Atypicality of most few-body observables

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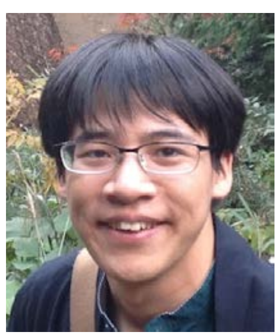

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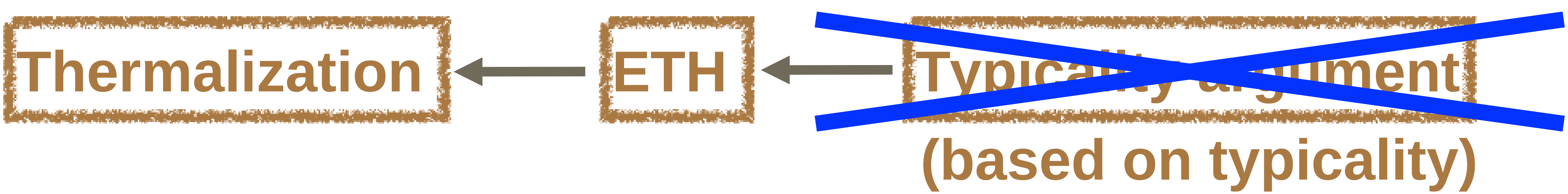
Outline

1. A brief review on

- thermalization in isolated quantum systems
- typicality and the typicality argument as a possible scenario for the eigenstate thermalization hypothesis

2. Atypicality of most few-body observables

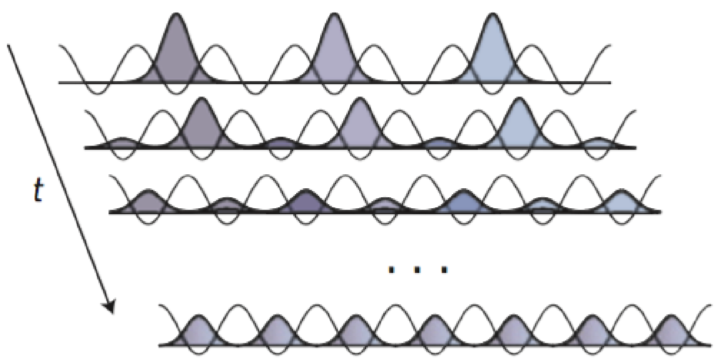
→ The typicality argument cannot be regarded as an actual mechanism of the ETH.

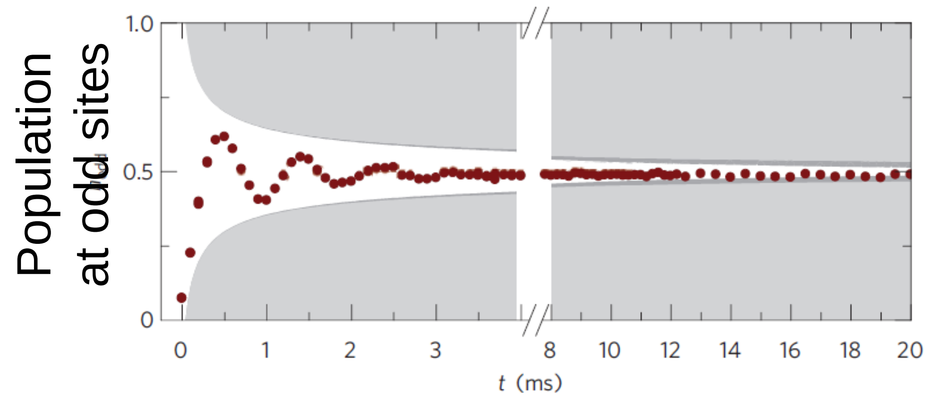


Thermalization in isolated quantum systems

Ultracold atoms   S. Trotzky, et al. Nat. Phys. **8**, 325 (2012)

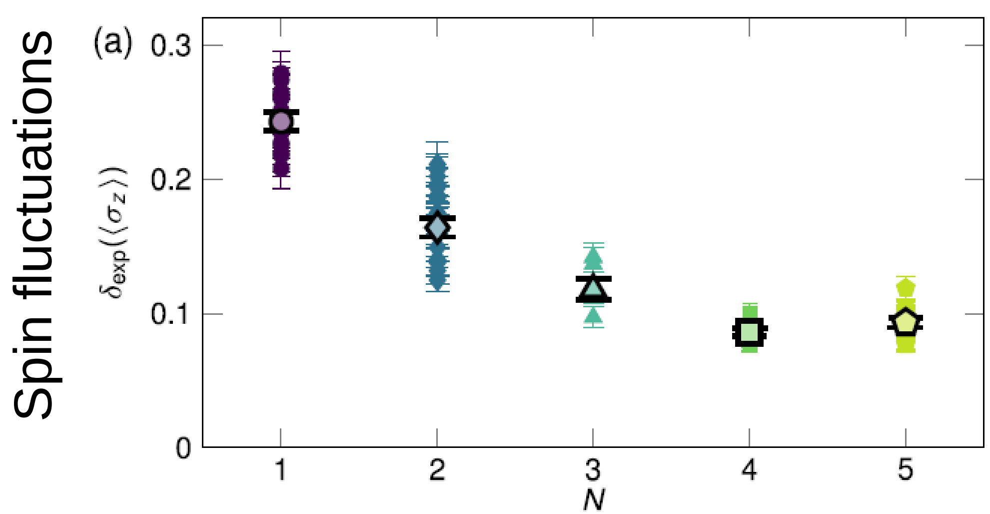
Population relaxation of an isolated Bose-Hubbard model



