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Reversibility and Irreversibility in Quantum Many-Body Systems

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1. Boltzmann vs. Loschmidt: Irreversible vs. reversible dynamics

2. Thermalization of closed quantum many-body systems

3. Definitions of irreversibility in quantum many-body systems

4. Echos in the transverse field Ising model
   [M. Schmitt, S. Kehrein, arXiv: 1607.02272]

5. Echos in interacting models

6. Conclusions & Outlook

1. Boltzmann vs. Loschmidt: Irreversible vs. reversible dynamics

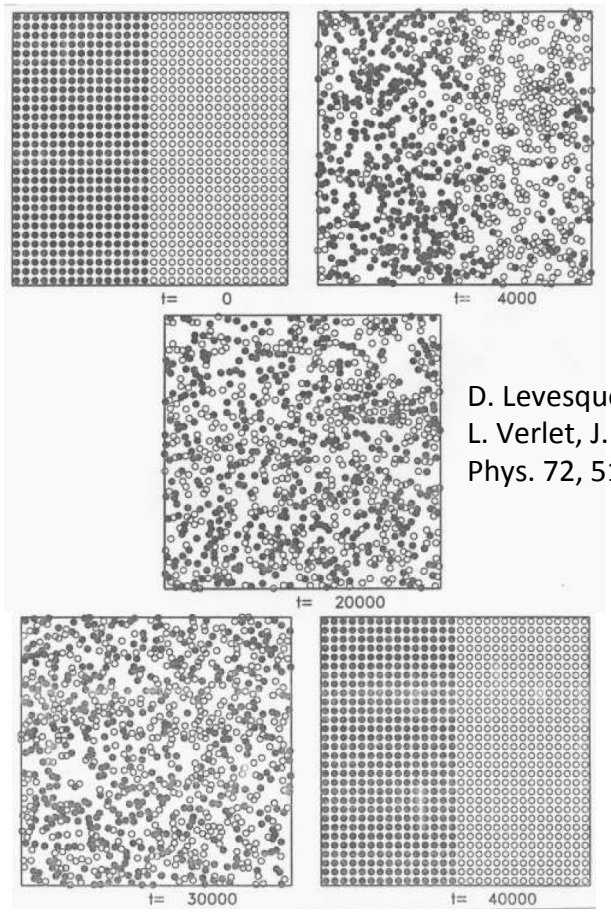
How to reconcile the second law of thermodynamics/the arrow of time with microscopic time-reversal invariance?

- Thomson (1874):

  If we allowed this equalization to proceed for a certain time, and then reversed the motions of all the molecules, we would observe a disequalization. However, if the number of molecules is very large, as it is in a gas, any slight deviation from absolute precision in the reversal will greatly shorten the time during which disequalization occurs.

- In modern language:

  Classical chaotic system
  → Positive Lyapunov exponent
  → Mixing and exponential sensitivity to initial conditions
  → Time-reversal operation requires exponentially increasing accuracy with waiting time



D. Levesque and L. Verlet, J. Stat. Phys. 72, 519 (1993)

Integer arithmetics!

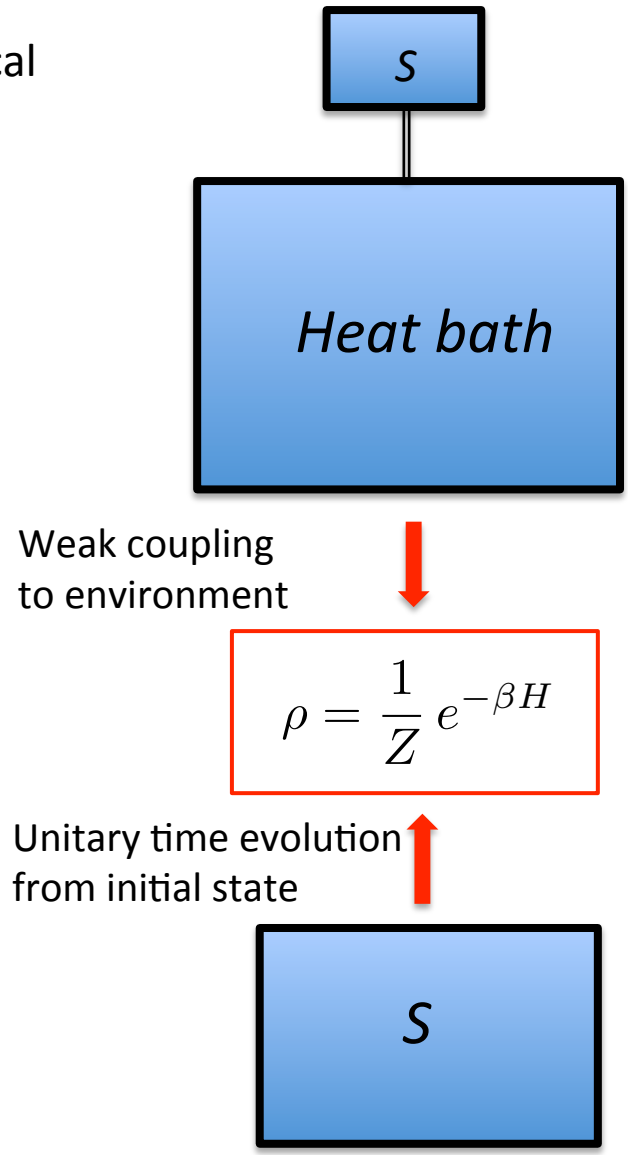
<u>Goal: Understand irreversibility in quantum many-body systems</u>

