Regression relation for pure quantum states and its implications for efficient computing

Boris Fine

Institute for Theoretical Physics
Heidelberg Graduate School of Fundamental Physics
University of Heidelberg

fine@uni-heidelberg.de

Universität Heidelberg Zukunft. Seit 1386.

HGSFP

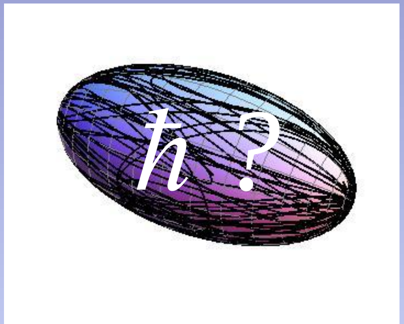
Center for Quantum Dynamics

Innovationsfonds FRONTIER/DFG

Motivation:

$$P(E) \cong e^{-\frac{E}{k_B T}}$$

Gibbs distribution



Energy shell in the phase space

Definition and implications of quantum chaos?

How to assign statistical weight to quantum superpositions that are not allowed classically?

Outline:

1. Regression relation for pure quantum states and its implication for efficient computing.
2. Properties of Lyapunov instabilities in classical spin systems.
3. Implications of microscopic chaos for the relaxation behavior in quantum spin systems.
4. Quantum ensemble with fixed energy expectation value and unrestricted participation of eigenstates

Regression relation for pure quantum states and its implications for efficient computing [T. A. Elsayed and B. F., arXiv:1208.4652]

Onsager's regression hypothesis (1931):

"*the average regression of fluctuations will obey the same laws as the corresponding macroscopic irreversible process*"

Today's view: ORH = high-temperature limit of the fluctuation-dissipation theorem.

$$\mathrm{Tr}\left\{\hat{A}(t)\rho_{\mathrm{neq}}\right\} = \frac{\alpha}{N}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$$

$$\rho_{\mathrm{neq}} = \frac{1}{N}\exp(\alpha\hat{A})$$

Felix Israilev:

What is the practicality of typicality?

Quantum typicality:

One quantum superposition is enough to represent the entire ensemble.

microcanonical ensemble

J. Gemmer, M. Michel, and G. Mahler, *Quantum Thermodynamics*

S. Goldstein, J. L. Leibowitz, R. Tumulka, and N. Zanghi, Phys. Rev. Lett. **96**, 050403 (2006)

S. Popescu, A. J. Short, and A. Winter, Nature Physics **2**, 754 (2006)

relaxation

C. Bartsch and J. Gemmer, Phys. Rev. Lett. **102**, 110403 (2009)

equilibrium fluctuations

C. Bartsch and J. Gemmer, Europhys. Lett. **96**, 60008 (2011)

quantum parallelism

G. A. Álvarez, E. P. Danieli, P. R. Levstein, and H. M. Pastawski, Phys. Rev. Lett. **101**, 120503 (2008)

Onsager's regression hypothesis:

$$\mathrm{Tr}\left\{\hat{A}(t)\rho_{\mathrm{neq}}\right\} = \frac{\alpha}{N}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$$

Relaxation of QM expectation value in a pure state:

$$\langle\Psi_{\mathrm{neq}}|\hat{A}(t)|\Psi_{\mathrm{neq}}\rangle = \mathrm{Tr}\left\{\hat{A}(t)\rho_{\mathrm{neq}}\right\}\left[1 + O\left(\frac{1}{\alpha\sqrt{N}}\right)\right]$$

C. Bartsch and J. Gemmer, Phys. Rev. Lett. **102**, 110403 (2009)

Fluctuations of QM expectation value in a pure state:
[T. A. Elsayed and B. F., arXiv:1208.4652] :

$$C(t,T) = \frac{1}{N^2}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\} + \Delta_1$$

$$C(t,T) \equiv \frac{1}{2T}\int_{-T}^{T} dt' \langle\Psi_{\mathrm{eq}}|\hat{A}(t+t')|\Psi_{\mathrm{eq}}\rangle\langle\Psi_{\mathrm{eq}}|\hat{A}(t')|\Psi_{\mathrm{eq}}\rangle$$

$$|\Psi_{\mathrm{eq}}\rangle = \sum_{k=1}^{N} a_k|\phi_k\rangle$$

$$P(|a_k|^2) = N\exp(-N|a_k|^2)$$

with random phases

$$\overline{\Delta_1^2} \approx \frac{1}{2\sqrt{2}\,TN^4}\int_{-T\sqrt{2}}^{T\sqrt{2}} dt_2 \left(\left[\mathrm{Tr}\left\{\hat{A}(t_2)\hat{A}(0)\right\}\right]^2 + \mathrm{Tr}\left\{\hat{A}(t-t_2)\hat{A}(0)\right\}\mathrm{Tr}\left\{\hat{A}(t+t_2)\hat{A}(0)\right\}\right)$$

$$C(t,T) \equiv \frac{1}{2T}\int_{-T}^{T} dt' \langle \Psi_{\rm eq}|\hat{A}(t+t')|\Psi_{\rm eq}\rangle \langle \Psi_{\rm eq}|\hat{A}(t')|\Psi_{\rm eq}\rangle$$

$$\mathrm{Tr}\left\{\hat{A}(t)\rho_{\rm neq}\right\} = \frac{\alpha}{N}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\}$$

$$\langle \Psi_{\rm neq}|\hat{A}(t)|\Psi_{\rm neq}\rangle = \mathrm{Tr}\left\{\hat{A}(t)\rho_{\rm neq}\right\}\left[1 + O\left(\frac{1}{\alpha\sqrt{N}}\right)\right]$$

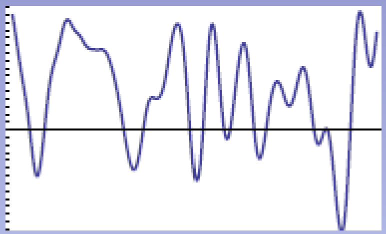
$$C(t,T) = \frac{1}{N^2}\mathrm{Tr}\left\{\hat{A}(t)\hat{A}(0)\right\} + \Delta_1$$

$$\Downarrow$$

Regression relation for pure states:

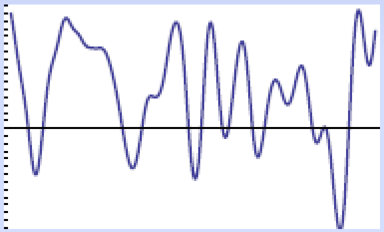
$$\lim_{N\to\infty} \langle \Psi_{\rm neq}|\hat{A}(t)|\Psi_{\rm neq}\rangle = \alpha \lim_{T\to\infty, N\to\infty} N C(t,T)$$

Equilibrium magnetization noise in a system of n <u>classical</u> spins



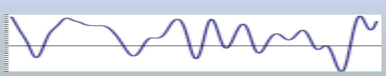
$\updownarrow$ $\sqrt{n\left\langle S_{iz}^2\right\rangle}$

Equilibrium noise of <u>monitored</u> magnetization in a system of n <u>spins 1/2</u>



$\updownarrow$ $\sqrt{n\left\langle S_{iz}^2\right\rangle}$

Equilibrium noise of the <u>magnetization expectation value</u> in a random pure state for a system of n <u>spins 1/2</u>



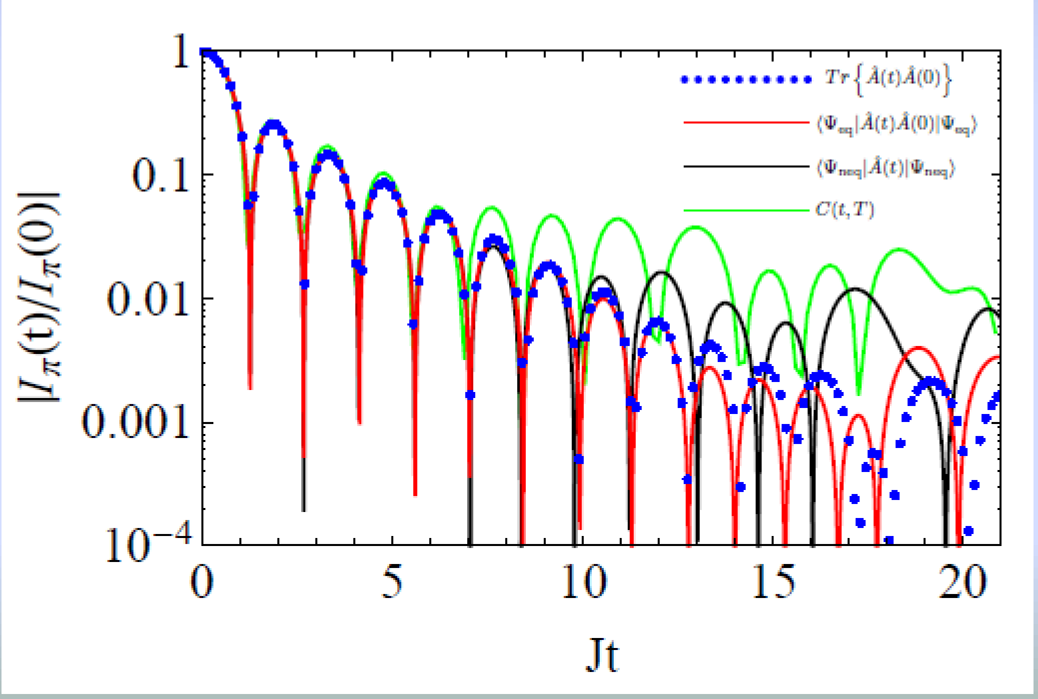
$\updownarrow$ $\dfrac{\sqrt{n\left\langle S_{iz}^2\right\rangle}}{2^{n/2}}$

Direct sampling of the trace:

$$\langle \Psi_{\rm eq} | \hat{A}(t) \hat{A}(0) | \Psi_{\rm eq} \rangle = \frac{1}{N} {\rm Tr} \left\{ \hat{A}(t) \hat{A}(0) \right\} + \Delta_2$$

$$\overline{\Delta_2^2} = \frac{1}{N^2} {\rm Tr} \left\{ \hat{A}(t) \hat{A}(0) \hat{A}(t) \hat{A}(0) \right\}$$

Intermediate dynamic structure factor $I_\pi(t)$ for the Heisenberg chain of 20 spins 1/2



Direct integration of the Schrödinger equation – 4th order Runge-Kutta

$$|\Psi(t+\Delta t)\rangle = |\Psi(t)\rangle + |v_1\rangle + |v_2\rangle + |v_3\rangle + |v_4\rangle$$

$$|v_1\rangle = -i\mathcal{H}|\Psi(t)\rangle\Delta t$$

$$|v_2\rangle = -\tfrac{1}{2}i\mathcal{H}|v_1\rangle\Delta t$$

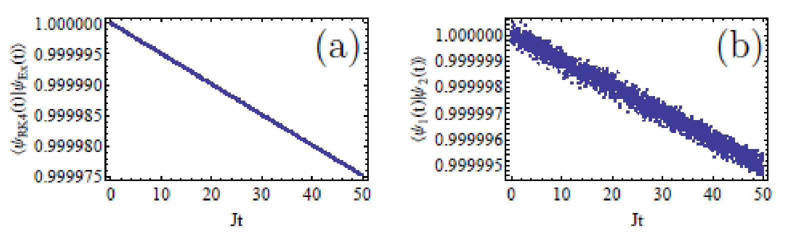
$$|v_3\rangle = -\tfrac{1}{3}i\mathcal{H}|v_2\rangle\Delta t$$

$$|v_4\rangle = -\tfrac{1}{4}i\mathcal{H}|v_3\rangle\Delta t$$

Memory requirement:
~ $N \log N$ for short-range interactions
~ $N \log^2 N$ for long-range interactions

Complete diagonalization: ~ N^2

Tests:



Calculations of time correlation functions require propagating two pure states:

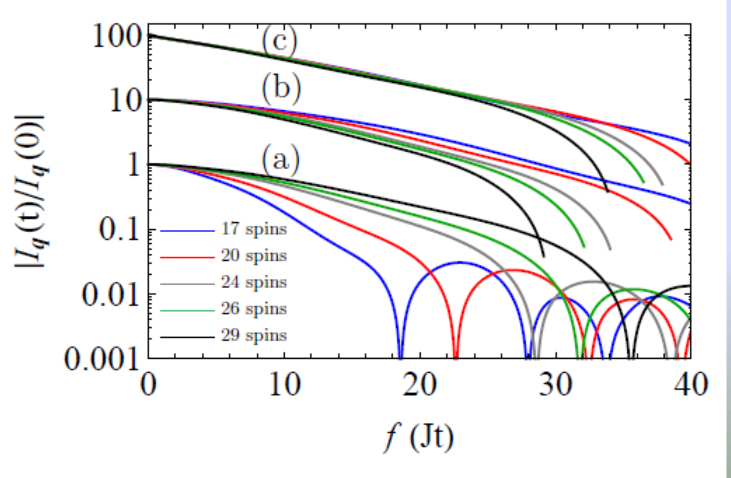
$$\langle\Psi_{eq}|\hat{A}(t)\hat{A}(0)|\Psi_{eq}\rangle = \langle\Psi_{eq}(t)|\hat{A}|\Phi(t)\rangle$$

$$|\Psi_{eq}(t)\rangle = \exp(-i\mathcal{H}t)|\Psi_{eq}(0)\rangle$$

$$|\Phi(t)\rangle = \exp(-i\mathcal{H}t)|\Phi(0)\rangle$$

$$|\Phi(0)\rangle = \hat{A}|\Psi_{eq}(0)\rangle$$

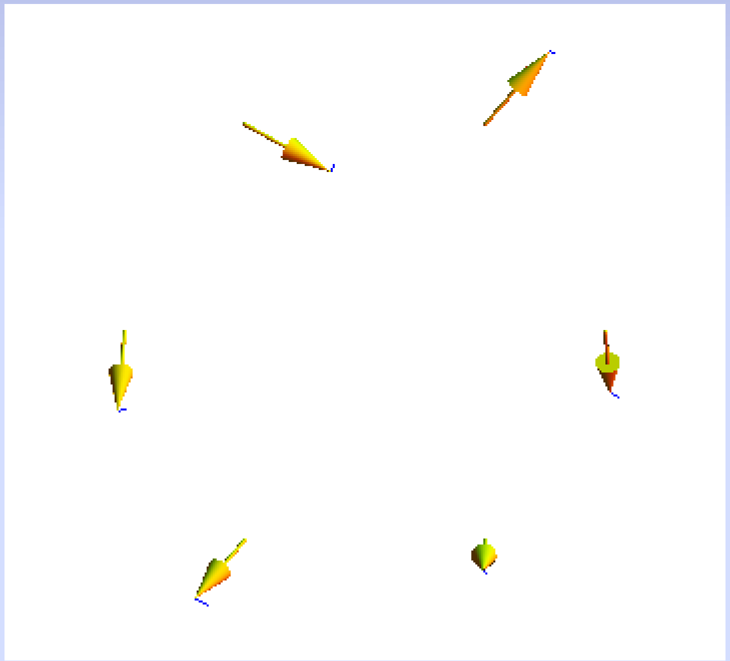
$I_{2\pi/n}(t)$

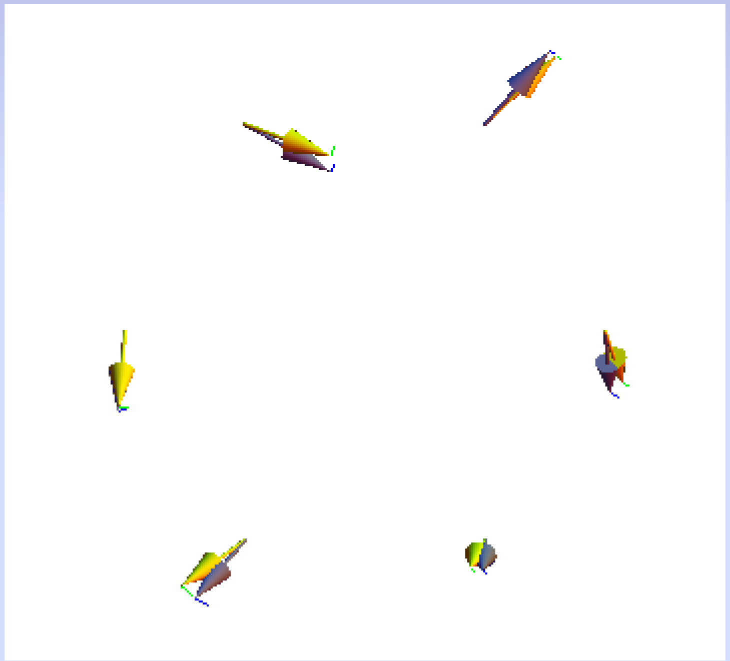


Part 2: Properties of Lyapunov instabilities in classical spin systems

[A. de Wijn, B. Hess, and B. F., Phys. Rev. Lett. **109**, 034101 (2012)]

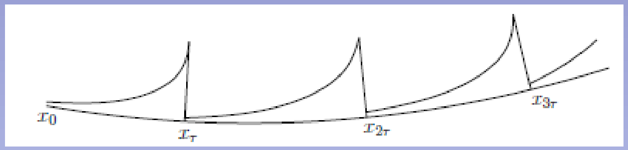
$$H = \sum_{i<j}^{\mathrm{NN}} J_x S_{ix} S_{jx} + J_y S_{iy} S_{jy} + J_z S_{iz} S_{jz}$$





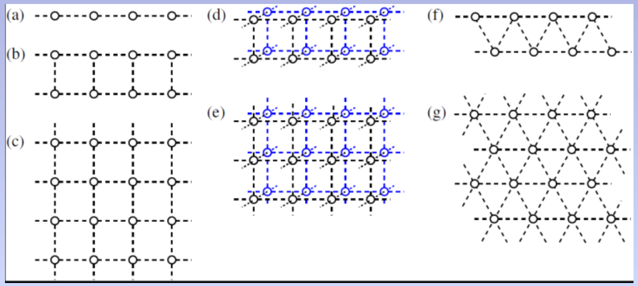
Survey of the largest Lyapunov exponents

$$\mathcal{H} = \sum_{m<n}^{NN} J_x S_m^x S_n^x + J_y S_m^y S_n^y + J_z S_m^z S_n^z$$



Interaction constants are randomly sampled

on a "sphere" $J_x^2 + J_y^2 + J_z^2 = 1$



Lessons learned:

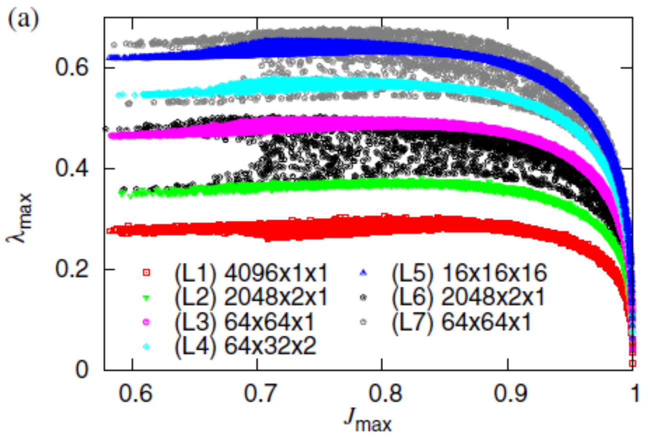
- No integrable cases for large spin lattices besides the case of $J_x = J_y = 0; \; J_z = 1.$

- The largest Lyapunov exponent is mostly controlled by $J_{max} = \max\left[|J_x|, |J_y|, |J_z| \right]$

- The dependence on J_{max} is mostly universal .
  For $J_{max} < 0.85,$ it is nearly flat.