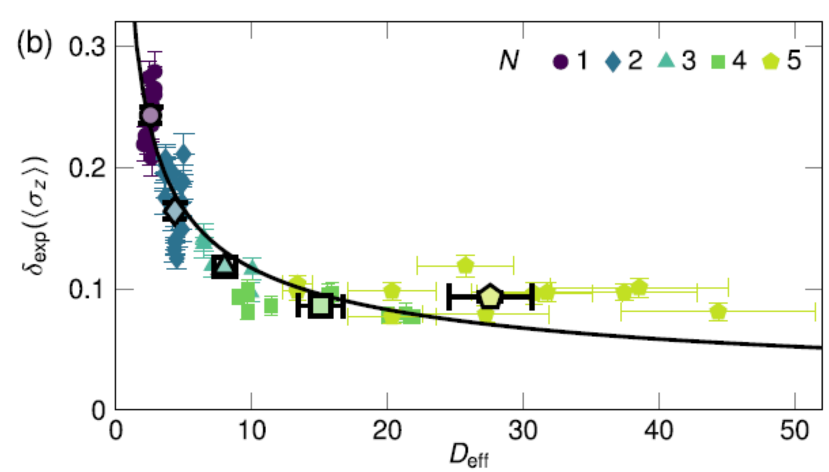


Ionic crystals   G. Clos, et al. PRL **117**, 170401 (2016)

Relaxation of a single spin toward a microcanonical ensemble



Bath (phonon) degrees of freedom



Effective Hilbert-space dimensions

Thermalization via unitary evolution

In an isolated quantum system, the state evolution is unitary.

But how does a nonequilibrium initial state unitarily approach thermal equilibrium described by a microcanonical ensemble?

$$\langle \psi(t)|\hat{\mathcal{O}}|\psi(t)\rangle \simeq \mathrm{Tr}[\hat{\rho}_{\mathrm{mic}}\hat{\mathcal{O}}] \qquad (t \to \infty)$$

microcanonical ensemble

This is a long-standing fundamental problem dating back to von Neumann in 1929.

Derive statistical mechanics from QM

J. von Neumann, “Proof of the Ergodic Theorem and the H-Theorem in Quantum Mechanics” (1929)

1. Decomposition of the Hilbert space
   In terms of macroscopic observables
2. A sufficient condition for thermalization
   similar in spirit to eigenstate thermalization hypothesis
3. As a justification for the condition:
   typicality argument

Eigenstate thermalization hypothesis (ETH)

J. M. Deutsch (1991), M. Sredniciki (1994, 1999); M. Rigol et al. (2008)

widely studied as a possible mechanism of thermalization

The ETH focuses on $\mathcal{O}_{\alpha\alpha} = \langle E_\alpha | \hat{\mathcal{O}} | E_\alpha \rangle$ with respect to energy eigenstates, and makes the following statement:

For all $|E_\alpha\rangle, |E_\beta\rangle \in \mathcal{H}_{\mathrm{sh}}$ with mean *E* and subextensive width *ΔE*, $|\mathcal{O}_{\alpha\alpha} - \mathcal{O}_{\beta\beta}|$ is negligible in the thermodynamic limit.

If the ETH holds true, the long-time average can be described by the microcanonical ensemble for all initial states with subextensive energy fluctuations.

Other definitions of the strong ETH

There are several other definitions of the ETH:
e.g.,

M. Sredniciki, J. Phys. A (1999); Rigol et al., Nature (2008)

Diagonal matrix elements are smooth functions of energy plus exponentially small diagonal & off-diagonal fluctuations.

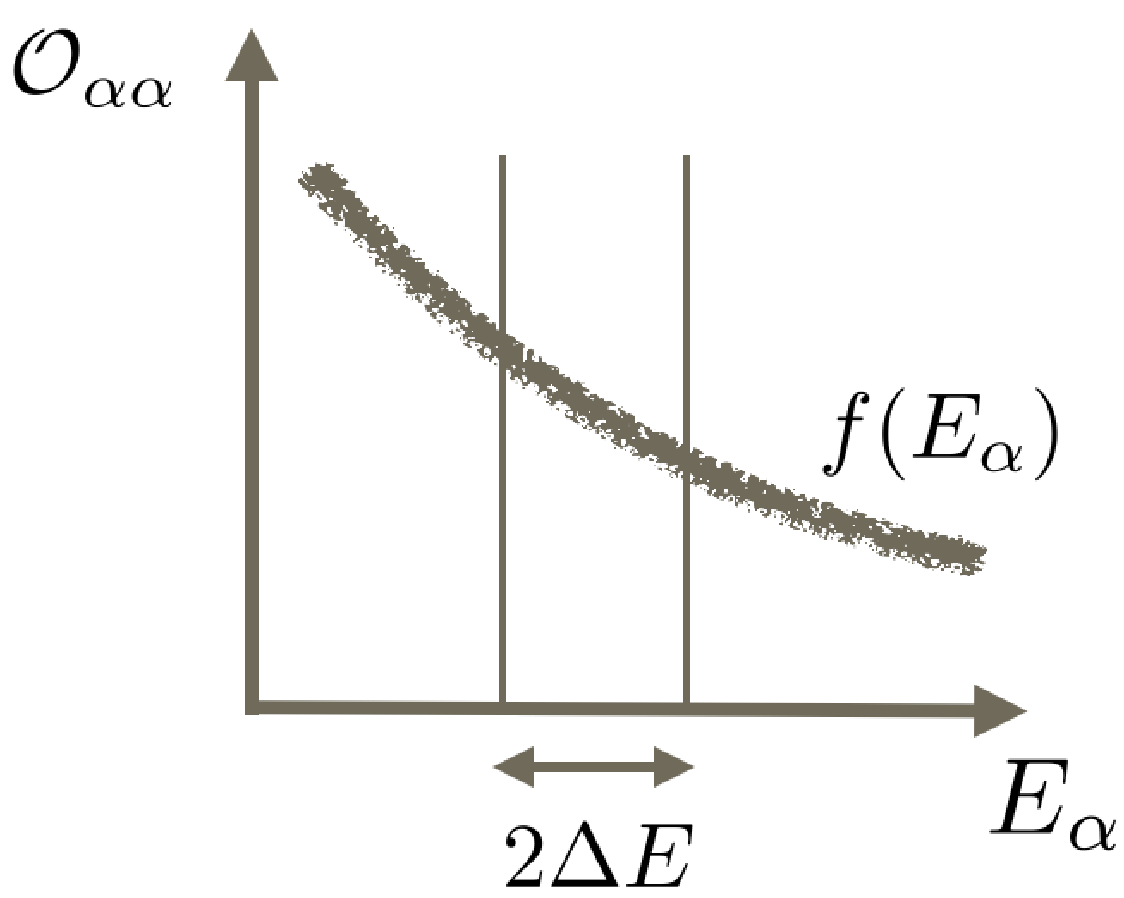
$$\mathcal{O}_{\alpha\beta} = f(E_\alpha)\delta_{\alpha\beta} + g\left(E_\alpha, E_\beta\right) e^{-S\left(\frac{E_\alpha + E_\beta}{2}\right)/2} R_{\alpha\beta}$$