2. Thermalization of closed quantum many-body systems

Goal: Dynamical justification of equilibrium statistical mechanics for closed quantum systems

Key questions:

- What is the intrinsic time scale of a closed system to thermalize?
- What are the conditions for a closed system to thermalize?
- What do we really mean by thermalization?

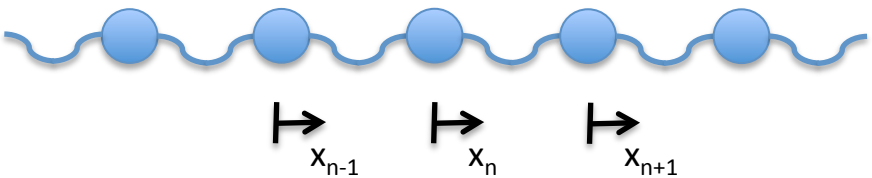


The Fermi-Pasta-Ulam-Tsingou problem

E. Fermi, J. Pasta, S. Ulam; Los Alamos Report (1955)

Closed classical system: Harmonic chain with anharmonic perturbations
(weakly nonlinearly coupled harmonic oscillators)

$$\frac{d^2x_n}{dt^2} = (x_{n+1} - 2x_n + x_{n-1}) + \alpha\left[(x_{n+1}-x_n)^2 - (x_n - x_{n-1})^2\right] + \beta\left[(x_{n+1}-x_n)^3 - (x_n - x_{n-1})^3\right]$$



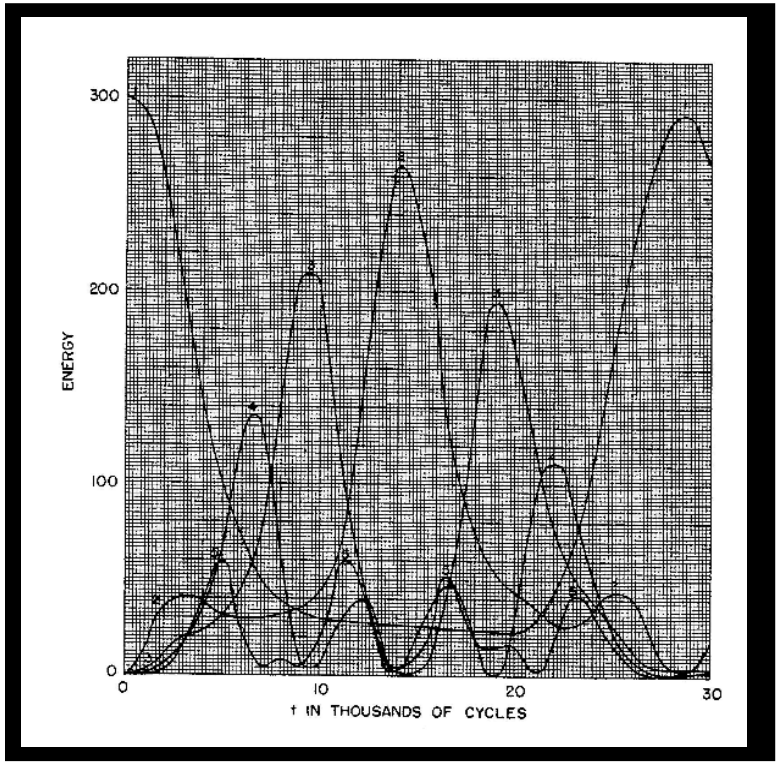
Goal: Dynamical justification of the assumptions of classical equilibrium statistical mechanics

Initial state: Mode k=1 excited

⇒ Recurrences

⇒ Violation of equipartiation theorem

⇒ No thermalization (?!)