- Near the integrable limit $J_{max} = 1$, the scaling is universal :

$$\lambda_{max} \cong (1 - J_{max})^{1/3}$$

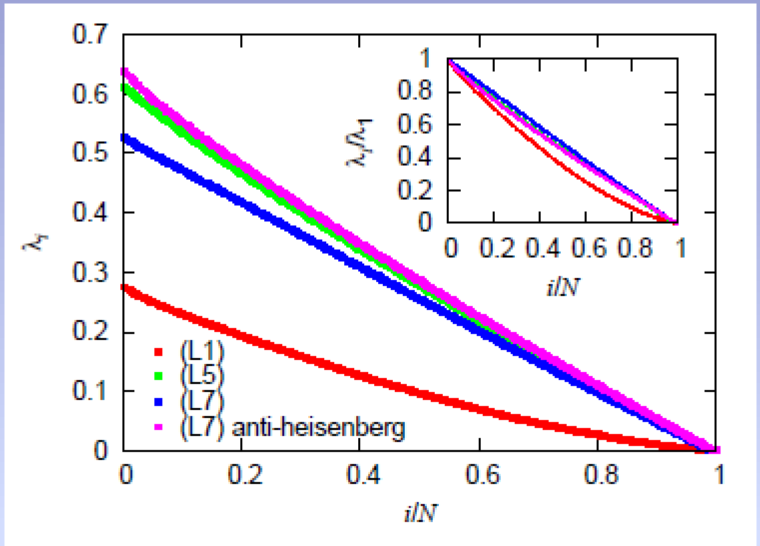


A. de Wijn, B. Hess, and B. F.,
Phys. Rev. Lett. **109**, 034101 (2012)

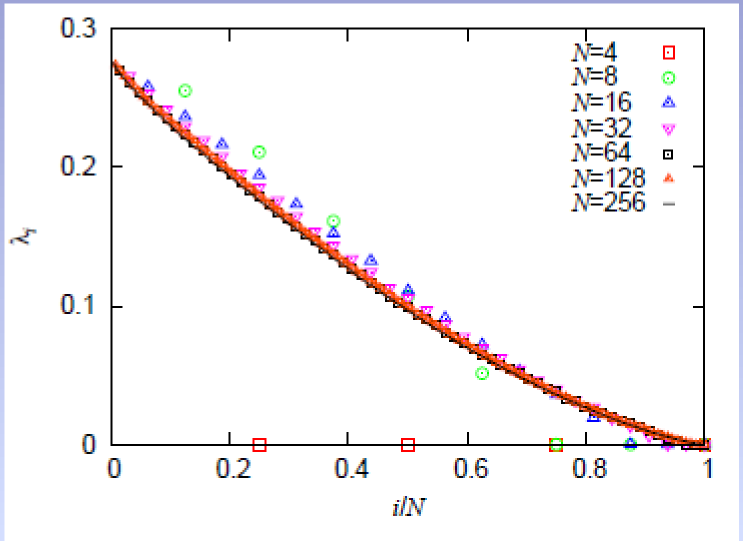
Lyapunov spectra

[A. de Wijn, B. Hess, and B. F., in preparation]

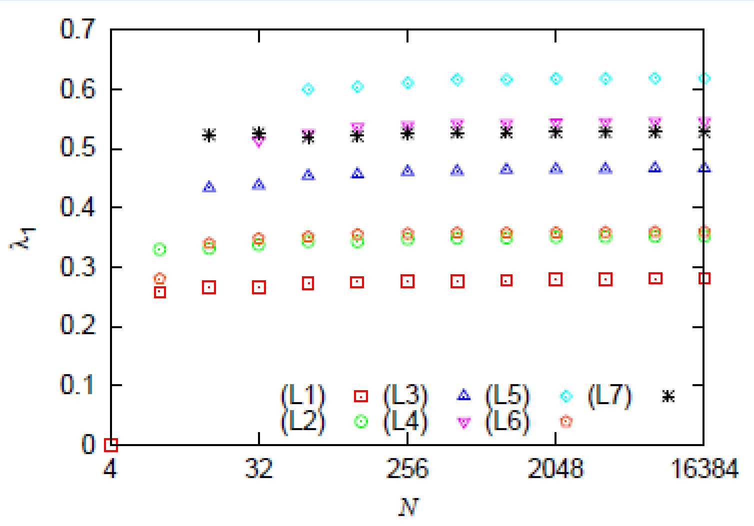
Four different lattices



Same lattice, different number of spins



Size dependence of the largest Lyapunov exponent



Part 3: Implications of microscopic chaos for the <u>observable</u> behavior of many-spin systems.

Level spacing statistics in not observable in many-body quantum systems

Lyapunov instabilities are not observable in many-body classical systems

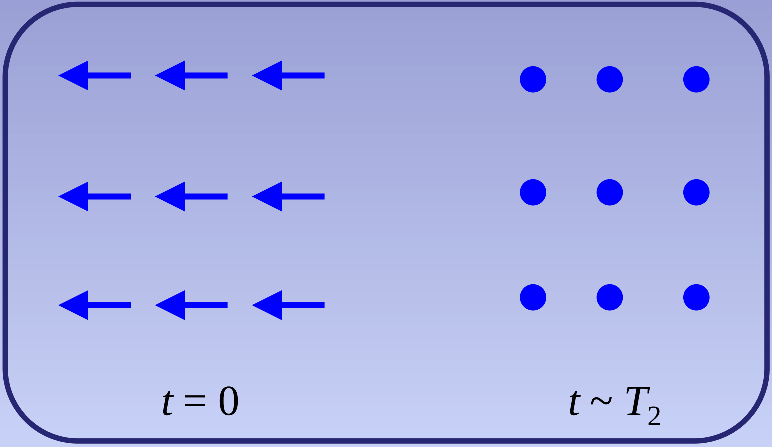
Can the notion of chaos be used as a quantitative resource for solving non-perturbative relaxation problems?