smooth functions of energy

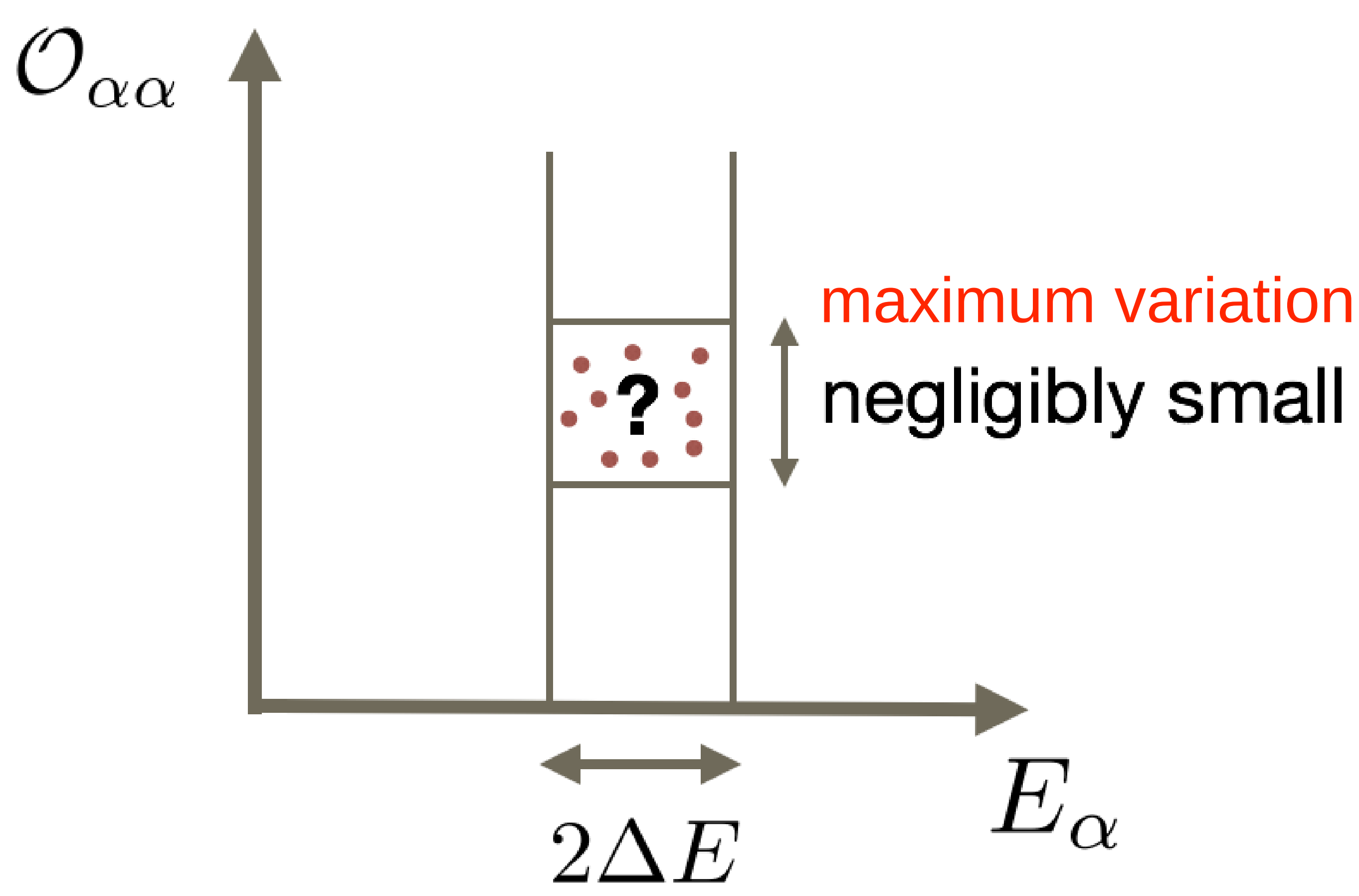
exponentially small diagonal & off-diagonal fluctuations

Comparison

Srednicki's ansatz



Our ansatz



We do not assume smoothness but assume that the maximum variation in each subextensive energy shell is negligible. → weaker but sufficient to show thermalization

von Neumann, Z. Phys. (1929); P. Reimann, PRL (2015)

Strong ETH and the typicality argument

The strong ETH has been verified numerically for small systems, but its mathematical justification has yet to be established.

A popular approach based on mathematical rigor is the typicality argument:

originally put forth by von Neumann for macrospaces;

von Neumann, Z. Phys. (1929); S. Goldstein, Eur. Phys. J. H. (2010)

later generalized to arbitrary observables.