Basic issues in closed quantum systems

- A pure state always remains pure:

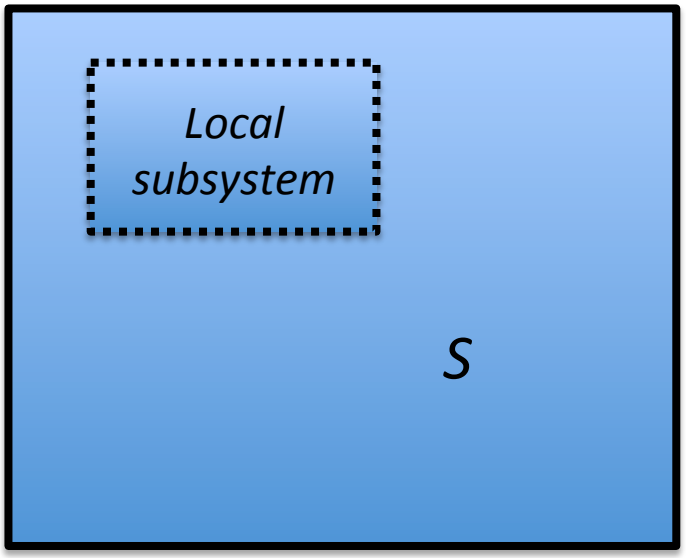
$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle$$ never becomes a Gibbs state $$\rho = \frac{1}{Z}\,e^{-\beta H}$$

- Definition of thermalization:

For "all" physically relevant observables O

$$\lim_{t\to\infty} \langle\psi(t)|O|\psi(t)\rangle = \mathrm{Tr}(\rho\, O)$$

→ time evolved pure state in practise indistinguishable from thermal or generalized Gibbs state



Possibilities:

- Observables in local subsystem (system acts as its own heat bath)
- Few-body operators

- Quantum quench:

- Prepare system in ground state of H_0 : $$H_0\,|\psi(0)\rangle = E_{\mathrm{GS}}\,|\psi(0)\rangle$$
- Time evolve with H : $$[H_0, H] \neq 0$$

Eigenstate thermalization hypothesis (ETH)

Time evolution:

$$
\begin{aligned}
|\psi(t)\rangle &= e^{-iHt}\,|\psi_0\rangle \\
&= \sum_n e^{-iE_n t}\, c_n\,|E_n\rangle \quad \text{with} \quad c_n \stackrel{\text{def}}{=} \langle E_n|\psi_0\rangle \\
\Rightarrow \quad A(t) &= \langle\psi(t)|A|\psi(t)\rangle \\
&= \sum_{n,m} c_m^* c_n\, e^{-i(E_n-E_m)t}\,\langle E_m|A|E_n\rangle
\end{aligned}
$$

Thermalization: Initial states with the same total energy

E_{tot} + O(many-body level spacing)

should have the same long-time limit for physically "relevant"/few body operators A

$$\lim_{t\to\infty} A(t) = A_{E_{tot}}$$

How is this possible for different realizations of $\{c_n\}$?

How is this possible for different realizations of $\{c_n\}$?

Eigenstate thermalization hypothesis (ETH):

$$\boxed{\langle E_m|A|E_n\rangle = \delta_{nm} A_{E_n} + O((\dim\mathcal{H})^{-1})}$$

$$\Rightarrow \quad \lim_{t\to\infty} A(t) = \underbrace{\sum_n |c_n|^2}\ A_{E_{tot}}$$

$$= \quad 1 \times \quad A_{E_{tot}} \qquad \forall\ |\psi_0\rangle$$

Eigenstate thermalization hypothesis (ETH): J. M. Deutsch 1991, M. Srednicki 1994

