Thermalization of isolated quantum systems and pure state statistical physics

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Why pure state stat. phys.?

Stat. phys. was developed before QM

We fix some issues of classical SM using QM (black body radiation, Gibbs paradox etc.), but what if a more fundamental "derivation" is necessary? (magnetic systems etc.)

Even if we don't worry about potential problems, QM can still provide a new perspective on SM.

"Although the subject has been under development for many years, we still do not have a complete and satisfactory theory, in the sense that there is no line of argument proceeding from the laws of microscopic mechanics to macroscopic phenomena, that is generally regarded by physicists as convincing in all respects."

E. T. Jaynes, Phys. Rev. **106**, 620 (1957)

"Statistical physics has not yet developed a set of generally accepted formal axioms."
"[It] has developed into a number of different schools, each with its own programme and technical apparatus. Unlike quantum theory or relativity, this field lacks a common set of assumptions that is accepted by most of the participants [...] But one common denominator seems to be that nearly all schools claim the founding fathers, Maxwell, Boltzmann and Gibbs as their champions.

J. Uffink, Compendium of the foundations of statistical physics (2006)

- ensembles: when and why do they work?
- classical SM: subjective lack of knowledge, coarse graining. In QM we have objective lack of knowledge! (Jaynes' Bayesian approach in the quantum world?)
- ergodicity: time scale is exp. large, very hard to prove

Take home message

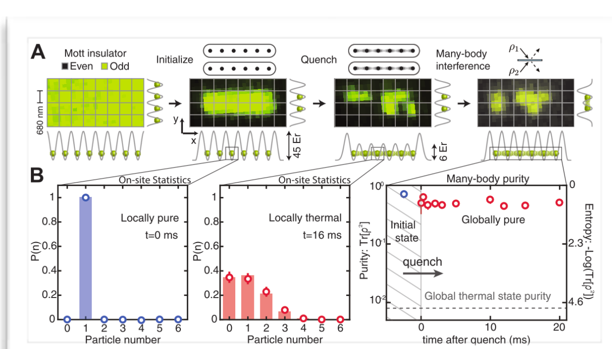
Individual quantum states can exhibit statistical properties.

Recommended literature

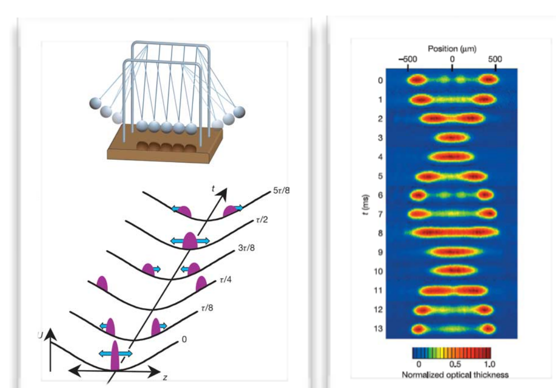
- C. Gogolin, J. Eisert, Rep. Prog. Phys. **79**, 056001 (2016): rigorous theorems and bounds
- C. Gogolin, Ph.D. thesis, arXiv:1003.5058
- J. Gemmer J, M. Michel, G. Mahler, "Quantum thermodynamics" (2009)

- A. Polkovnikov et al., Rev. Mod. Phys. **83** 863 (2011): many-body physics
- M. A. Cazalilla, M. Rigol, New J. Phys. **12** 55006 (2010)   (editorial of focus issue)
- L. D'Alessio et al., Adv. Phys. **65**, 239 (2016): many-body systems, ETH and more
- J. Eisert, M. Friesdorf, C. Gogolin, Nat. Phys. **11**, 124 (2015): many body systems

Remark: experiments! (e.g. cold atoms)



A. Kaufman et al., Science **353**, 794 (2016)



T. Kinoshita et al., Nature **440**, 900 (2006)

Typicality

Almost all pure states of a system is such that its (small enough) subsystems are in equilibrium.

- E. Schrödinger, Ann. Phys. **388**, 956 (1927); "Statistical Thermodynamics" (1952)
- J. Neumann, Z. Phys. **57**, 30 (1929); Eur. Phys. J. H **35**, 201 (2010); S. Goldstein et al., Proc. Roy. Soc. A **466**, 3203 (2010);
- S. Goldstein et al., "Canonical Typicality", Phys. Rev. Lett. **96**, 50403 (2006) (Aharonov!)
- Popescu et al., Nat. Phys. **2**, 754 (2007)

Theorem 1 *For a randomly chosen state* $|\phi\rangle \in \mathcal{H}_R \subseteq \mathcal{H}_S \otimes \mathcal{H}_E$ *and arbitrary* $\epsilon > 0$, *the distance between the reduced density matrix of the system* $\rho_S = \mathrm{Tr}(|\phi\rangle\langle\phi|)$ *and the canonical state* $\Omega_S = \mathrm{Tr}\, \mathcal{E}_R$ *is given probabilistically by*

$$\mathrm{Prob}\big[\, \|\rho_S - \Omega_S\|_1 \geq \eta \big] \leq \eta', \tag{9}$$

where

$$\eta = \epsilon + \sqrt{\frac{d_S}{d_E^{\mathrm{eff}}}}, \tag{10}$$

$$\eta' = 2 \exp\left(-C d_R \epsilon^2\right). \tag{11}$$

In these expressions, C *is a positive constant (given by* $C = (18\pi^3)^{-1}$*),* d_S *and* d_R *are the dimensions of* $\mathcal{H}_S$ *and* $\mathcal{H}_R$ *respectively, and* d_E^{eff} *is a measure of the effective size of the environment, given by*

$$d_E^{\mathrm{eff}} = \frac{1}{\mathrm{Tr}\,\Omega_E^2} \geq \frac{d_R}{d_S}, \tag{12}$$