P. Reimann, PRL (2015); M. Rigol and M. Srednicki, PRL (2012)

Typicality Argument

J. von Neumann (1929)
S. Goldstein et al. (2011)
P. Reimann (2015)

We first project an observable onto the energy shell and diagonalize it.

$$\hat{\mathcal{P}}_{\rm sh}\hat{\mathcal{O}}\hat{\mathcal{P}}_{\rm sh} = \sum_{i=1}^{d_{\rm sh}} a_i |a_i\rangle\langle a_i| \qquad d_{\rm sh} = \dim[\mathcal{H}_{\rm sh}]$$

Projection operator

Then we take the expectation value over an energy eigenstate and rewrite it in terms of a unitary matrix:

$$\mathcal{O}_{\alpha\alpha} = \langle E_\alpha|\hat{\mathcal{O}}|E_\alpha\rangle = \sum_{i=1}^{d_{\rm sh}} a_i |\langle E_\alpha|a_i\rangle|^2$$

$$\mathcal{O}_{\alpha\alpha} = \sum_{i=1}^{d_{\rm sh}} a_i |U_{\alpha i}|^2 \qquad U_{\alpha i} = \langle E_\alpha|a_i\rangle$$

$d_{\rm sh} \times d_{\rm sh}$ unitary matrix

If $\{a_i\}$ is given, $\mathcal{O}_{\alpha\alpha}$ is determined solely by *U*.

Typicality of diagonal matrix elements

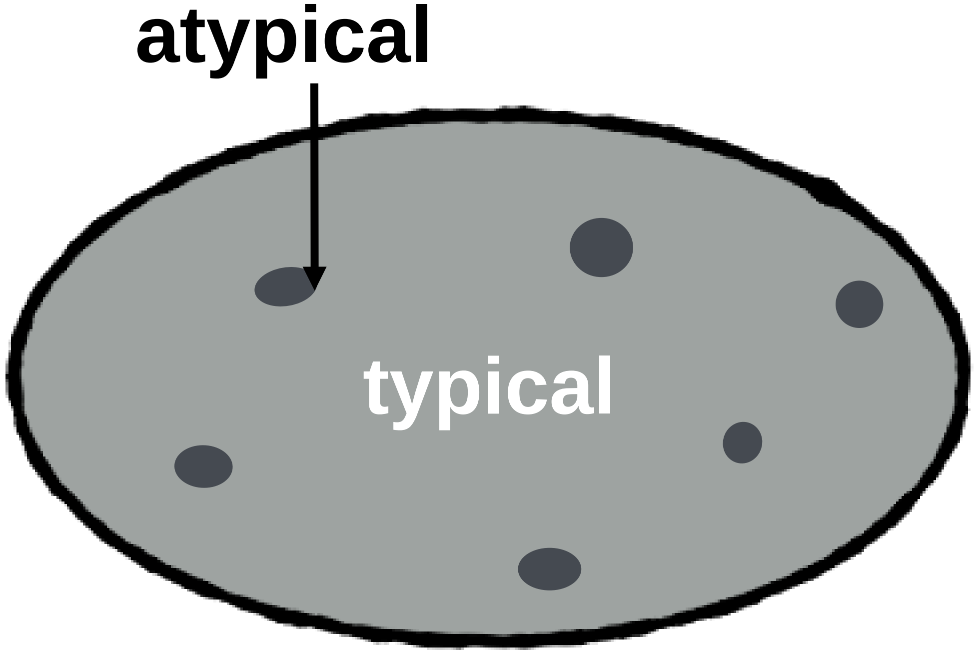
J. von Neumann (1929); P. Reimann (2015)

Very difficult to find *U* in macroscopic quantum systems. If one takes a unitary Haar measure, then the following rigorous result, which is called typicality, follows:

For almost all (or typical) *U* over the unitary Haar measure,

$$\max_{|E_\alpha\rangle, |E_\beta\rangle \in \mathcal{H}_{\rm sh}} |\mathcal{O}_{\alpha\alpha} - \mathcal{O}_{\beta\beta}|$$

decreases exponentially.



Space of unitary matrices

Note that this property, which is called typicality, is mathematically rigorous.

Typicality argument

J. von Neumann (1929); P. Reimann (2015)

The typicality argument asserts that the mathematically rigorous property

–typicality–

applies to real physical systems.

To be more precise, …

J. von Neumann (1929); P. Reimann (2015)

Consider realistic Hamiltonian & observables

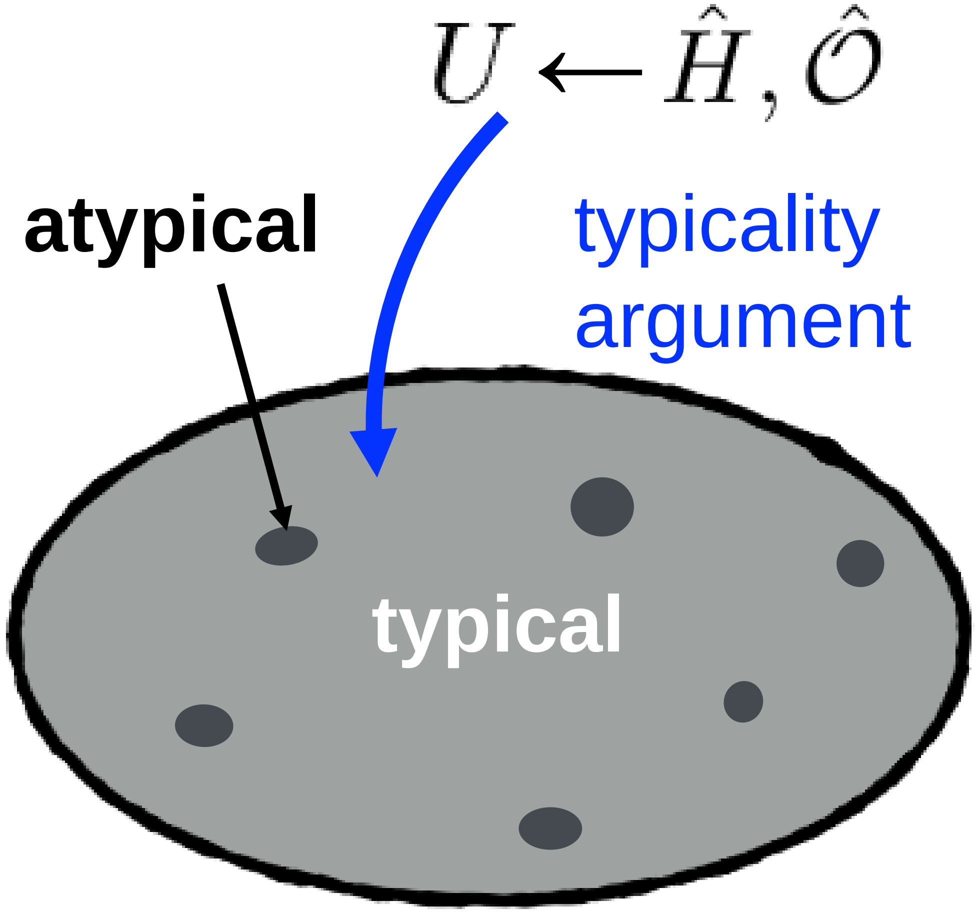
- We can calculate U from realistic $\hat{O}$ and $\hat{H}$.
- Is such U typical? $U_{\alpha i} = \langle E_\alpha | a_i \rangle$