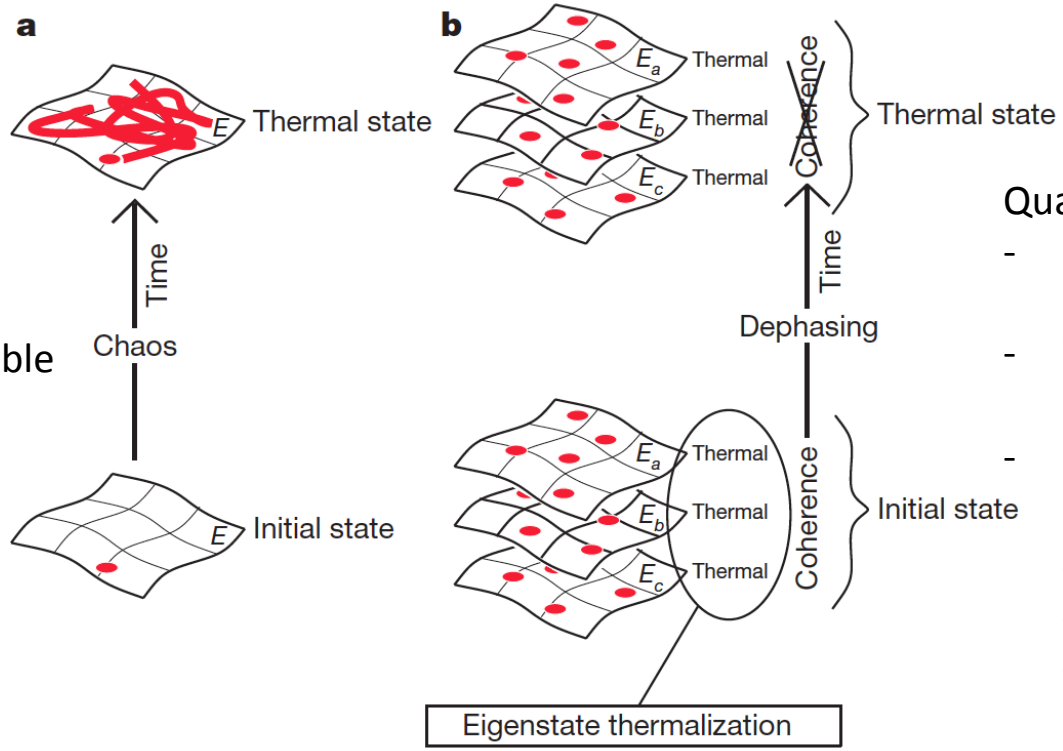
In a <u>non-integrable</u> quantum many-body system the expectation value of physically relevant observables does not depend on the specific eigenstate with energy E of the Hamiltonian

→ a single eigenstate is typical, no need for thickened microcanonical ensemble and hypothesis of equal probabilities / Jaynes approach

→ physical observables (few body operators) cannot distinguish nearby many-body eigenstates

M. Rigol et al., Nature 452 (2008)

Classical thermalization: Thermal state does not resemble initial state



Quantum thermalization (ETH):

- Every eigenstate of the Hamiltonian is thermal
- Thermal nature initially hidden due to coherences
- Dephasing leads to effectively incoherent superposition of thermal states, weights of these states unimportant

Source: M. Rigol et al., Nature 452 (2008)

Integrable models

Integrability: Existence of infinitely many conserved quantities I_k

$$[H, I_k] = 0 \ , \ [I_k, I_l] = 0$$

→ constrain dynamics

$$\langle I_k(t) \rangle = \langle \psi(t) | I_k | \psi(t) \rangle = \langle \psi(0) | I_k | \psi(0) \rangle = \langle I_k(0) \rangle$$

Describe asymptotic state $|\psi(t=\infty)\rangle \langle \psi(t=\infty)|$

as "generalized Gibbs ensemble (GGE)" (Rigol et al., 2007)

$$\rho = \frac{1}{Z} e^{-\beta H - \sum \lambda_k I_k}$$

with additional Lagrange multipliers λ_k

$$\langle I_k(0) \rangle = \mathrm{Tr}(\rho \, I_k)$$

- Very successful for describing integrable non-equilibrium systems for local observables (Essler et al.)
- ETH-like picture holds when observable expectation values are considered as functions of all conserved quantities (not only energy) [Cassidy et al., PRL (2011)]

3. Definitions of irreversibility in quantum many-body systems

a) Loschmidt echo [Peres, 1984]

b) OTO correlations functions [Kitaev, 2014; Maldacena et al., 2014]