- Objective "lack of knowledge"
- role of entanglement

P. Reimann, Phys. Rev. Lett. **99**, 160404 (2007):

- generalizes the distribution of states we draw from
- the state of the full system is indistinguishable from the average state with reasonable measurements

Instead of simply postulating that a certain ensemble yields a reasonable description of a certain physical situation, typicality shows, in a mathematically very well-defined way, when and why details do not matter. If most states anyway exhibit the same or very similar properties, then this does provide a heuristic, but pretty convincing, argument in favour of the applicability of ensembles. It is hence an argument supporting a description of large systems with ensembles.

Equilibration

Non-equilibrium states are non-generic

A time dependent property equilibrates on average if for most times during the evolution its value is close to some equilibrium value.

$$\mathrm{Tr}[\rho(t)A] = \sum_{n,m} \langle n|\rho(0)|m\rangle\langle m|A|n\rangle e^{-i(E_n-E_m)t} \longrightarrow \sum_n \langle n|\rho(0)|n\rangle\langle n|A|n\rangle = \mathrm{Tr}[\omega A] \qquad \omega = \sum_n \rho_{nn}(0)|n\rangle\langle n|$$

Theorem 1 (Generalization of Reimann's result [1]). *Consider a d-dimensional quantum system evolving under a Hamiltonian $H = \sum_n E_n P_n$, where P_n is the projector onto the eigenspace with energy E_n. Denote the system's density operator by $\rho(t)$, and its time-averaged state by $\omega \equiv \langle \rho(t)\rangle_t$. If H has non-degenerate energy gaps, then for any operator A,*

$$\sigma_A^2 \equiv \langle |\mathrm{tr}(A\rho(t)) - \mathrm{tr}(A\omega)|^2\rangle_t \leqslant \frac{\Delta(A)^2}{4d_{\mathrm{eff}}} \leqslant \frac{\|A\|^2}{d_{\mathrm{eff}}} \qquad (2)$$

where $\|A\|$ is the standard operator norm[1],

$$\Delta(A) \equiv 2 \min_{c\in\mathbb{C}} \|A - cI\|, \qquad (3)$$

and

$$d_{\mathrm{eff}} \equiv \frac{1}{\sum_n (\mathrm{tr}(P_n\rho(0)))^2}. \qquad (4)$$

[1] $\|A\| = \sup\{\sqrt{\langle v|A^\dagger A|v\rangle} : |v\rangle \in \mathcal{H} \text{ with } \langle v|v\rangle = 1\}$, or equivalently $\|A\|$ is the largest singular value of A.

Corollary 1. *Consider a quantum system evolving under a Hamiltonian with non-degenerate energy gaps. The average distinguishability of the system's state $\rho(t)$ from ω, given a finite set of measurements $\mathcal{M}$, satisfies*

$$\langle D_{\mathcal{M}}(\rho(t),\omega)\rangle_t \leqslant \frac{\sum_{M\in\mathcal{M}}\sum_r \Delta(M_r)}{4\sqrt{d_{\mathrm{eff}}}} \leqslant \frac{N(\mathcal{M})}{4\sqrt{d_{\mathrm{eff}}}}, \qquad (14)$$

where $N(\mathcal{M})$ is the total number of outcomes for all measurements in $\mathcal{M}$.

$$\langle D(\rho_S(t),\omega_S)\rangle_t \leqslant \frac{1}{2}\sqrt{\frac{d_S^2}{d_{\mathrm{eff}}}}.$$

P. Reimann, Phys. Rev. Lett. **101**, 190403 (2008)

Linden et al., Phys. Rev. E **79**, 061103 (2009)

A. Short, New J. Phys. **12**, 053009 (2011)

- Subsystem is completely general
- Energy can be non-extensive
- Interactions can be strong
- Eigenvalues and form of eigenvectors do not matter