Typicality argument assumes that U is typical. Then

For realistic $\hat{H}$ and $\hat{O}$

$$\max_{|E_\alpha\rangle, |E_\beta\rangle \in \mathcal{H}_{\rm sh}} |\mathcal{O}_{\alpha\alpha} - \mathcal{O}_{\beta\beta}|$$

would be exponentially small (by the mathematical typicality).



Space of unitary matrices

Typicality vs. Typicality argument

J. von Neumann (1929); P. Reimann (2015)

Note that the typicality is a mathematical property, but the typicality argument is a physical conjecture.

Aim of this study

We revisit the typicality argument by focusing on realistic few-body observables.

Our finding

For an arbitrary few-body Hamiltonian and randomly chosen few-body observables, the typicality argument does NOT hold if the energy width changes at most polynomially with increasing the size of the system.

R. Hamazaki and MU, PRL **120**, 080603 (2018)

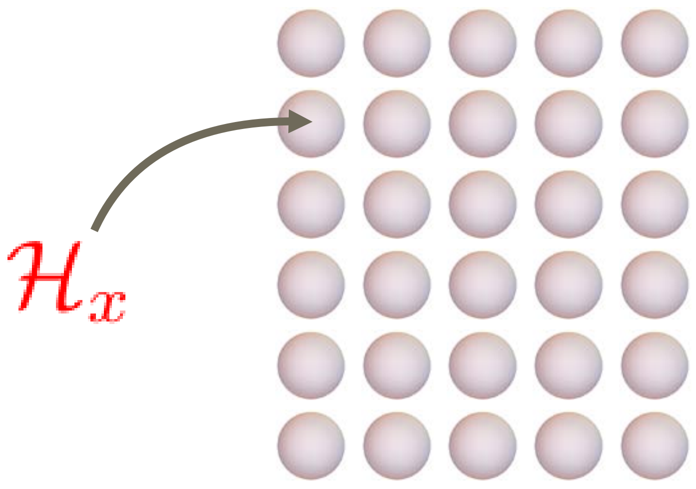
Setup I: Hilbert Space

- A system of *N* spins on a lattice

$$\mathcal{H} = \bigotimes_{x=1}^{N} \mathcal{H}_x$$

local Hilbert space $\dim[\mathcal{H}_x] = S$

e.g. *S*=2 for spin 1/2



- Energy shell $\mathcal{H}_{\rm sh} \subset \mathcal{H}$ with mean *E* and width *ΔE*

spanned by $|E_\alpha\rangle$ with $E_\alpha \in [E - \Delta E, E + \Delta E]$

- We assume

ΔE changes at most polynomially with *N*;
the Hilbert-space dimension is exponentially large.

$$d_{\rm sh} = \dim[\mathcal{H}_{\rm sh}]$$

Setup II: Operator Spaces

Basis set of operators $\mathcal{L}(\mathcal{H}_x)$ acting on local Hilbert space

$$\left\{\hat{\lambda}_x^0 := \hat{\mathbb{I}}_x, \hat{\lambda}_x^1, \cdots, \hat{\lambda}_x^{S^2-1}\right\}$$

S x *S* Hermitian matrices

normalization $\mathrm{Tr}_x[\hat{\lambda}_x^{\mu}\hat{\lambda}_x^{\mu'}] = S\delta_{\mu\mu'}$

e.g. spin 1/2 $\left\{\hat{I}, \hat{\sigma}^x, \hat{\sigma}^y, \hat{\sigma}^z\right\}$

Basis set $\mathcal{L}(\mathcal{H})$ acting on entire Hilbert space

$$\mathcal{B}_N = \left\{\hat{\Lambda}'_{\mu_1,\cdots,\mu_N} = \bigotimes_{x=1}^N \hat{\lambda}_x^{\mu_x} | 0 \leq \mu_x \leq S^2 - 1\right\}$$

$$\mathrm{Tr}[\hat{\Lambda}_{\mu_1\cdots\mu_N}\hat{\Lambda}_{\mu'_1\cdots\mu'_N}] = S^N \prod_{x=1}^N \delta_{\mu_x\mu'_x}$$

e.g. spin 1/2

$$\mathcal{B}_N = \left\{\hat{I}, \hat{\sigma}_1^x, \hat{\sigma}_1^y, \hat{\sigma}_1^z, \hat{\sigma}_2^x, \cdots, \hat{\sigma}_N^z, \hat{\sigma}_1^x\hat{\sigma}_2^x, \hat{\sigma}_1^x\hat{\sigma}_2^y, \cdots, \hat{\sigma}_{N-1}^z\hat{\sigma}_N^z, \cdots, \hat{\sigma}_1^z\cdots\hat{\sigma}_N^z\right\}$$

