Assigning temperatures to eigenstates

isolated many-body quantum systems

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Maynooth University
Dept. Theoretical Physics

Maynooth, Ireland

Maynooth University
National University of Ireland Maynooth

Max Planck Institute for Physics of Complex Systems (MPI-PKS)

mpipks

Dresden, Germany

Assigning temperatures to eigenstates

isolated many-body quantum systems

Burke, Nakerst, Haque, PRE 2023

Assigning temperatures to eigenstates

Burke and Haque, PRE 2023

Entropy & temperature in finite isolated quantum systems

Haque, McClarty, Khaymovich, PRE 2022

Entanglement in mid-spectrum eigenstates

Khaymovich, Haque, McClarty, PRL 2019

Eigenstate Thermalization, Random Matrix Theory and Behemoths

Beugeling, Bäcker, Moessner, Haque, PRE 2018

Eigenstate amplitudes (coefficients)

Beugeling, Moessner, Haque, PRE 2014

Finite-size scaling of eigenstate thermalization

Phillip Cussen Burke

Goran Nakerst

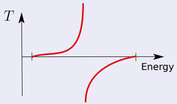
Punchline

Eigenvalue-based T vs eigenstate-based T

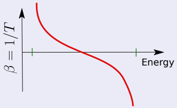
Temperature from eigenvalues

$$E = \langle H \rangle \ = \ \frac{\mathrm{tr}(e^{-\beta H} H)}{\mathrm{tr}(e^{-\beta H})}$$

$$= \ \frac{\sum_j e^{-\beta E_j} E_j}{\sum_j e^{-\beta E_j}}$$



Invert: $\beta_C(E)$



Canonical temperature

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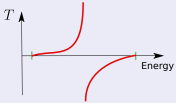

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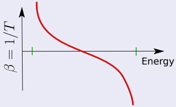

Canonical temperature

Temperature from full eigenstate

Compare

$\rho = |E_n\rangle\langle E_n|$ with $\rho_C = e^{-\beta H}$

Which β minimizes distance?

$$\beta_E = \operatorname*{argmin}_{\beta} d_p(\rho, \rho_C)$$

"Eigenstate temperature"

Punchline

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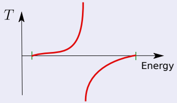

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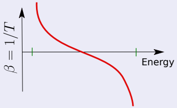

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"Eigenstate temperature"

$\beta_E \sim \beta_C$ for all systems

Distance measure important

Punchline continued

Temperature from eigenvalues

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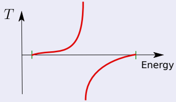

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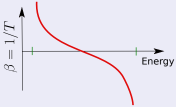

Canonical temperature

Punchline continued

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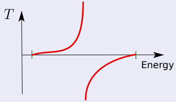

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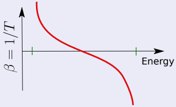
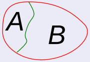


Canonical temperature

Temp from traced eigenstate

Spatial partition,



Compare $\rho^A = \mathrm{tr}_B(\rho) = \mathrm{tr}_B \, |E_n\rangle\langle E_n|$

with $\rho_C^A = \mathrm{tr}_B(e^{-\beta H})$ or $e^{-\beta H_A}$

Which β minimizes distance?

$$\beta_S = \underset{\beta}{\mathrm{argmin}} \, d_p\left(\rho^A, \rho_C^A\right)$$

"Subsystem temperature"

Punchline continued

Temperature from eigenvalues

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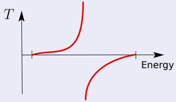

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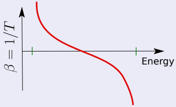

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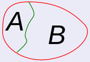

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Which β minimizes distance?

$$\beta_S = \underset{\beta}{\mathrm{argmin}}\, d_p\left(\rho^A, \rho^A_C\right)$$

"Subsystem temperature"

$\beta_S \longrightarrow \beta_C$ in t.d. limit

for chaotic local Hamiltonians

Context

Experiments
in the limit of "isolation":

time of measurement $\ll$ time scale of environment effects

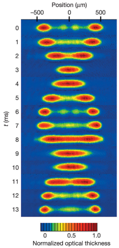
Context

Non-Equilibrium dynamics of isolated quantum systems

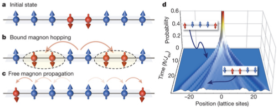
Experiments
in the limit of "isolation":

time of measurement $\ll$ time scale of environment effects

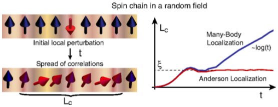
- Ultracold trapped atoms/ions
- NMR quantum computing
- Ultrafast pump-probe spectroscopy



Weiss group,
Nature 2006



Bloch group,
Nature Phys 2013



Wei, Ramanathan, Cappellaro,
PRL 2018

Isolated system, no external bath. Can it thermalize?

Answer:

No thermalization of full system

Context

Isolated system, no external bath. Can it thermalize?

Answer:

No thermalization of full system

Pure state $|\psi(t)\rangle$ remains pure under isolated evolution.
Will never turn into a mixed thermal state

$$\rho_C = \mathrm{tr}\, e^{-\beta H} = \sum_j e^{-\beta E_j} \, |E_j\rangle\langle E_j|$$

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Isolated system, no external bath. Can it thermalize?