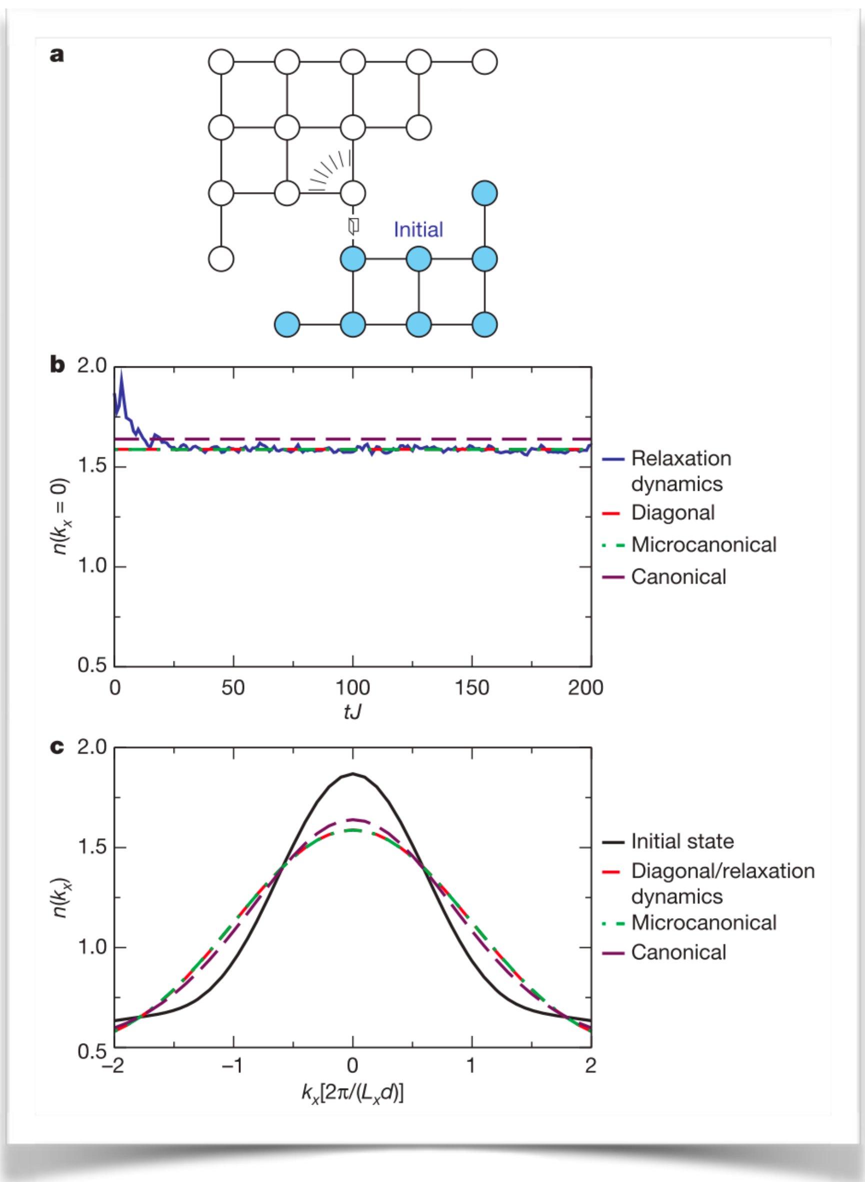
The last statement about subsystems does not have a classical analogue.

Subsystem equilibrates to the same state for almost all initial states of the bath.

Thermalization

1. Equilibration
2. subsystem initial state independence
3. bath state independence
4. diagonal form of subsystem equilibrium state (decoherence)
5. Gibbs state

M. Rigol, V. Dunjko, M. Olshanii, Nature **452**, 854 (2008) (1100+ citations and counting)



5 hardcore bosons on a 2D lattice of 21 sites (dim=20349)

if A thermalizes:

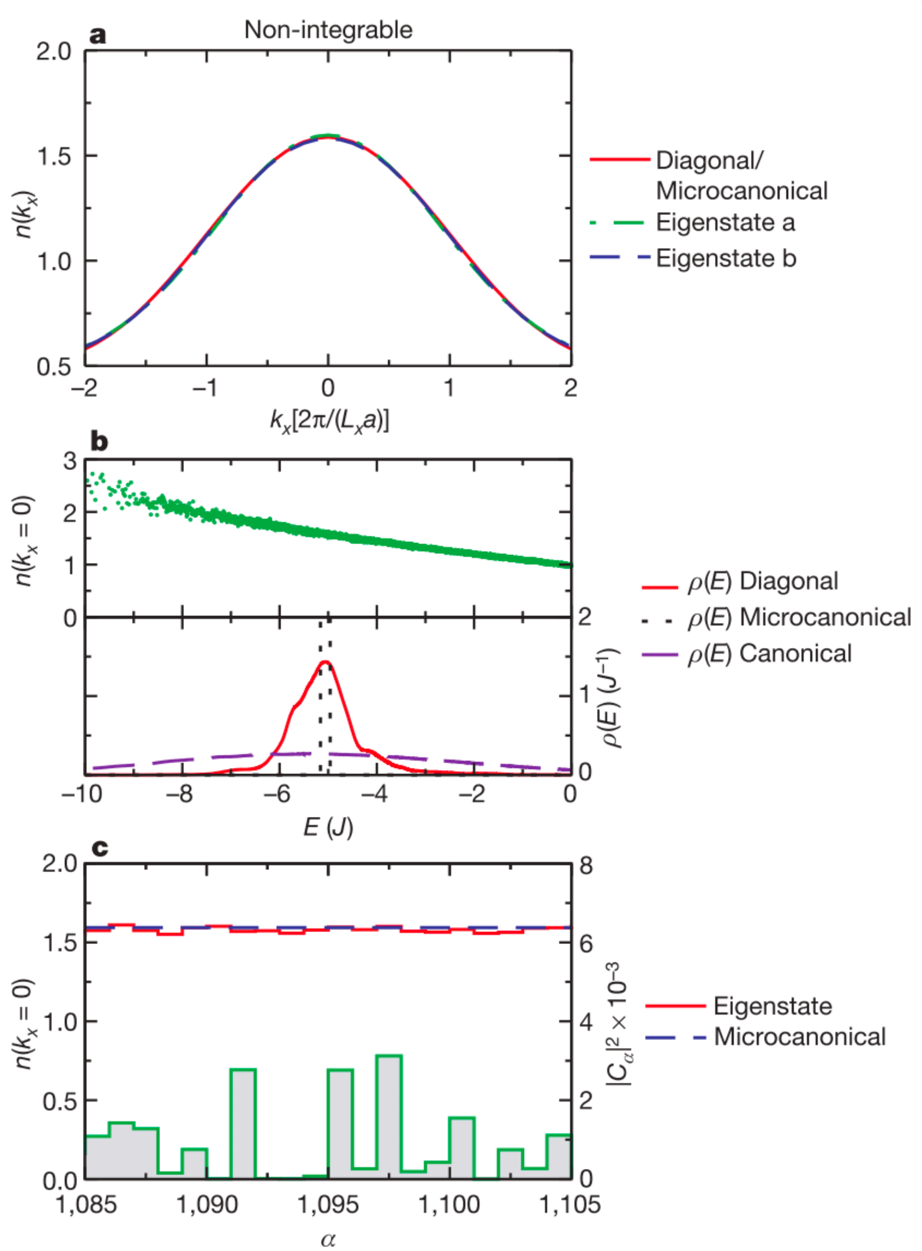
$$\sum_{\alpha} |C_\alpha|^2 A_{\alpha\alpha} = \langle A \rangle_{\text{microcan}}(E_0) \equiv \frac{1}{\mathcal{N}_{E_0,\,\Delta E}} \sum_{\substack{\alpha \\ |E_0 - E_\alpha| < \Delta E}} A_{\alpha\alpha}$$