Setup III: *m*-body observables

Basis set of operators acting on at most *m* sites

$$\mathcal{B}_m = \left\{ \bigotimes_{i=1}^{q} \hat{\lambda}_{x_i}^{\alpha_{x_i}} \middle| 1 \le q \le m, 1 \le x_i \le N, 1 \le \alpha_{x_i} \le S^2 - 1 \right\}$$

e.g. spin 1/2 and *m* =2 — at most two Pauli operators

$$\mathcal{B}_m = \left\{ \hat{I}, \hat{\sigma}_1^x, \hat{\sigma}_1^y, \hat{\sigma}_1^z, \hat{\sigma}_2^x, \cdots, \hat{\sigma}_N^z, \hat{\sigma}_1^x\hat{\sigma}_2^x, \hat{\sigma}_1^x\hat{\sigma}_2^y, \cdots, \hat{\sigma}_{N-1}^z\hat{\sigma}_N^z \right\}$$

m-body observables

defined as linear combinations of elements in $\mathcal{B}_m$, but not in $\mathcal{B}_{m-1}$ alone

e.g. spin 1/2 and *m*=2

O $\sum_{i=1}^{N} \hat{\sigma}_i^z + \hat{\sigma}_1^x \hat{\sigma}_5^y, \ \sum_{i=1}^{N-1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z, \ \hat{\sigma}_1^x \hat{\sigma}_2^x + \hat{\sigma}_1^x + 2$

2-body operators

× $\sum_{i=1}^{N} \hat{\sigma}_i^z, \ \hat{\sigma}_3^z + 1, \ \hat{\sigma}_3^z \hat{\sigma}_5^y \hat{\sigma}_6^z$

1-body 3-body

Few-body observables

At most *m*-body observables

expressed as linear combinations of elements in $\mathcal{B}_m$

e.g. spin 1/2 and *m*=2

O $\sum_{i=1}^{N}\hat{\sigma}_i^z+\hat{\sigma}_1^x\hat{\sigma}_5^y,\ \sum_{i=1}^{N-1}\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z,\ \hat{\sigma}_1^x\hat{\sigma}_2^x+\hat{\sigma}_1^x+2,\ \sum_{i=1}^{N}\hat{\sigma}_i^z,\ \hat{\sigma}_3^z+1$ ✕ $\hat{\sigma}_3^z\hat{\sigma}_5^y\hat{\sigma}_6^z$

e.g. spin 1/2 and *m*=*N*

O $\sum_{i=1}^{N}\hat{\sigma}_i^z+\hat{\sigma}_1^x\hat{\sigma}_5^y,\ \sum_{i=1}^{N-1}\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z,\ \hat{\sigma}_1^x\hat{\sigma}_2^x+\hat{\sigma}_1^x+2,\ \sum_{i=1}^{N}\hat{\sigma}_i^z,\ \hat{\sigma}_3^z+1,\hat{\sigma}_3^z\hat{\sigma}_5^y\hat{\sigma}_6^z,\prod_{i=1}^{N}\hat{\sigma}_i^x$

Few-body observables

m-body observables with $m\,(\ll N)$ & *N*-independent

e.g.

O $m=1, m=2, m=3$ ✕ $m=N,\ m=N/2,\ m=\sqrt{N}$

Randomly chosen observables

Denote elements of $\mathcal{B}_m$ as $\hat{\Lambda}_1, \cdots, \hat{\Lambda}_n$. $n = \sum_{q=0}^{m} \frac{N!(S^2-1)^q}{q!(N-q)!}$

Let $\mathcal{L}_m$ be a set of at most *m*-body observables $(\subset \mathcal{L}(\mathcal{H}))$ expressed as a linear combination of $\{\hat{\Lambda}_f\}_{f=1}^n$

Randomly chosen observables $\hat{G} \in \mathcal{L}_m$

$$\hat{G} = \sum_{f=1}^{n} G_f \hat{\Lambda}_f$$

$\vec{G} = (G_1, \cdots, G_n)$: real variables randomly taken from $P(\vec{G})$

probability distribution

We assume that $P(\vec{G})$ is invariant under *n* x *n* orthogonal transformations.

Reminder: typicality vs. typicality argument

Typicality over the Haar measure

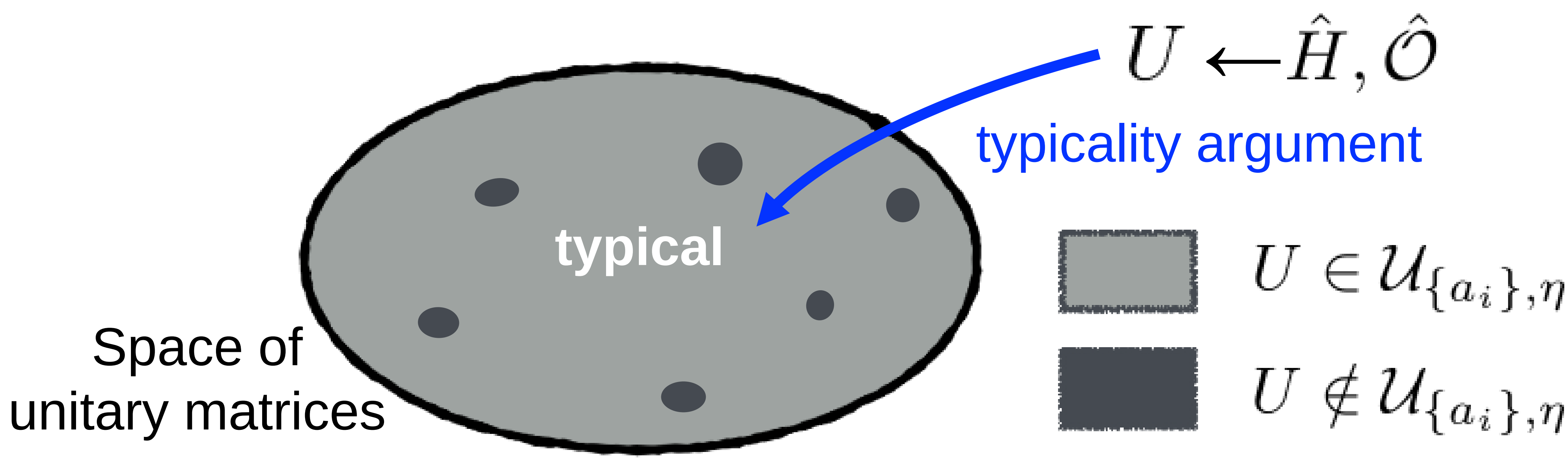
$$\mathcal{O}_{\alpha\alpha} = \sum_{i=1}^{d_{\rm sh}} a_i |U_{\alpha i}|^2$$

$$U \in \mathcal{U}_{\{a_i\},\eta} \Leftrightarrow \max_{|E_\alpha\rangle,|E_\beta\rangle \in \mathcal{H}_{\rm sh}} |\mathcal{O}_{\alpha\alpha} - \mathcal{O}_{\beta\beta}| < ||\hat{\mathcal{O}}||_{\rm op} d_{\rm sh}^{-\eta}$$