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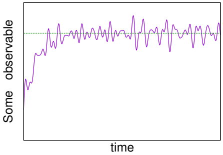
However:

observables could thermalize

sub-regions of the isolated system could thermalize

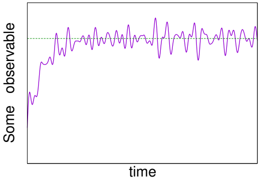


Context

Thermalization in isolated many-body systems

An observable thermalizes

$\Longrightarrow$ relaxes to value dictated by thermal ensemble



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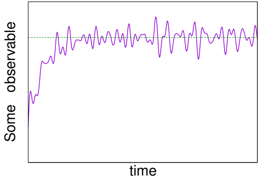

⋆ Initial state $|\psi(0)\rangle = \sum_j c_j |E_j\rangle$ relaxes to

$$\langle O(t)\rangle = \langle\psi(t)|\hat{O}|\psi(t)\rangle \xrightarrow{t\to\infty,\ \langle . \rangle} \sum_j |c_j|^2 \langle E_j|\hat{O}|E_j\rangle$$

⋆ Prediction from thermal ensemble:

$$\langle O\rangle_{\text{therm}} = \frac{1}{Z(\beta)} \operatorname{tr}\left(\hat{O}e^{-\beta\hat{H}}\right) = \frac{1}{Z(\beta)} \sum_j e^{-\beta E_j} \langle E_j|\hat{O}|E_j\rangle$$

Context   Thermalization in isolated many-body systems

$$\sum_j |c_j|^2 \langle E_j | \hat{O} | E_j \rangle = \frac{1}{Z(\beta)} \sum_j e^{-\beta E_j} \langle E_j | \hat{O} | E_j \rangle$$

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- ⋆ ETH $\longrightarrow$ $\langle E_j | \hat{O} | E_j \rangle$'s are smooth functions of E_j

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Deutsch, P.R.A (1991); Srednicki, P.R.E (1994)

Rigol, Dunjko, Olshanii, Nature (2008)

.... + many others

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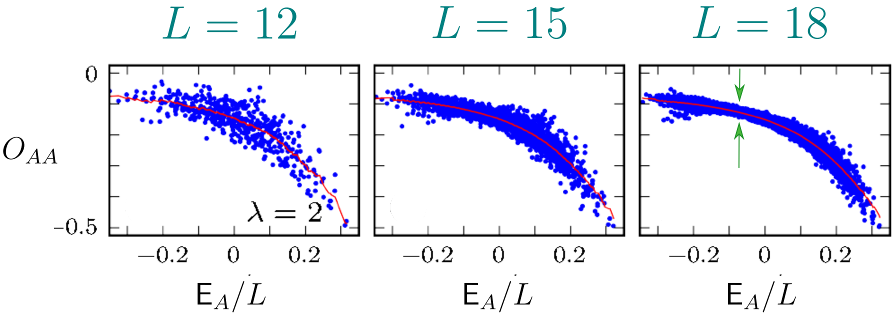
Beugeling, Moessner, Haque, P.R.E (2014)

Finite-Size Scaling of ETH

$$H = H_{XXZ} + \lambda \sum_j (j - j_0)^2 S_j^z$$

E.T.H. Scaling

$$O_{jj} = \langle E_j | \hat{O} | E_j \rangle = \langle E_j | S^z_{\rm middle} | E_j \rangle$$



Scaling of E.T.H. fluctuations: $\sigma \sim \mathcal{D}^{-1/2} \sim e^{-\alpha L}$

$\mathcal{D}$ = dimension of Hilbert space

Beugeling, Moessner, Haque, P.R.E (2014)

$$\sum_j |c_j|^2 \langle E_j | \hat{O} | E_j \rangle = \frac{1}{Z(\beta)} \sum_j e^{-\beta E_j} \langle E_j | \hat{O} | E_j \rangle$$

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- ⋆ Related idea: in every eigenstate, dens.mat. of subsystem A is close to

$$\rho_C^A = \mathrm{tr}_B \left(e^{-\beta H} \right) \qquad \text{or} \qquad e^{-\beta H_A}$$

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- ⋆ Temperature β required. Usual choice: canonical temperature β_C.

Canonical temperature

Pretend: system is described by canonical dens.mat. $\rho_C = e^{-\beta H}$

$$E = \langle H \rangle \; = \; \frac{\mathrm{tr}(e^{-\beta H} H)}{\mathrm{tr}(e^{-\beta H})} = \frac{\sum_j e^{-\beta E_j} E_j}{\sum_j e^{-\beta E_j}} = \frac{\sum_j e^{-\beta E_j} E_j}{Z(\beta)}$$

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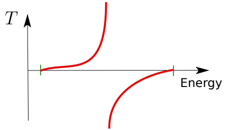

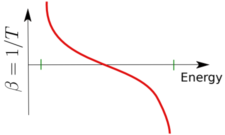

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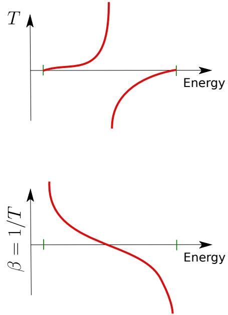

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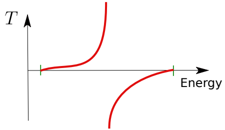

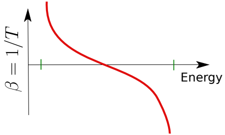

- ⋆ Provides a map, temperature ↔ energy
- ⋆ Also for finite Hilbert space: negative temp!
- ⋆ Based on eigenvalues only
- ⋆ Doesn't care about eigenstate physics!
- ⋆ E.g., works for a random matrix,
- ⋆ or for an arbitrarily generated sequence $\{E_1, E_2, \ldots\}$

Context "Many-body Hamiltonians are Random Matrices"

- ⋆ Mid-spectrum eigenstates are somewhat 'random'

  $\longrightarrow$ one path to justifying ETH.