?

3 possible explanations...

Thermalization and ETH

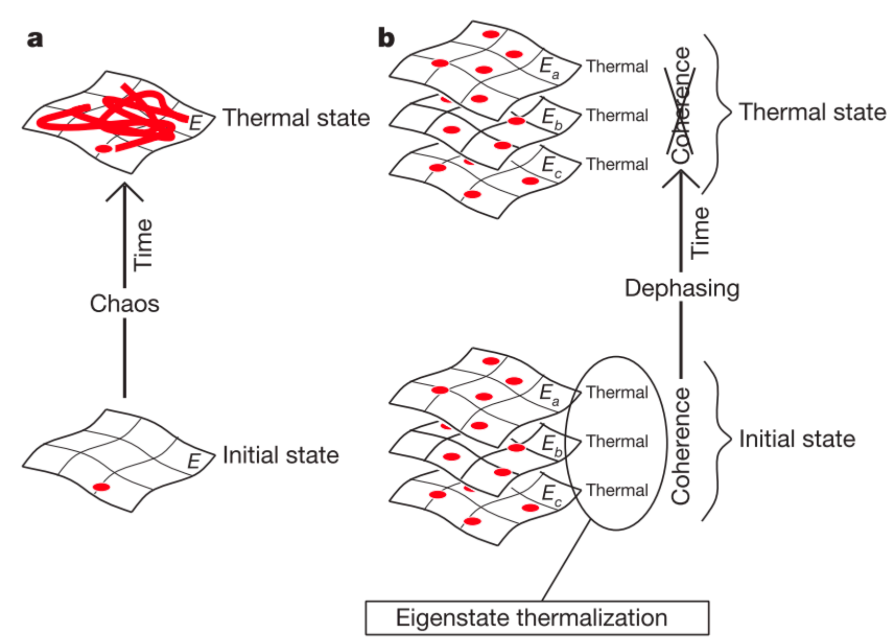
M. Rigol, V. Dunjko, M. Olshanii, Nature **452**, 854 (2008)



Eigenstate Thermalization Hypothesis:
the expectation value of an observable in an energy-E eigenstate is equal to the thermal average of the observable at mean energy E

J. M. Deutsch, Phys. Rev. A **43**, 2046 (1991); M. Srednicki, Phys. Rev. E **50**, 888 (1994)
R. Jensen, R. Shankar, Phys. Rev. Lett. **54**, 1879 (1985)

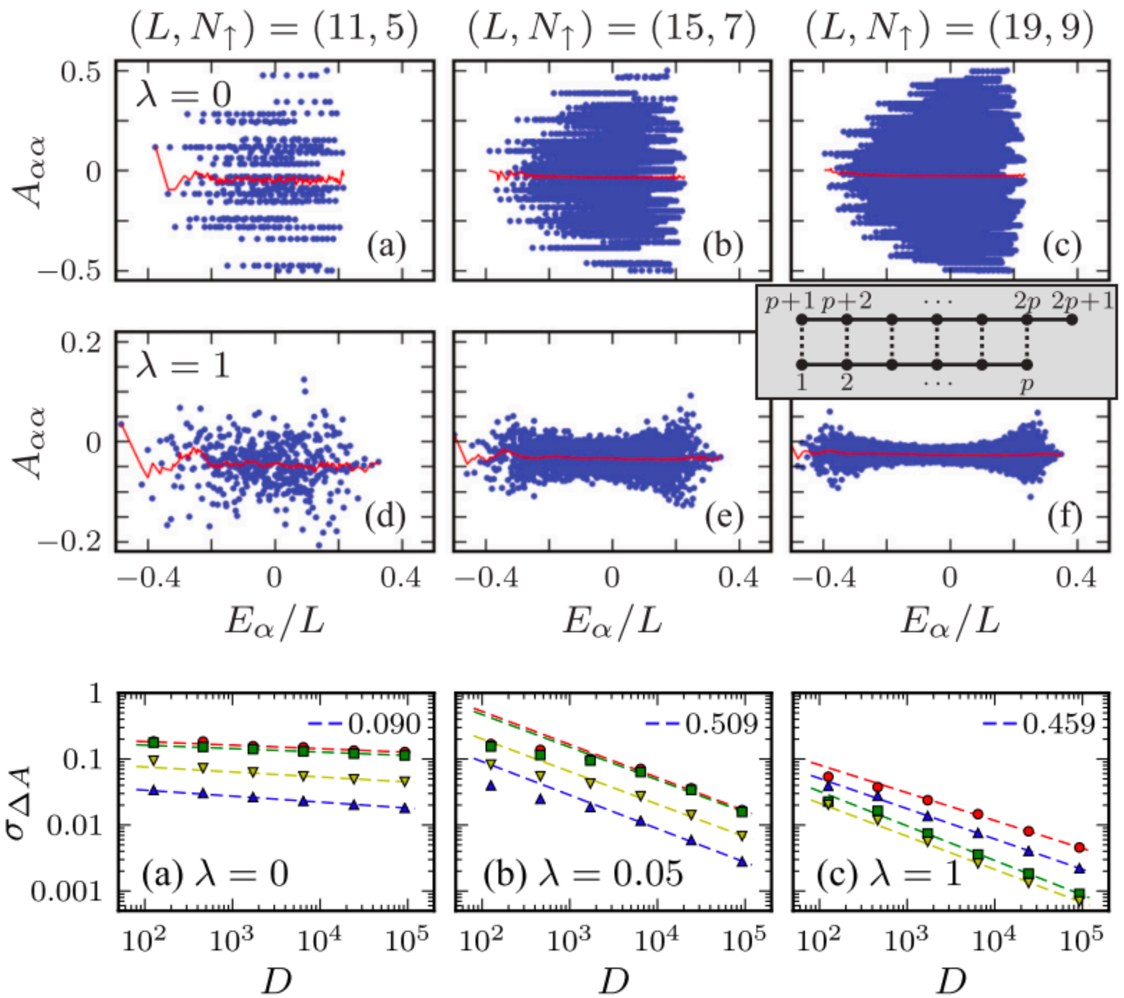
ETH suggests that classical and quantum thermal states have very different natures