$(0 < \eta < 1/2)$ maximum difference exponentially small

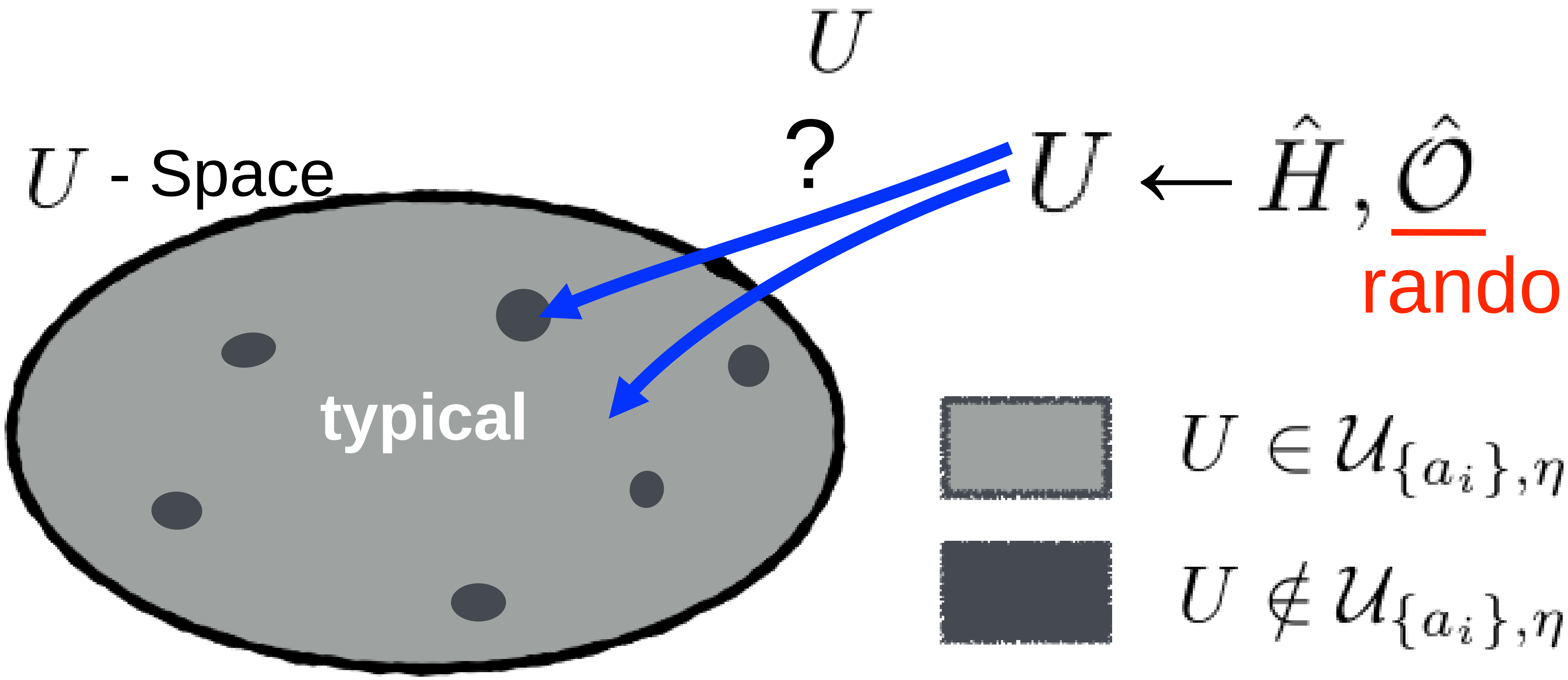
Typicality: almost all U 's belong to $\mathcal{U}_{\{a_i\},\eta}$ for $N \to \infty$

Typicality argument: *U* is typical for realistic *H* and *O.*



Are randomly chosen observables typical?

We fix Hamiltonian and randomly choose observables from $\mathcal{L}_m$, and then ask if the corresponding *U* is typical.



Main Theorem

We fix *k*-body $\hat{H}$ & randomly choose $\hat{O}$ from $\mathcal{L}_m$.

Let m $(k \leq m \ll N)$ be independent of *N*. → few-body

$\Lambda = \max_f ||\hat{\Lambda}_f||_{\mathrm{op}} \leq S^{\frac{m}{2}}$

$$\mathbb{P}_{\mathcal{L}_m}[U \in \mathcal{U}_{\{a_i\},\eta}] \leq \frac{\sqrt{\pi n}||\hat{H}||_{\mathrm{op}}\Lambda}{2\Delta E} \frac{\Gamma\left(\frac{n}{2}\right)}{\Gamma\left(\frac{n-1}{2}\right)} d_{\mathrm{sh}}^{-\eta}$$

probability associated with $P(\vec{G})$

The probability that *U* is typical is exponentially small unless $||\hat{H}||_{\mathrm{op}}$ is exponentially large or *ΔE* is exponentially small with respect to the size of the system *N.*

R. Hamazaki & MU, Phys. Rev. Lett. **120**, 080603 (2018)

Atypicality of most few-body observables

Most few-body observables have atypical diagonal matrix elements: $U \notin \mathcal{U}_{\{a_i\},\eta}$

$$\max_{|E_\alpha\rangle, |E_\beta\rangle \in \mathcal{H}_{\rm sh}} |\mathcal{O}_{\alpha\alpha} - \mathcal{O}_{\beta\beta}| \geq ||\hat{\mathcal{O}}||_{\rm op} d_{\rm sh}^{-\eta}$$

Fluctuations of diagonal matrix elements are larger than what the unitary Haar measure predicts.