- ⋆ Many-body Hamiltonians behave like random matrices

  (when complex, chaotic, enough)

  $\longrightarrow$ one 'definition' of quantum chaos

Context "Many-body Hamiltonians are Random Matrices"

Random matrices (GOE & GUE classes)

Eigenstates: coefficients are gaussian-distributed

Eigenvalues: level spacings have Wigner-Dyson statistics

Coefficients of many-body eigenstates

$$|E_A\rangle = \sum_{\boldsymbol{n}} c_{\boldsymbol{n}} |\boldsymbol{n}\rangle$$

$|\boldsymbol{n}\rangle$'s $\longrightarrow$ many-body configurations

Context

"Many-body Hamiltonians are Random Matrices"

Coefficients of many-body eigenstates

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$|\boldsymbol{n}\rangle$'s $\longrightarrow$ many-body configurations

$$H = J_1 \sum_{i=1}^{L-1} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + \Delta_1 S_i^z S_{i+1}^z \right) + J_2 \sum_{i=2}^{L-2} \left(S_i^+ S_{i+2}^- + S_i^- S_{i+2}^+ + \Delta_2 S_i^z S_{i+2}^z \right)$$

$J_2 = 0 \longrightarrow$ integrable XXZ chain

$J_2 \approx J_1 \longrightarrow$ non-integrable ('chaotic' or 'ergodic')

$|\boldsymbol{n}\rangle$'s $\longrightarrow$

$|\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\rangle$
$|\downarrow\downarrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow\rangle$
$|\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\rangle$
$\vdots$

Context "Many-body Hamiltonians are Random Matrices"

Coefficients of many-body eigenstates

$$|E_A\rangle = \sum_{\boldsymbol{n}} c_{\boldsymbol{n}} |\boldsymbol{n}\rangle \qquad z = c_{\boldsymbol{n}}\sqrt{\mathcal{D}}$$

Beugeling, Moessner, Bäcker, Haque, P.R.E (2018)

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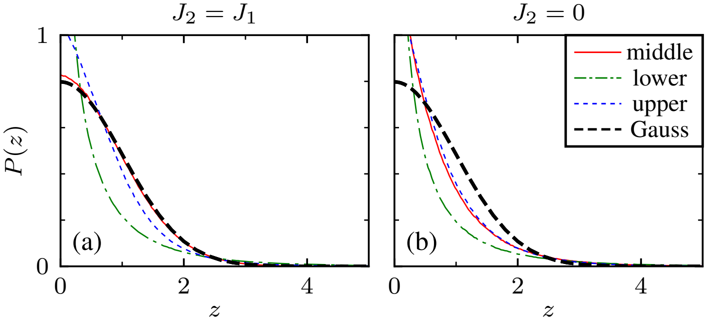
Beugeling, Moessner, Bäcker, Haque, P.R.E (2018)

NON-INTEGRABLE

INTEGRABLE



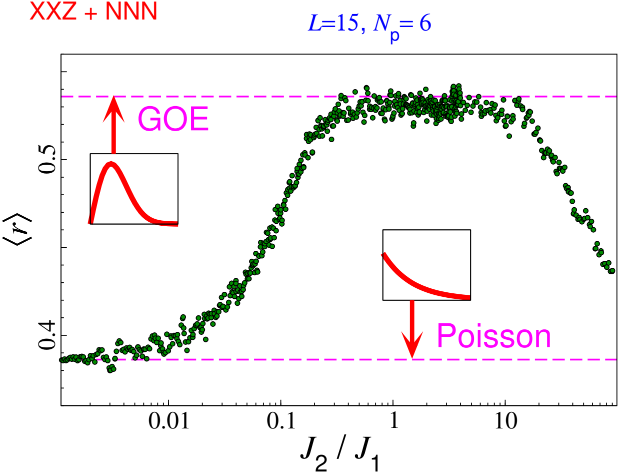
Level statistics of many-body spectra

Context

"Many-body Hamiltonians are Random Matrices"

Level statistics of many-body spectra

XXZ + NNN



$\langle r \rangle$ distinguishes GOE, GUE, Poisson

$$r_i = \min\left(\frac{s_{i+1}}{s_i}, \frac{s_i}{s_{i+1}}\right)$$

Integrable systems usually have Poisson statistics

Context “Many-body Hamiltonians are Random Matrices”

Entanglement entropy of many-body eigenstates

Context

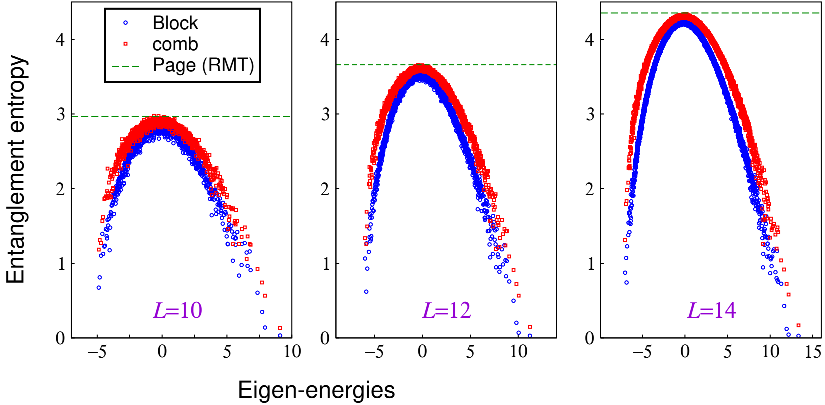
"Many-body Hamiltonians are Random Matrices"

Entanglement entropy of many-body eigenstates

XYZ + NNN

(both: $\eta = 0.5$, $\Delta = 0.9$)
+ h_x-field (0.8) + h_z-field (0.2)

Haque, McClarty, Khaymovich, PRE 2022



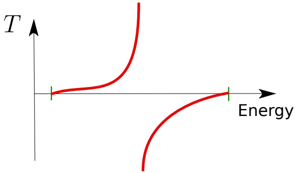
Only the middle of the spectrum?

Context

"Many-body Hamiltonians are Random Matrices"

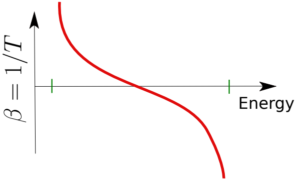
Only the middle of the spectrum?