<u>In this part:</u>

- manifestations of chaos in the long-time behavior of nuclear spin decays in solids

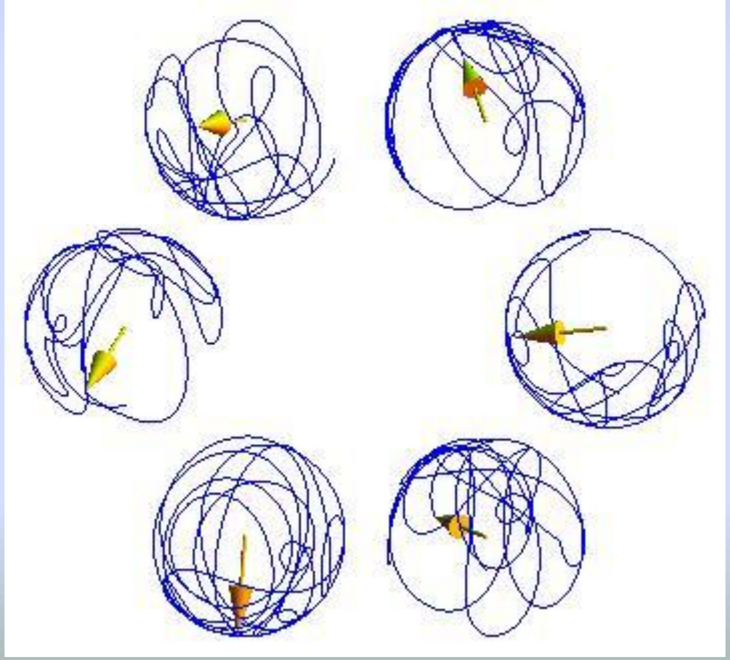
Formulation of NMR free induction decay problem

$$\mathcal{H} = \sum_{m<n} J^{z}_{mn} S^{z}_{m} S^{z}_{n} + J^{\perp}_{mn} \left(S^{x}_{m} S^{x}_{n} + S^{y}_{m} S^{y}_{n} \right)$$

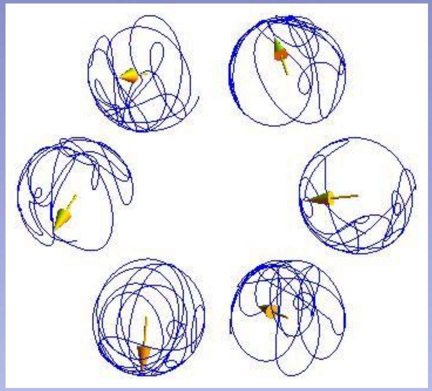


magnetic dipolar interaction:

$$J^{z}_{mn} = -2\, J^{\perp}_{mn} = \frac{g^2 \hbar^2 \left(1 - 3\cos^2\theta_{mn}\right)}{r^3_{mn}}$$



Generic long-time behavior of nuclear spin decays:
[*B. F.*, Int. J. Mod. Phys. B **18**, 1119 (2004)]



$$G(t) \sim e^{-\gamma t} \cos(\omega t + \phi), \quad \text{where} \quad \gamma, \omega \sim J\sqrt{N_{nn}}$$

Markovian behavior on non-Markovian time scale is a manifestation of chaos.

Chaotic eigenmodes of the time evolution operator:
Pollicott-Ruelle resonances [D. Ruelle, PRL **56**, 405 (1986)]

Expansion-contraction picture in the phase space:

Correlated diffusion equation for one-spin distribution function:

$$\frac{\partial f(t,\mathbf{x})}{\partial t} = \frac{\partial}{\partial \mathbf{x}} \left\{ D(\mathbf{x}) \frac{\partial f(t,\mathbf{x})}{\partial \mathbf{x}} - \int_{V_{\mathbf{x}'}} K(\mathbf{x},\mathbf{x}')\, f(t,\mathbf{x}')\, d\mathbf{x}' \right\}$$

Asymptotic behavior of many-spin density matrices:

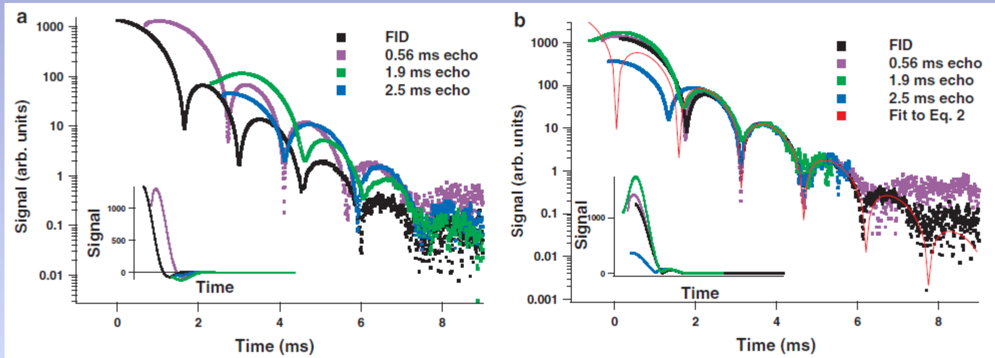
$$\rho_{kl}(t) = \rho_{0,kl}\, e^{-(\gamma + i\omega)t} + \rho^{+}_{0,kl}\, e^{-(\gamma - i\omega)t}$$

Quantitative relations between NMR free induction decays and spin echoes [B.F. PRL 94, 247601 (2005)]

$$\rho_{kl}(t) = \rho_{0,kl}\, e^{-(\gamma + i\omega)t} + \rho^{+}_{0,kl}\, e^{-(\gamma - i\omega)t}$$