R. Hamazaki & MU, Phys. Rev. Lett. **120**, 080603 (2018)

Atypicality of most few-body observables

Most few-body observables have atypical diagonal matrix elements: $U \notin \mathcal{U}_{\{a_i\},\eta}$

→Typicality argument does not explain the ETH in realistic setups (few-body $\hat{H}$ and $\hat{O}$) if energy width decreases at most polynomially

Note: we do not claim the breakdown of the ETH itself

than what the unitary Haar measure predicts.

R. Hamazaki & MU, Phys. Rev. Lett. **120**, 080603 (2018)

Typicality to *N*-body observables

The typicality argument actually applies to *N*-body observables.

R. Hamazaki & MU, Phys. Rev. Lett. **120**, 080603 (2018)

Typicality to *N*-body observables

In fact, most observables randomly chosen from $\mathcal{L}_{m=N}$ are typical. That is, *U* belongs to the typical region.

$$U \in \mathcal{U}_{\{a_i\},\eta}$$

$$\downarrow$$

$$\max_{|E_\alpha\rangle,|E_\beta\rangle\in\mathcal{H}_{\mathrm{sh}}} |\mathcal{O}_{\alpha\alpha} - \mathcal{O}_{\beta\beta}| \ < \ ||\hat{\mathcal{O}}||_{\mathrm{op}} d_{\mathrm{sh}}^{-\eta}$$

$$\downarrow$$

$$\mathbb{P}_{\mathcal{L}_N}[U \notin \mathcal{U}_{\{a_i\},\eta}] \leq 2d \exp\left[-\frac{d d_{\mathrm{sh}}^{-2\eta}}{72\pi^3}\right] \to 0 \ (N \to \infty)$$

$$d = \dim[\mathcal{H}] = S^N$$

R. Hamazaki & MU, Phys. Rev. Lett. **120**, 080603 (2018)

Underlying physics

In operator space, *m*-body operators become exponentially dominant as *m* increases toward *N*.

What is typical in operator space is *N*-body operators.

What is typical for human beings is few-body.

Unfortunately, few-body operators are mathematically atypical.

Typicality for *N*-body observables

This result for *N*-body observables is actually highly nontrivial, since previous numerical results on ETH mainly focused on few-body observables.

The typicality for *N*-body observables suggests that many-body observables indeed satisfy the ETH.

Do *N*-body observables satisfy ETH?

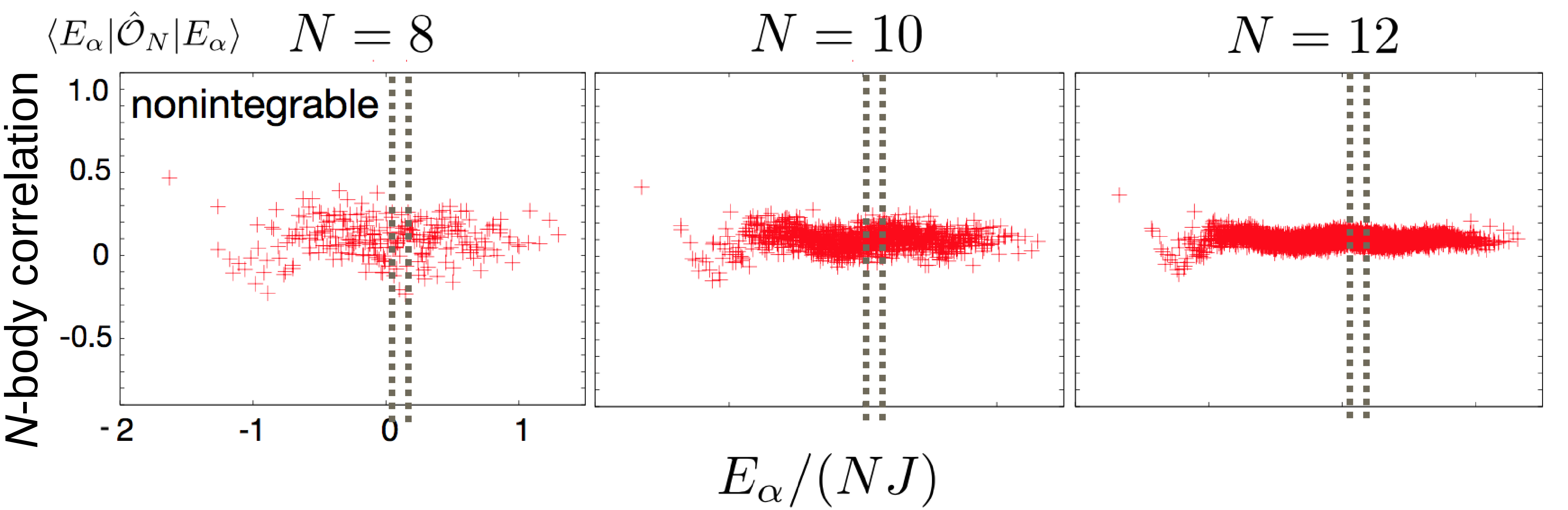
$$\hat{H} = -\sum_{i=1}^{N-1} J(1+\epsilon_i)\hat{\sigma}_i^z\hat{\sigma}_{i+1}^z - \sum_{i=1}^{N} h'\hat{\sigma}_i^x - \sum_{i=1}^{N} h\hat{\sigma}_i^z$$

nonintegrable spin model

random

$$\hat{\mathcal{O}}_N = \prod_{l=1}^{N} \hat{\sigma}_l^z$$

N-body correlation



The ETH holds true for the many-body observables!

A caveat on ETH

We have not excluded the possibility that the maximum variation of diagonal matrix elements decreases algebraically with increasing the size of the system.

If this is the case, the ETH holds true and thermalization occurs in the thermodynamic limit.

Conclusion

For few-body Hamiltonians, matrix elements of most few-body observables are atypical if the energy width changes at most polynomially with the system size.

The typicality argument does not apply to realistic few-body systems; it actually applies to *N*-body observables.

Lesson: what is comprehensible to human beings is simple few-body observables which are unfortunately atypical from a mathematical point of view.