Thermalization and ETH

System size dependence of the distribution of eigenstate expectation values

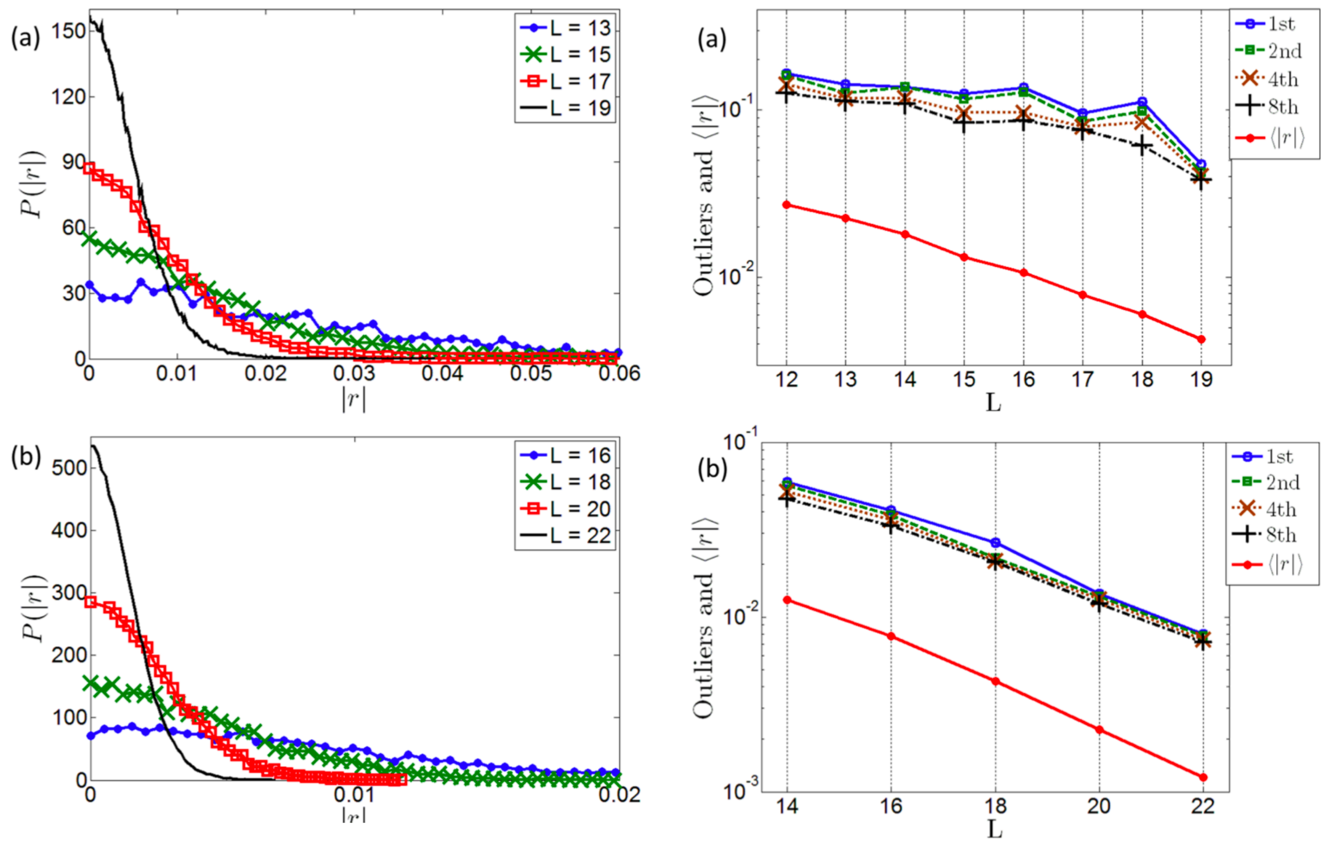
Variance scales as $[\dim(\mathcal{H})]^{-1/2}$