Introduce (canonical) temperature



mid-spectrum eigenstates $\equiv$ infinite-temperature states

Mid-spectrum eigenstates
$\longrightarrow$ well-described by $|\psi_{\mathrm{rand}}\rangle$



Finite-temperature eigenstates
$\longrightarrow$ well-described by $\exp\left[-\frac{\beta}{2}\hat{H}\right]|\psi_{\mathrm{rand}}\rangle$

Context "Many-body Hamiltonians are Random Matrices"

Not just the middle of the spectrum

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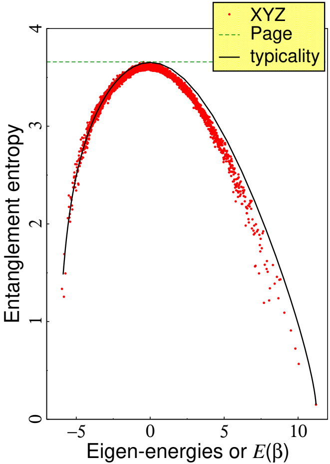
Eigenstates as $\quad \sim \exp\left[-\frac{\beta}{2}\hat{H}\right]|\psi_{\mathrm{rand}}\rangle$



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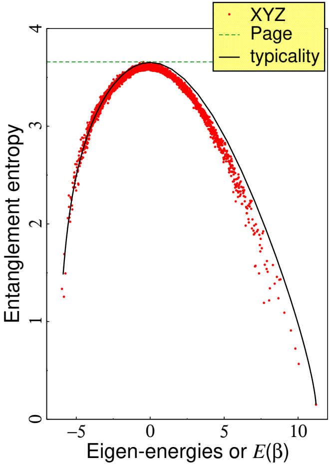

'Concentration of measure' phenomenon:

$$\langle\psi_{\rm rand}|\, e^{-\frac{\beta}{2}\hat{H}}\hat{O}e^{-\frac{\beta}{2}\hat{H}}\,|\psi_{\rm rand}\rangle$$
$$\approx \; {\rm tr}\left[e^{-\frac{\beta}{2}\hat{H}}\hat{O}e^{-\frac{\beta}{2}\hat{H}}\right] \;=\; {\rm tr}\left[\hat{O}e^{-\beta\hat{H}}\right]$$

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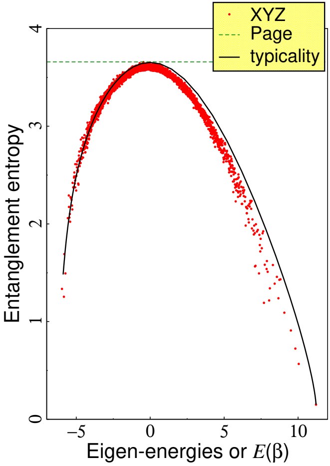

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Justifying ETH:

$$\langle E_A|\,\hat{O}\,|E_A\rangle \approx \langle\psi_{\rm rand}|\, e^{-\frac{\beta}{2}\hat{H}}\hat{O}e^{-\frac{\beta}{2}\hat{H}}\,|\psi_{\rm rand}\rangle$$

should depend smoothly on β, hence on energy

ETH scaling — structure of operator matrices

Context "Many-body Hamiltonians are Random Matrices"

ETH scaling — structure of operator matrices

Operators as matrices in basis of configurations $\{|\boldsymbol{n}\rangle\}$ | Khaymovich, Haque, McClarty, PRL 2019

ETH scaling — structure of operator matrices

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Operators $\hat{\Omega}$ forming basis

$$\begin{pmatrix} 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 1 & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & 0 \end{pmatrix}$$

have the form

$$\hat{\Omega}_{\boldsymbol{n}\boldsymbol{n}'} \equiv |\boldsymbol{n}\rangle\langle\boldsymbol{n}'|$$

Changes one many-body configuration to another.

Highly nonlocal

Behemoth operators

Any operator is a sum of Behemoths.

(e.g. local observables, 2-point correlators)

Context

ETH Scaling from sparsity of operator matrices

Behemoth distribution $\sim K_0(\mathcal{D}x) \longrightarrow$ width $\sim \mathcal{D}^{-1} \longrightarrow$ super-ETH scaling

Local operators are sums of $M \sim O(\mathcal{D})$ Behemoths.

Using central limit theorem, width $\sim \sqrt{M}\mathcal{D}^{-1} \sim \mathcal{D}^{-1/2} \longrightarrow$ ETH scaling

A 'typical' operator is dense, $M > O(\mathcal{D})$

If $M \sim O\left(\mathcal{D}^{1+\beta}\right)$, width (using CLT) $\sim \mathcal{D}^{-1/2+\beta/2} \longrightarrow$ sub-ETH scaling

If $M \sim O\left(\mathcal{D}^{2}\right)$, width $\sim \mathcal{D}^{0}$

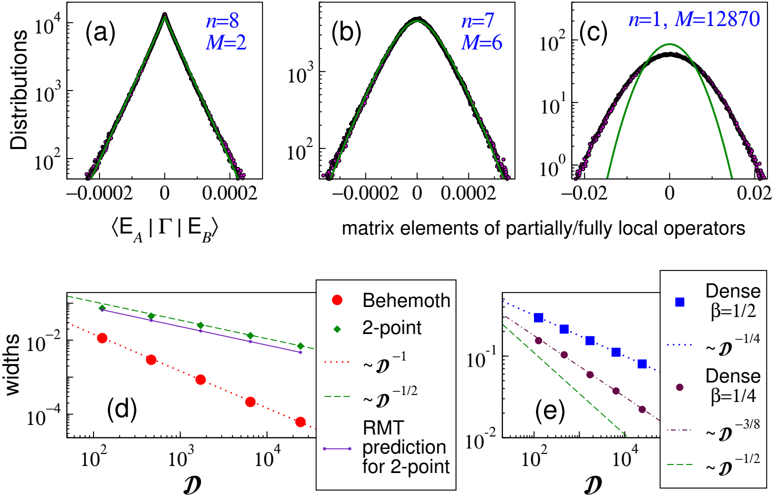
ETH works because physical operators are sparse.