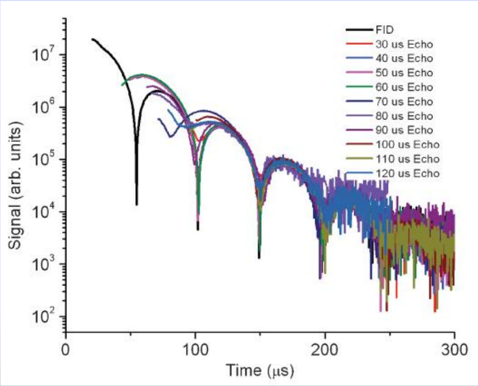
Identical constants γ and ω in $e^{-\gamma t} \cos(\omega t + \phi)$

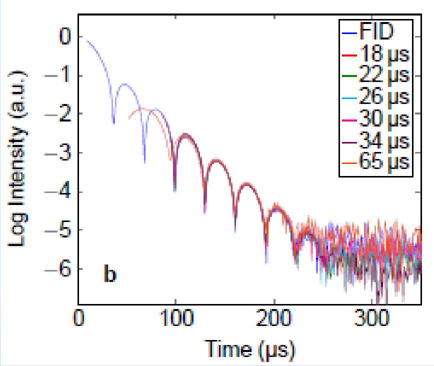
Experimental results for solid xenon:



S. W. Morgan et al, PRL **101**, 067601 (2008)

Experimental results for CaF_2:



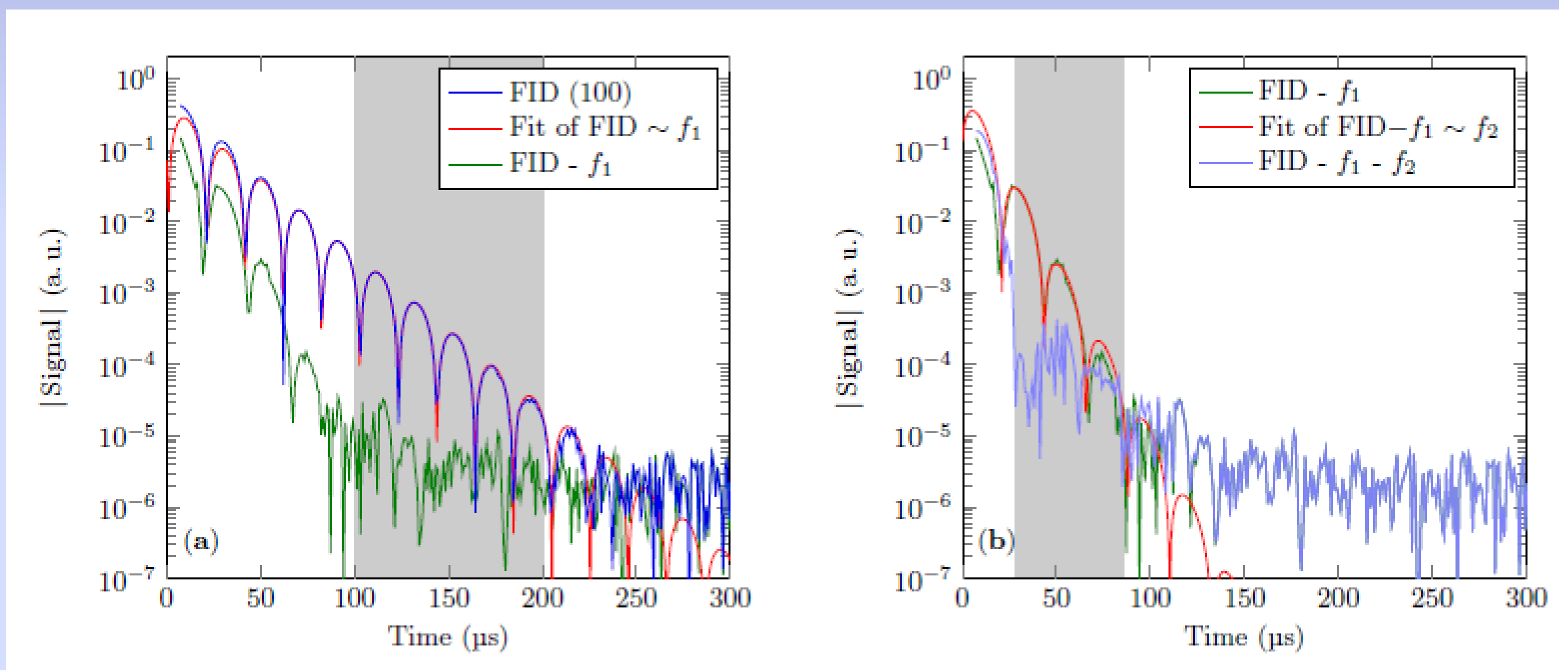


E. G. Sorte et al,
PRB **83**, 064302 (2011)

B. Meier et al,
Univ. of Leipzig, in preparation

Experimental observation of the second slowest relaxational eigenmode

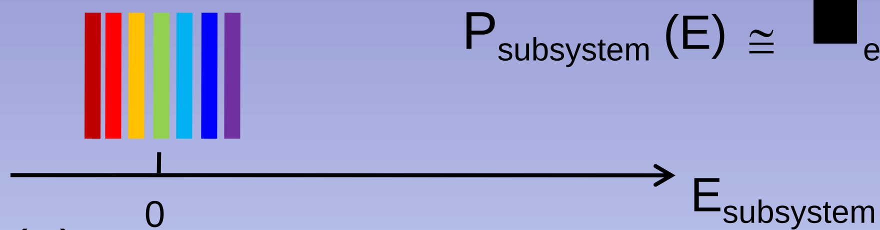
$$\frac{\partial f(t,\mathbf{x})}{\partial t} = \frac{\partial}{\partial \mathbf{x}} \left\{ D(\mathbf{x}) \frac{\partial f(t,\mathbf{x})}{\partial \mathbf{x}} - \int_{V_{\mathbf{x}'}} K(\mathbf{x},\mathbf{x}')\, f(t,\mathbf{x}')\, d\mathbf{x}' \right\}$$