XXZ spin ladder

Even outliers approach the average

$$r_n = \langle n+1|\hat{O}|n+1\rangle - \langle n|\hat{O}|n\rangle$$



Tilted Ising chain, h.c. bosons

strong ETH seems to hold: all eigenstates are thermal

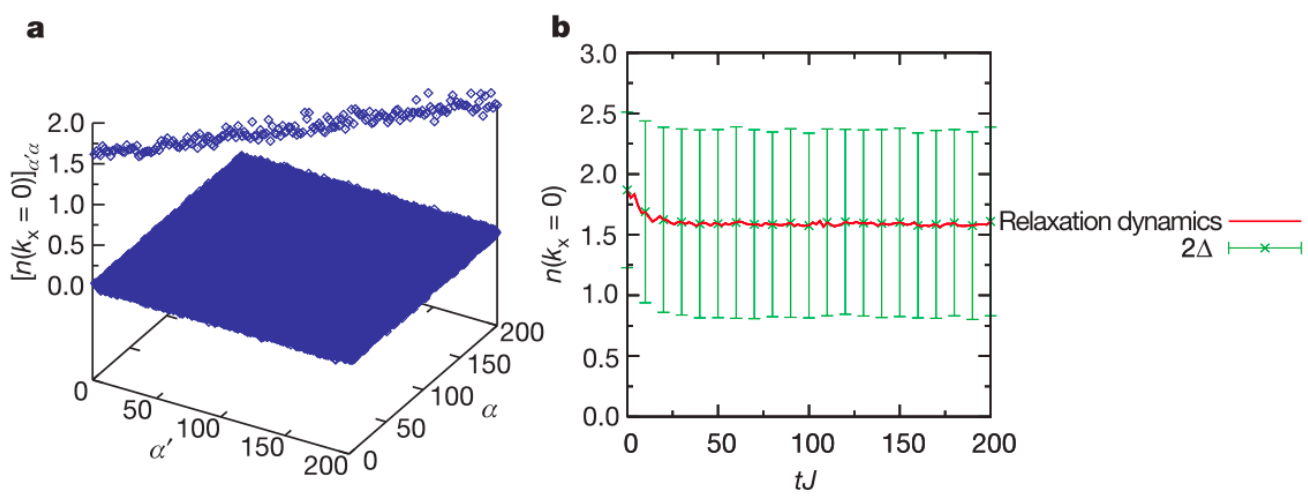
W. Beugeling, R. Moessner, M. Haque, Phys. Rev. E **89**, 042112 (2014)

H. Kim, T. Ikeda, D. Huse, Phys. Rev. E **90**, 052105 (2014)

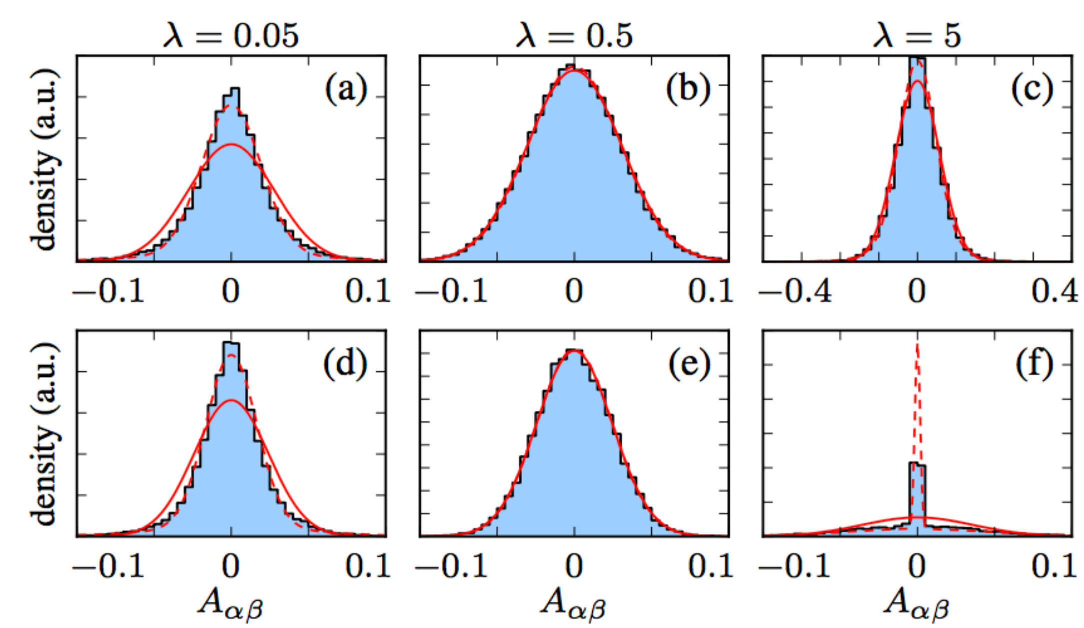
Thermalization and ETH

Off-diagonal matrix elements

Govern the temporal fluctuations: $\sigma_A^2 = \langle |\mathrm{tr}(A\rho(t)) - \mathrm{tr}(A\omega)|^2 \rangle_t \leq \max_{n \neq m} |\langle n|A|m\rangle^2$