$\mathcal{D}^{-1/2}$ scaling works because local operators have $M \sim O(\mathcal{D})$

ETH Scaling from sparsity of operator matrices

XXZ + NNN

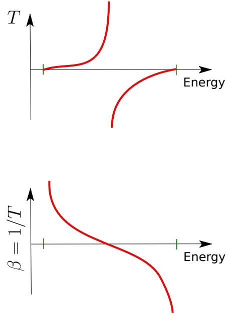
$(L,N_p)=(17,8)$. $J_1=J_2=1$, $\Delta_1=\Delta_2=0.8$



Temperature from Eigenvalues: Canonical temperature

Pretend: system is described by canonical dens.mat. $\rho_C = e^{-\beta H}$

$$E = \langle H \rangle \ = \ \frac{\mathrm{tr}(e^{-\beta H} H)}{\mathrm{tr}(e^{-\beta H})} = \frac{\sum_j e^{-\beta E_j} E_j}{\sum_j e^{-\beta E_j}} = \frac{\sum_j e^{-\beta E_j} E_j}{Z(\beta)}$$



- ⋆ Provides a map, temperature $\leftrightarrow$ energy
- ⋆ Based on eigenvalues only
- ⋆ Doesn't care about eigenstate physics!
- ⋆ Temperature from eigenstate?

Eigenstate-based temperatures — (1) full

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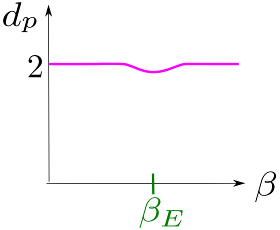

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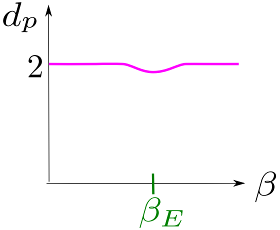

- ⋆ Expect $\min d_p \approx 2$
- ⋆ Minimum at correct temperature?
- ⋆ $\beta_E \approx \beta_C$? $\beta_E = \beta_C$?

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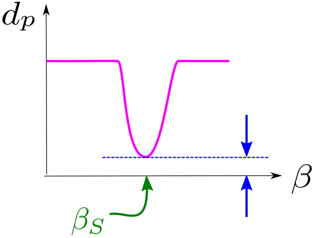

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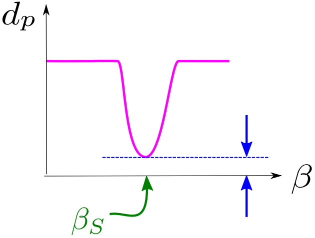

- ⋆ Minimum at correct temperature?
- ⋆ $\beta_S \approx \beta_C$? $\beta_S = \beta_C$? in some limit?
- ⋆ $\min d_p \approx 0$? $\min d_p \to 0$ in some limit?
- ⋆ Which limit?

Many-body Hamiltonians for this work

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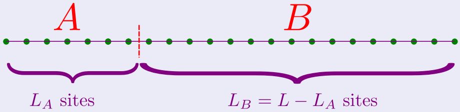

$D_A = 2^{L_A}$ $D_B = 2^{L_B}$

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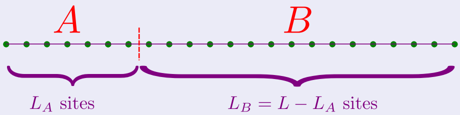

$D_A = 2^{L_A}$ $\qquad D_B = 2^{L_B}$

$D = D_A D_B$

- ⋆ Ising chain, transverse + longitudinal magnetic fields on each site
- ⋆ XXZ chain, staggered transverse + longitudinal fields
- ⋆ XXZ chain with disordered transverse + longitudinal magnetic fields

Distance measures

Schatten p-norm

⋆ Shatten p-norm of a matrix M, in terms of its singular values s_n:

$$\|M\|_p = \left(\sum_n s_n^p \right)^{1/p}$$

⋆ $p = 1 \quad \longrightarrow \quad$ trace norm

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Schatten p-distance

$$d_p(M, Q) = \left\| \frac{M}{\|M\|_p} - \frac{Q}{\|Q\|_p} \right\|_p \qquad \in [0, 2]$$

p-norm of difference between p-normalized matrices.

Eigenstate temperature — analytic result

- β_E minimizes $d_p\left(\rho, \rho_C\right) = d_p\left(|E_n\rangle\langle E_n|\, , e^{-\beta H}\right)$
- Express both DMs in eigenstate bases.
  Set derivative w.r.t. β to zero.

$$\longrightarrow \quad E_n = \frac{\mathrm{tr}(He^{-p\beta H})}{\mathrm{tr}(e^{-p\beta H})}$$

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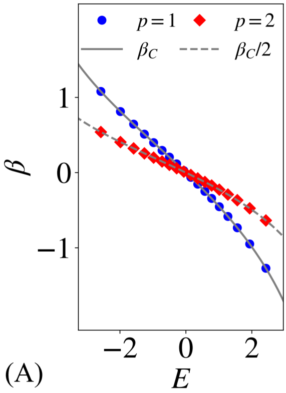
⋆ Determined by eigenvalues alone ☹

For small β_C

$$\min d_p \approx 2^{1/p}$$

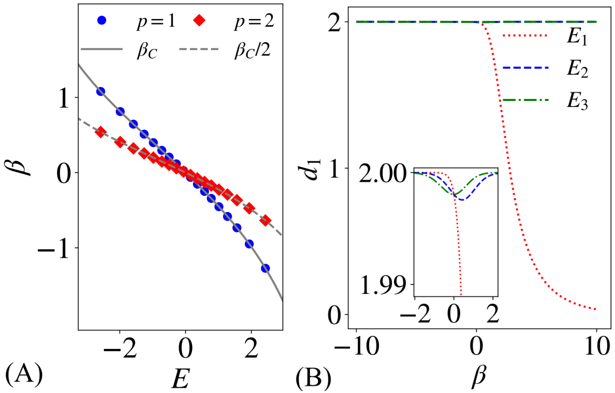
close to max for $p = 1, 2$

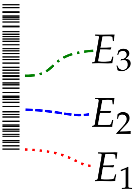
Eigenstate temperature — staggered-field XXZ



