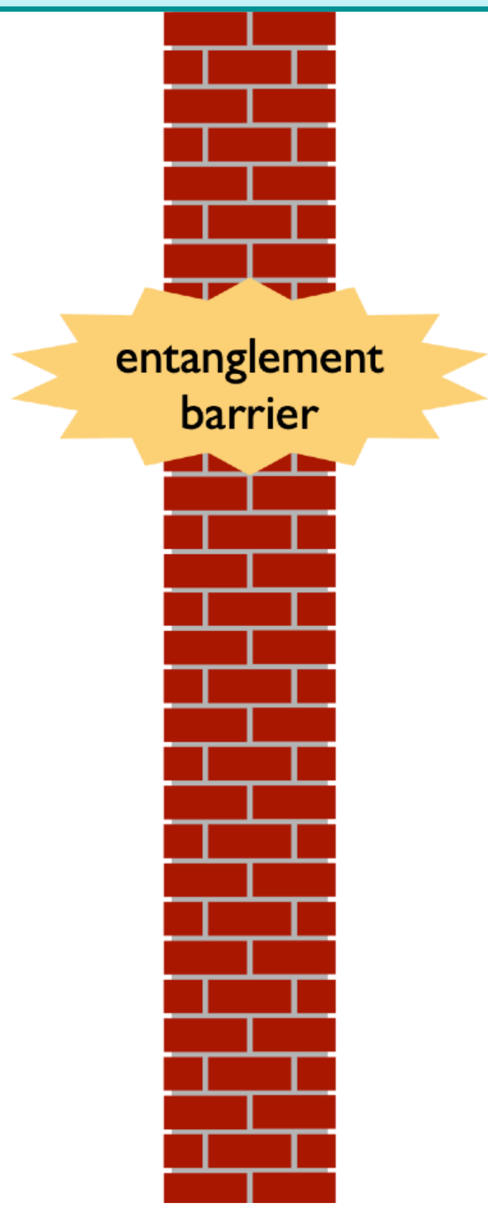

spectral properties of a QMB Hamiltonian

Yang, Iblisdir, Cirac, MCB, PRL124, 100602 (2020)
Lu, PRX Quantum 2, 020321 (2021)
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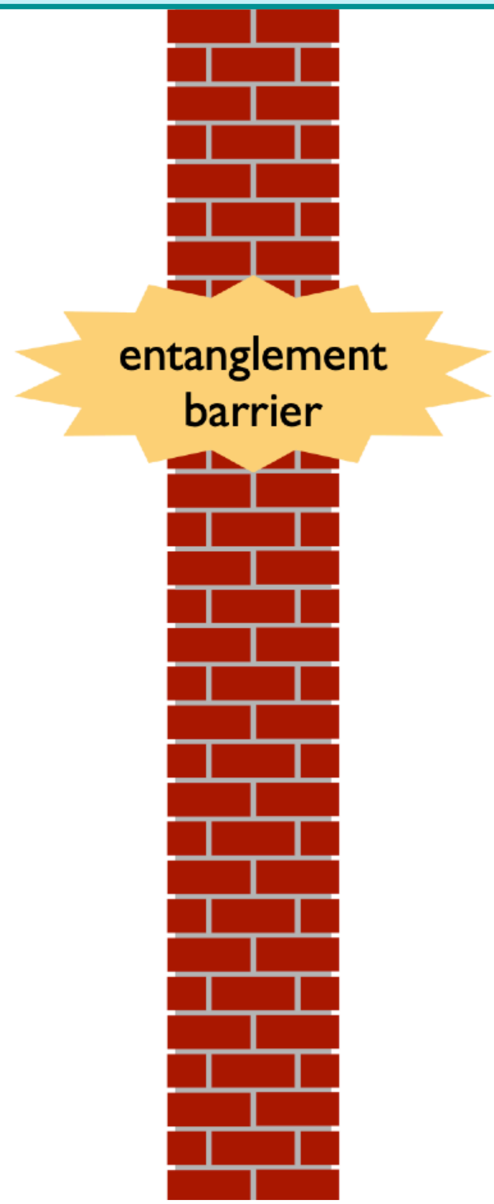

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further possibilities: apply to non-ergodic systems, probe fluctuation-dissipation relations, further explore off-diagonal matrix elements…

MCQST

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Thanks for your attention!

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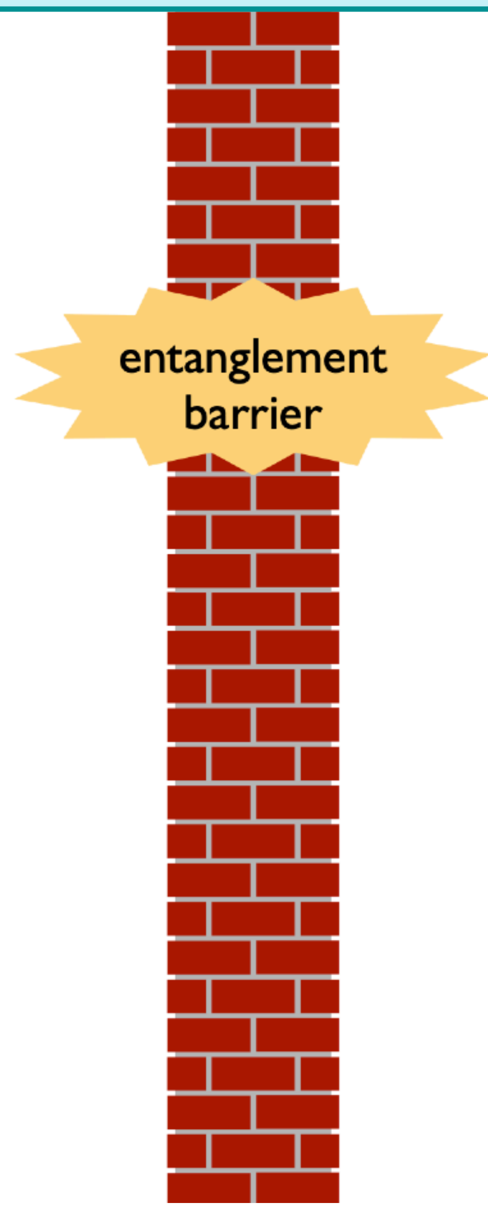

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