M. Rigol, V. Dunjko, M. Olshanii, Nature **452**, 854 (2008)



XXZ spin ladder $\hat{A} = S_2^z S_{2+p}^z$

W. Beugeling, R. Moessner, M. Haque, Phys. Rev. E **91**, 012144 (2015)

$|A_{nm}|^2 \sim [\dim(\mathcal{H})]^{-1}$

ETH can be formulated as an ansatz for the matrix elements of physical observables in the basis of the eigenstates of a Hamiltonian [28]:

$$O_{mn} = O\left(\bar{E}\right) \delta_{mn} + e^{-S(\bar{E})/2} f_O\left(\bar{E}, \omega\right) R_{mn} \qquad (54)$$

where $\bar{E} \equiv (E_m + E_n)/2$, $\omega \equiv E_n - E_m$, and $S(E)$ is the thermodynamic entropy at energy E. Crucially, $O\left(\bar{E}\right)$ and $f_O\left(\bar{E}, \omega\right)$ are smooth functions of their arguments, the value $O\left(\bar{E}\right)$ is identical to the expectation value of the micro-canonical ensemble at energy $\bar{E}$ and R_{mn} is a random real or complex variable with zero mean and unit variance ($R_{mn}^2 = 1$ or $|R_{mn}|^2 = 1$).

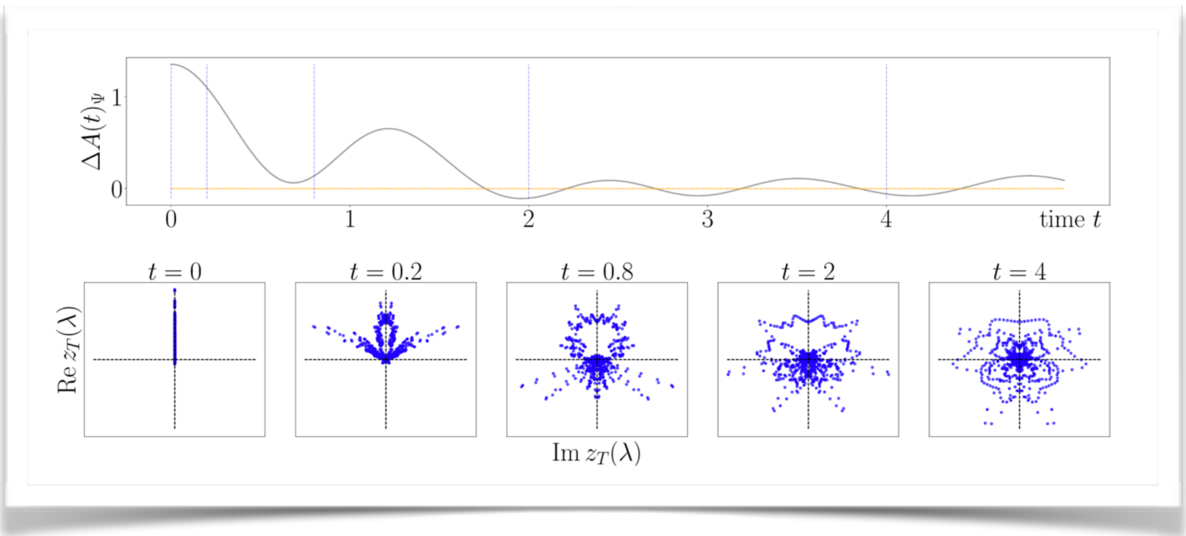
Time scale of equilibration

H. Wilming et al., arXiv:1704.06291
T. R. de Oliveira et al., arXiv:1704.06646

Equilibration as dephasing

$$\Delta A(t) = \mathrm{Tr}[\rho(t)A] - \langle \mathrm{Tr}[\rho(t)A]\rangle_t = \sum_{\Delta\neq 0} z_\Delta e^{i\Delta t}\,, \qquad z_\Delta = \sum_{E_m - E_n = \Delta} \langle n|\rho(0)|m\rangle\langle m|A|n\rangle$$

As $\Delta A(t)$ is large initially, the distribution of the complex numbers z_Δ must be anisotropic. The dispersion in the gaps makes them dephase, which leads to an isotropic configuration and a small $\Delta A(t)$.



Naively, $T \sim 2\pi/(\Delta_{\max} - \Delta_{\min})$. Better estimate:

$$\frac{2\pi}{T} \sim \sqrt{\frac{\sum_\Delta |z_\Delta|^2 \Delta^2}{\sum_\Delta |z_\Delta|^2}}$$

Example: uniformly distributed gaps, z_Δ follow a normal distribution independent of L

Need: smooth distribution z_Δ independent of L

Spectrum: distribution of gaps is roughly Gaussian of width $\sqrt{L}$, independent of integrability (!)

Initial state: can argue that most of the $\langle n|\rho(0)|m\rangle$ are small

Observable: for local H and A: $|\langle E_i|A|E_j\rangle| \leq \|A\|\,\mathrm{e}^{-\alpha(|E_i - E_j| - 2R)}$. Or invoke ETH form (without the "T").