(A)

Eigenstate temperature — staggered-field *XXZ*





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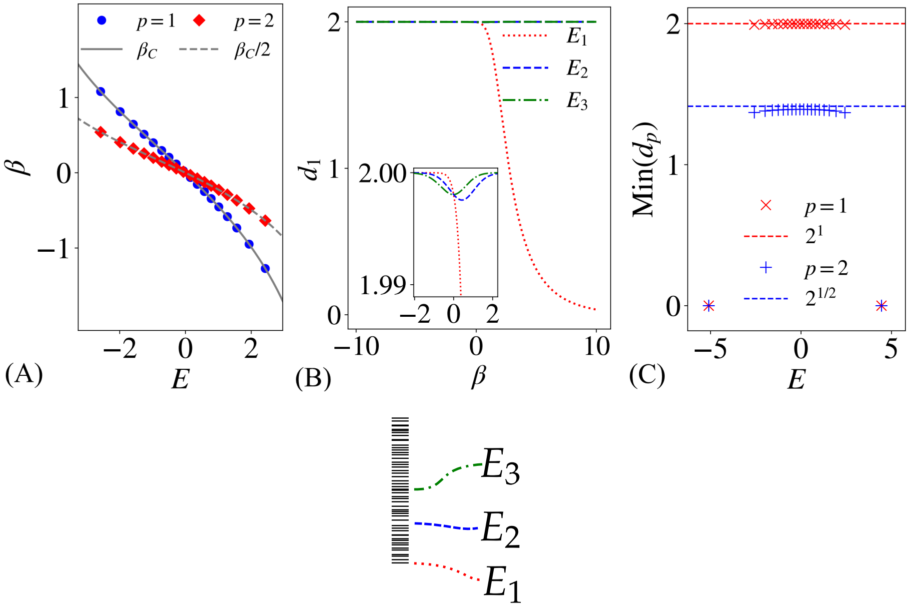
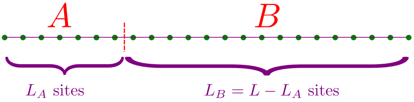


Subsystem temperature



$$\beta_S = \underset{\beta}{\text{argmin}}\, d_p\left(\rho^A, \rho^A_C\right)$$

$$\rho^A = \text{tr}_B\, |E_n\rangle\langle E_n| \text{ and } \rho^A_C = \text{tr}_B(e^{-\beta H})$$

⋆ No sweeping analytical results.

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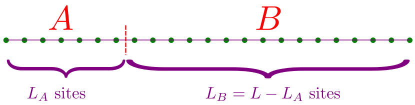

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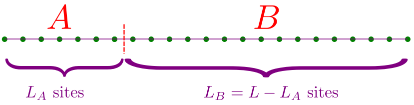

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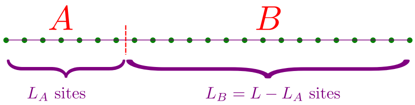

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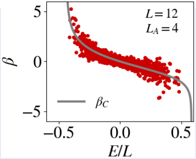
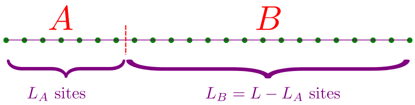


- ⋆ No sweeping analytical results. Trace operation tricky. Numerical observations only:
- ⋆ For $L_A \leq L/2$, β_S clusters around β_C

Subsystem temperature



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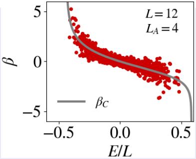

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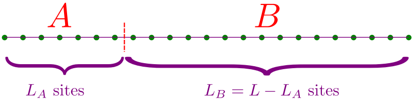

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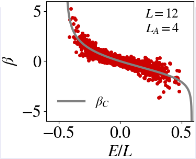

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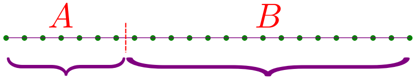

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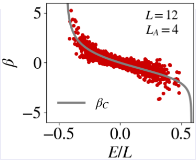

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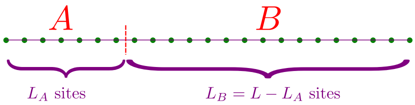

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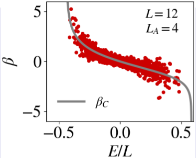

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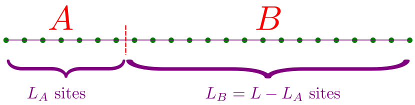

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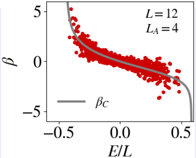

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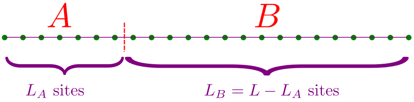

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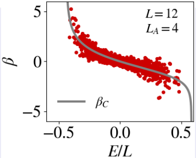

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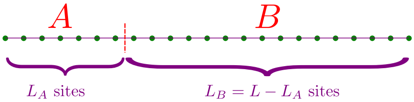
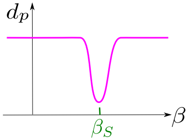
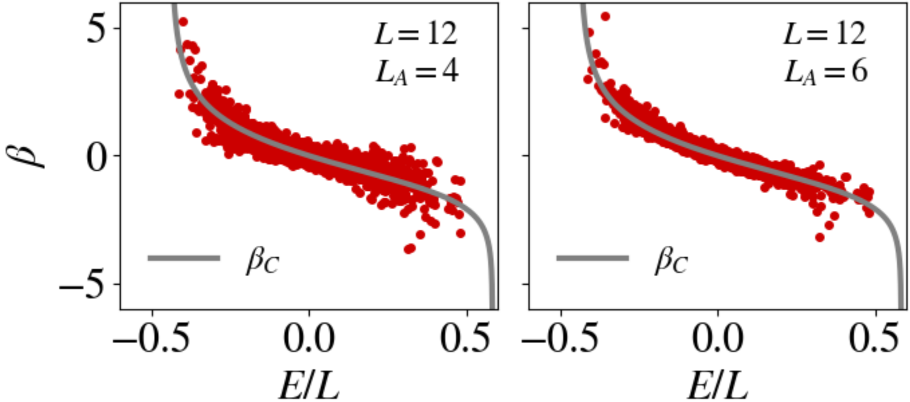
Subsystem temperature — chaotic Ising chain