B. Meier et al., Phys. Rev. Lett. **108**, 177602 (2012).

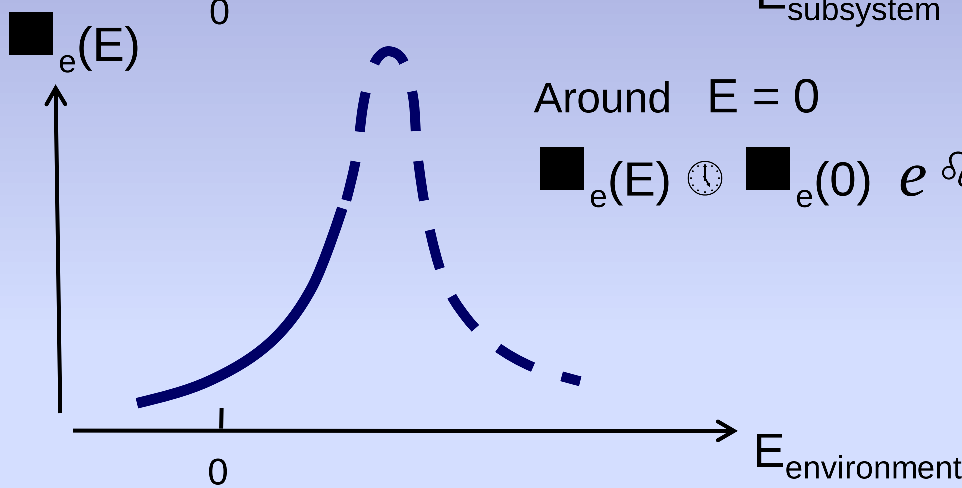
Part 4: Quantum ensemble with fixed energy expectation value and unrestricted participation of eigenstates

<u>Microcanonical ensemble</u>



$P_{subsystem}$ (E) ≅ ■$_e$(-E)~ $e^{-♌ E}$

Boltzmann-Gibbs



Around E = 0

■$_e$(E) 🕔 ■$_e$(0) $e^{♌ E}$

D. C. Brody and L. P. Hughston, (1998).

G. Aarts, G. F. Bonini, and C. Wetterich, (2000).

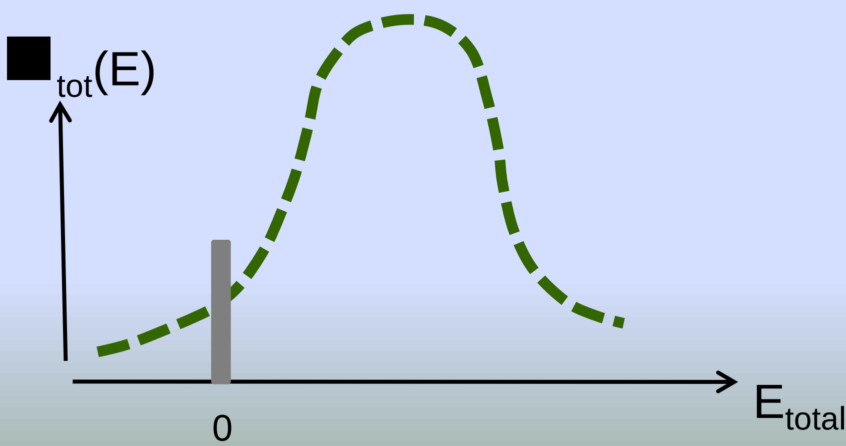
J. Naudts and E. Van der Straeten, (2006)

G. Jona-Lasinio and C. Presilla, (2006)

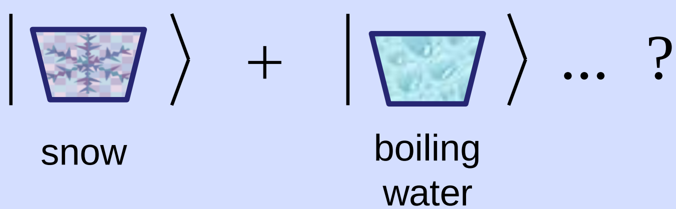
B.V. Fine, (2009).

B. Fresch and G. J. Moro, (2009).

M. Müller, D. Gross, and J. Eisert, (2011).



Why?

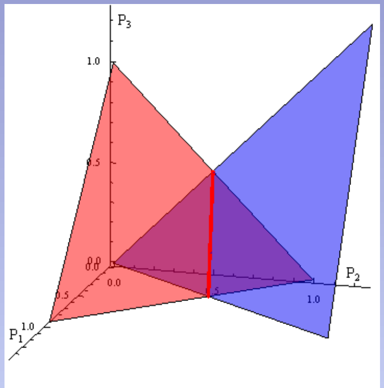


✡(t) = ♦ C_i $e^{-i E_i t}$ ♐$_i$

| C_i $e^{-i E_i t}$ | **do not depend on time.**

Quantum micro-canonical (QMC) ensemble:

$$\Psi = \sum_{i=1}^{N} C_i \phi_i$$



$$p_i = |C_i|^2$$

$$\sum_{i=1}^{N} E_i p_i = E_{\mathrm{av}}$$

unrestricted participation of eigenstates

$$\sum_{i}^{N} p_i = 1$$

$$p_i \geq 0, \qquad \forall i$$

W. K. Wootters, Found. Phys. **20**, 1365 (1990).

D. C. Brody and L. P. Hughston, J. Math. Phys. **39,** 6502 (1998).

C. M. Bender, D. C. Brody, and D. W. Hook, J. Phys. A **38,** L607 (2005).

B.V. Fine, Phys. Rev. E **80**, 051130 (2009).

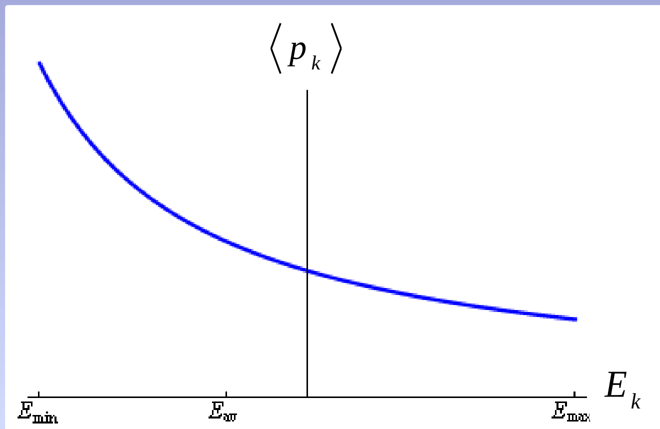
B. Fresch and G. J. Moro, J. Phys. Chem. A **113**, 14 502 (2009).