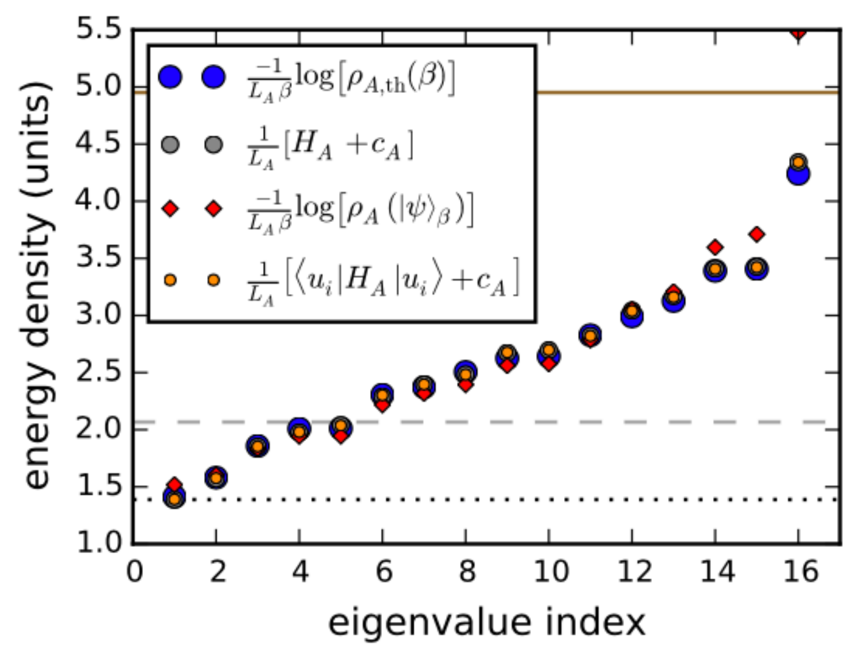
Thermalization and ETH

Which operators satisfy ETH?   Local? "Few-body"?

J. R. Garrison, T. Grover, "Does a single eigenstate encode the full Hamiltonian?", arXiv:1503.00729

"We conjecture and provide numerical evidence that ETH holds for all operators within a subsystem when the volume V_S of subsystem S satisfies $V_S \ll V$. [...] We also explore the more general condition $V_S < V/2$ and show that even in this case, ETH holds for a large class of operators."

"ETH allows one to calculate thermodynamical quantities as well as correlators at all temperatures/energy densities using only a single eigenstate."



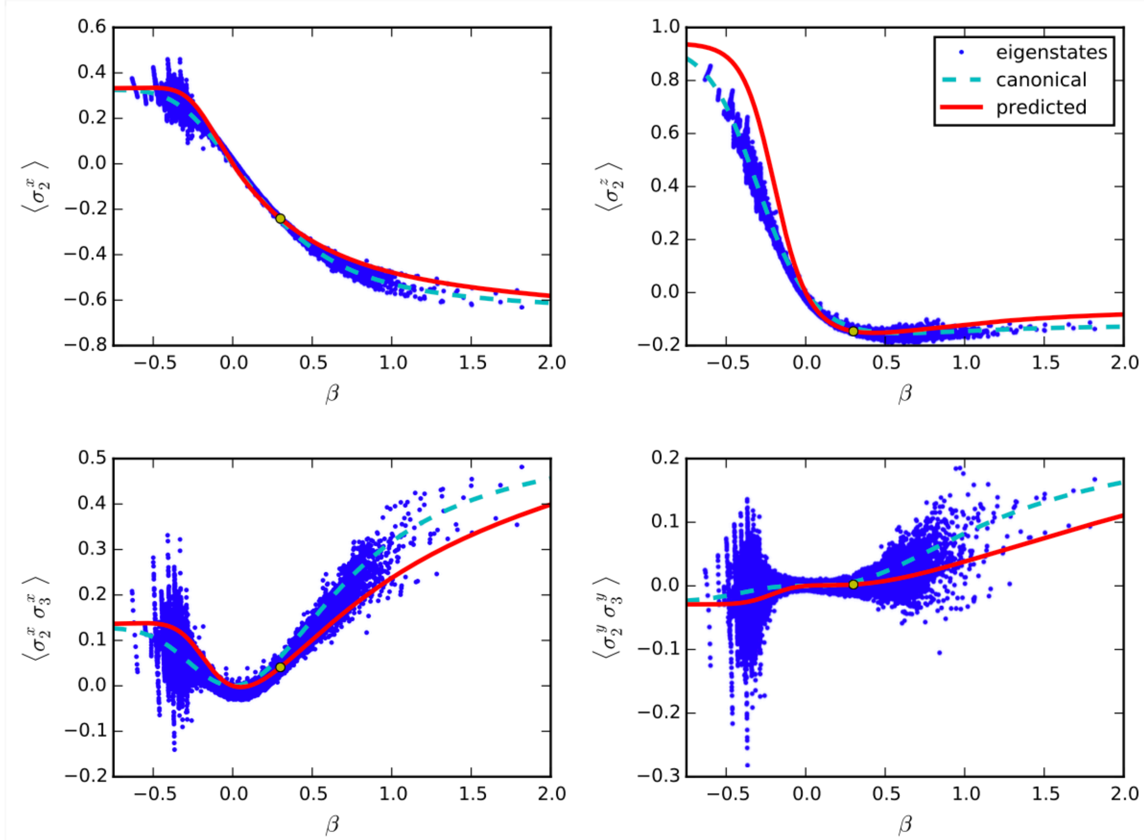


Figure 15: Equal time correlators for an $L = 21$ system plotted against inverse temperature β. The blue dots denote the expectation value with respect to each eigenstate, the dashed cyan curve plots the expectation value in the canonical ensemble, and the red curve plots the expectation value predicted from a single eigenstate at $\beta_0 = 0.3$ (yellow dot) by raising the $L_A = 4$ density matrix to the power β/β_0 and rescaling it to have unit trace.