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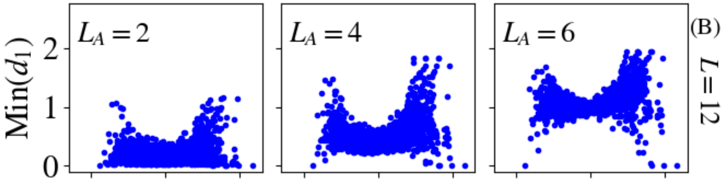

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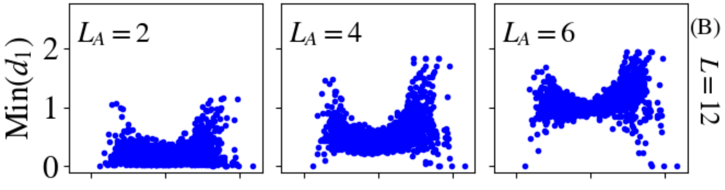

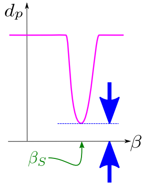

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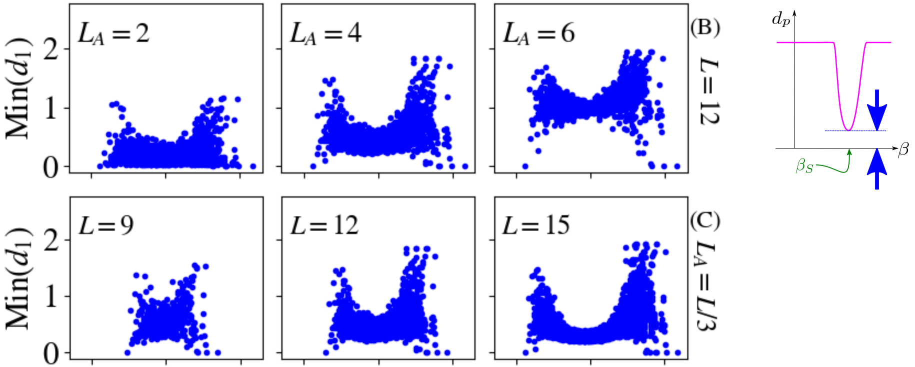

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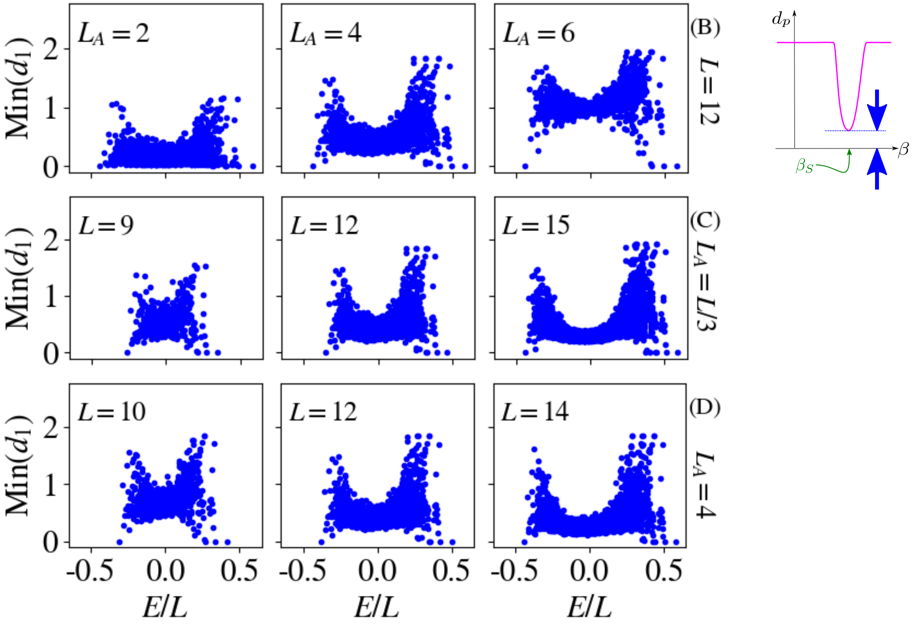

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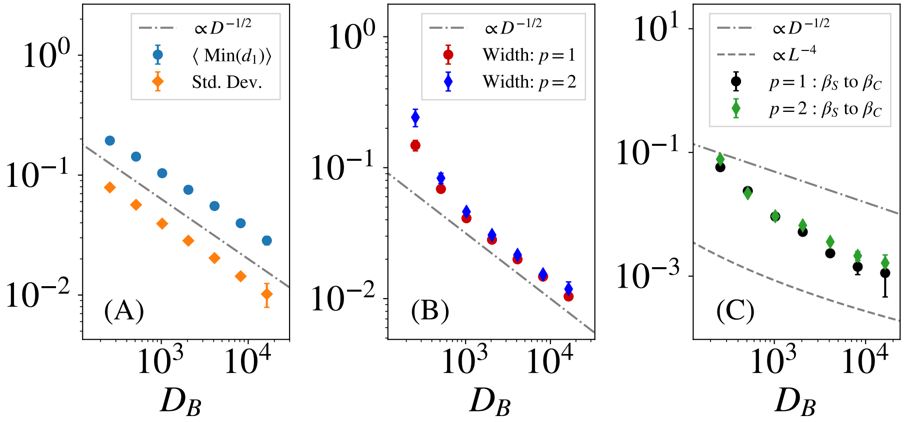
$L \to \infty$, const $L_A = 2$
Disordered XXZ chain