M. Müller, D. Gross, and J. Eisert, Commun. Math. Phys. **303**, 785 (2011).

Results: **QMC-based statistics for an isolated system with $N \gg 1$**

B.F., PRE 80, 051130 (2009)

$$V_k(p_k) = V_k(0)\exp\left\{(N-3)\left[\log(1-p_k) + \int_{E_{av}}^{E_{av}-\frac{(E_k-E_{av})p_k}{1-p_k}} \lambda[E]dE\right]\right\}$$



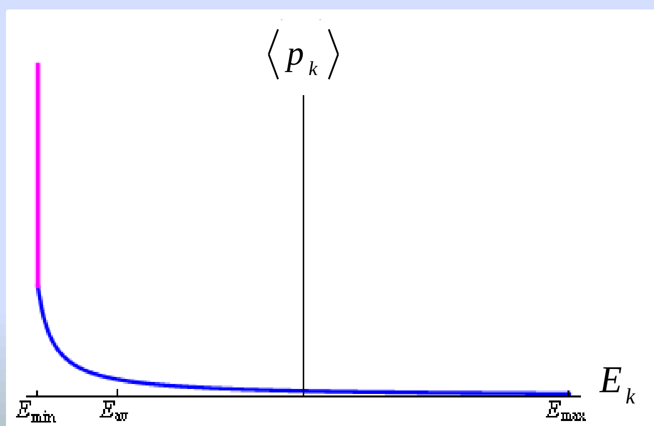
small-p_k approximation

$$V_k(p_k) = V_k(0)e^{-Np_k[1+\lambda(E_k-E_{av})]}$$

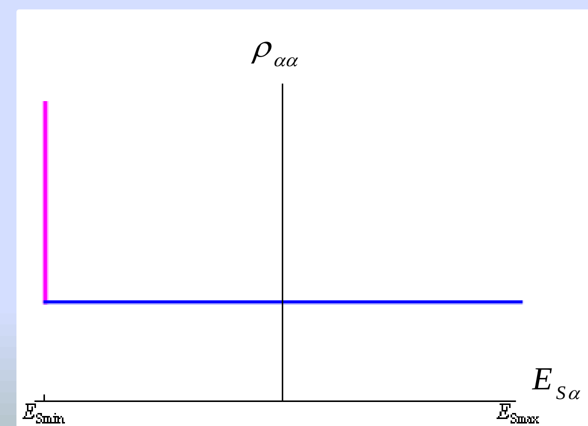
$$\langle p_k \rangle = \frac{1}{N[1+\lambda(E_k-E_{av})]}$$

confirmed by the direct Monte-Carlo sampling in B.F. and F. Hantschel, arXiv:1010.4673

Condensation for macroscopic systems



Density matrix elements for a small subsystem



Not Boltzmann-Gibbs!

Implications of the QMC result:

For macroscopic systems:

It implies the existence of a new fundamental limit for the applicability of conventional thermodynamics associated with the energy window for the eigenstates participating in statistical ensembles.

- Where is this limit located?
- What enforces it under everyday conditions?

For non-macroscopic systems with large number of quantum levels:

The QMC ensemble might be realizable under generic non-adiabatic perturbations.

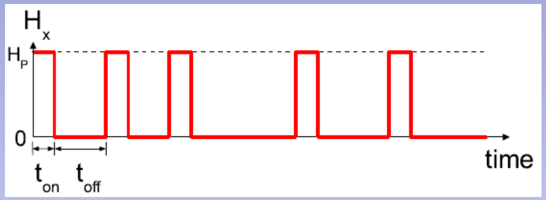
Two remarks:

1. Isolated quantum systems do not explore energy shells in the Hilbert space dynamically.

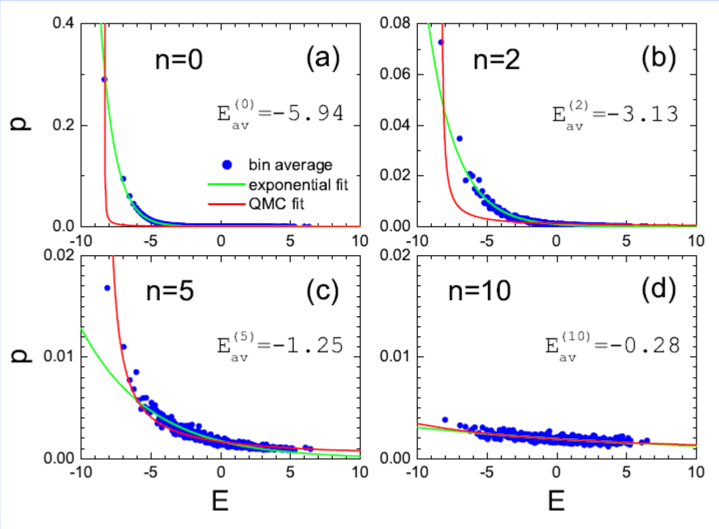
2. Energy shells in the Hilbert space grow with E_{av} exponentially faster than energy shells in the classical phase space

Ensembles emerging in thermally isolated clusters of spins ½ under multiple non-adiabatic perturbations [K. Ji & B.F., PRL 107, 050401 (2011)]

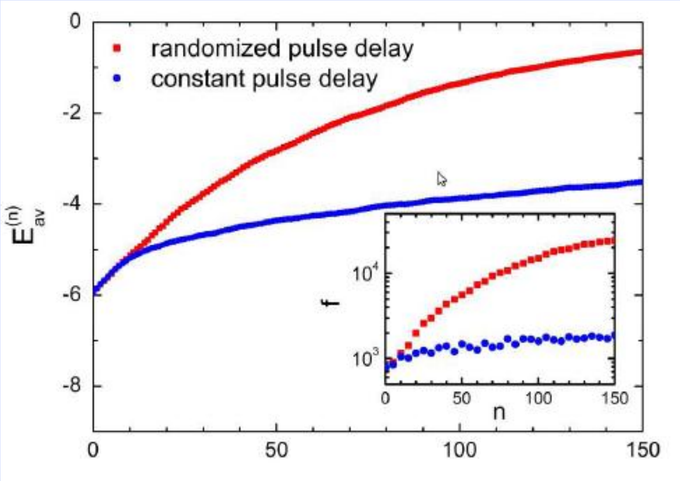
$$\mathcal{H} = \underbrace{\sum_{i=1}^{16} J_x S_i^x S_{i+1}^x + J_y S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z}_{\mathcal{H}_0} + \underbrace{H_x(t) \sum_{i=1}^{16} S_i^x}_{\mathcal{H}_p(t)}$$



16 spins ½ ~ 65 000 quantum states



Emergence of the QMC-like statistics



Evidence of dynamical localization?