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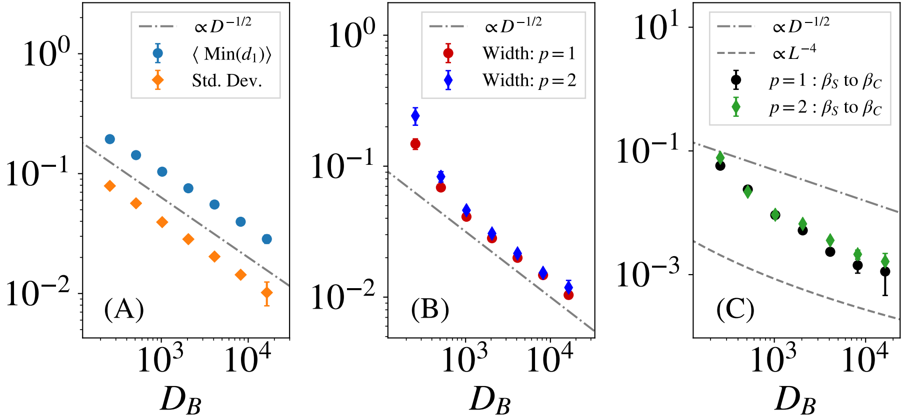

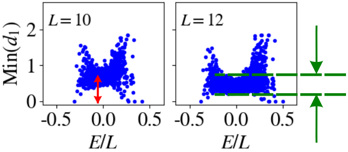

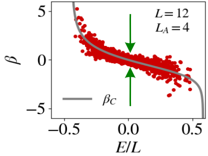

Summary

Temperature from full eigenstate

Compare

$\rho = |E_n\rangle\langle E_n|$ with $\rho_C = e^{-\beta H}$

Which β minimizes distance?

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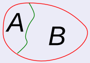

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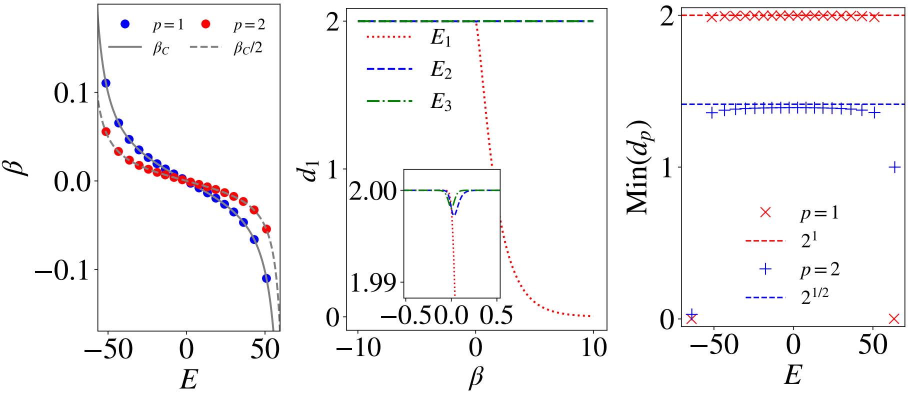
for chaotic systems

Eigenstate temperature — random (GOE) matrix



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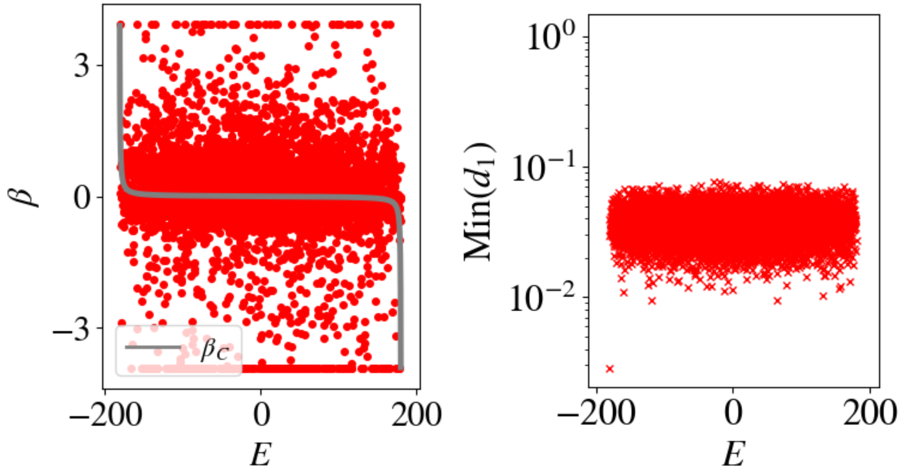

Eigenstate-based temperatures — full, 'microcanonical'

⋆ ETH $\longrightarrow$ "every eigenstate knows its temperature"

⋆ Is $\rho = |E_n\rangle\langle E_n|$ close to $e^{-\beta H}$, for some β? NO

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results ≈ same as for single eigenstate

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⋆ Option 1: Microcanonical entropy

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⋆ Option 2: Entanglement entropy

- If S_A is entanglement entropy of L_A-sized system, expect

$$S \approx S_A \left(\frac{L}{L_A} \right)$$

- another eigenstate-based temperature

Temperature from microcanonical entropy

- $\star$ $S = \log(\text{num. eigstates at energy } E)$

Temperature from microcanonical entropy

At energy E?
$\in (E, E + \Delta E)$

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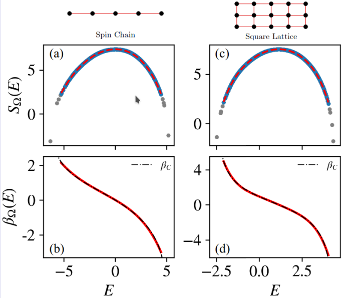

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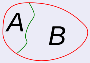
Spatial partition, 

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