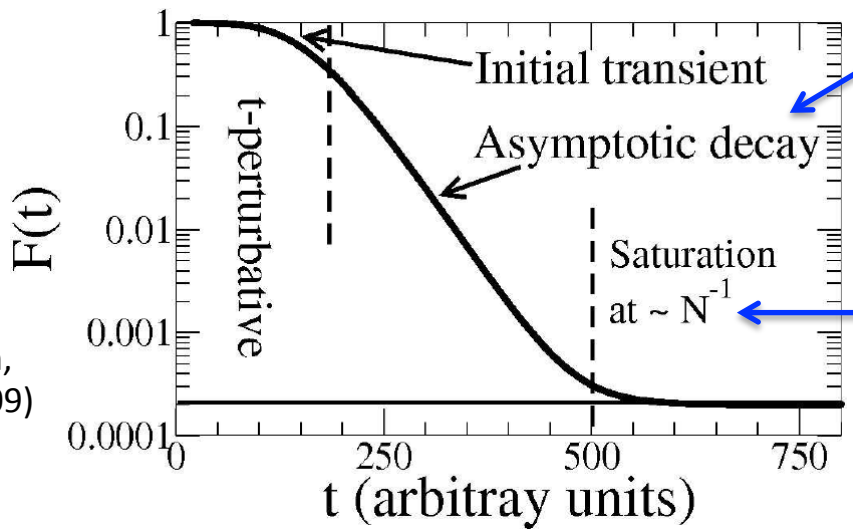
c) Echo dynamics

a) Loschmidt echo for characterizing quantum chaos & irreversibility (Peres, 1984)

Loschmidt echo $L(t) = |\langle\psi_i|\, e^{i(H+\Sigma)t}\, e^{-iHt}\, |\psi_i\rangle|^2$

backward forward
time evolution

Few-body systems:
(classically chaotic)



$\alpha\, e^{-\lambda t} + e^{-\Gamma t}$

Chaotic dynamics Dephasing

(Dimension of Hilbert space)$^{-1}$

Jacquod, Petitjean,
Adv. Phys. 58 (2009)

Few-body systems (non chaotic): Algebraic decay of L(t)

Quantum many-body systems:

ETH : "Physical" observables O cannot distinguish between nearby many-body eigenstates

$$\forall O \quad \langle\psi_0|O|\psi_0\rangle = \langle\psi_1|O|\psi_1\rangle + o(\dim\mathcal{H}^{-1})$$

but $\langle\psi_0|\psi_1\rangle = 0$

→ Orthogonality of states no useful criterion for "physically different"

→ Loschmidt echo not useful for characterizing irreversibility

Note: Large deviation form of Loschmidt echo $L(t) = e^{-V\,\ell(t)}$

→ generic exponential decay

b) Out-of-time-order (OTO) correlators

A. Kitaev, “Hidden Correlations in the Hawking Radiation and Thermal Noise,” talk given at Fundamental Physics Prize Symposium, Nov. 10, 2014

http://online.kitp.ucsb.edu/online/joint98/kitaev/rm/jwvideo.html

J. Maldacena, S. Shenker, D. Stanford, “A bound on chaos”, arXiv:1503.01409

P. Hosur, X.-L. Qi, D. Roberts, B. Yoshida, “Chaos in quantum channels”, arXiv:1511.04021, JHEP (2016)

Quantum chaos (Maldacena et al., 2015)

$$C(t) = -\langle\, [B(t), A(0)]^2 \,\rangle$$

thermal expectation value

commutator: effect of perturbation A
on later measurement of B

Definition of quantum chaos:

C(t) becomes large (of order $2\,\langle B\,B\rangle\,\langle A\,A\rangle$)

for all physically relevant observables A,B

Motivation:

- Semiclassical billiard, A=p, B(t)=q(t) [Larkin, Ovchinnikov, JETP 28 (1969)]
  → commutator gives dependence of final position on small changes of the initial position

$$C(t) \sim \hbar^2\, e^{2\lambda_L t}$$

- C(t) measures degree of non-commutativity of time-evolved observables

C(t) contains the out-of-time order (OTO) correlator

$$F(t) = \langle \{ B(t)\, A(0), B(t)\, A(0) \} \rangle$$
$$= \langle B(t)\, A(0)\, B(t)\, A(0) \rangle + \langle A(0)\, B(t)\, A(0)\, B(t) \rangle$$

Equivalent definition of quantum chaos:

F(t) decays and becomes small

- Initial decay $\dfrac{F(t)}{2\langle B^2 \rangle \langle A^2 \rangle} = g_0 - g_1\, e^{\lambda_L t}$

- For large-N CFT holographically described by Einstein gravity (t>>β)

$$g_0 = O(1) \quad , \; g_1 \propto \frac{1}{N^2} \quad , \quad \lambda_L = \frac{2\pi}{\beta}$$ [Shenker, Stanford (2014)]

- Conjecture [Maldacena et al. (2015)]:

Universal bound $\lambda_L \leq \dfrac{2\pi}{\beta}$

Quantum information [Hosur et al. (2016)]

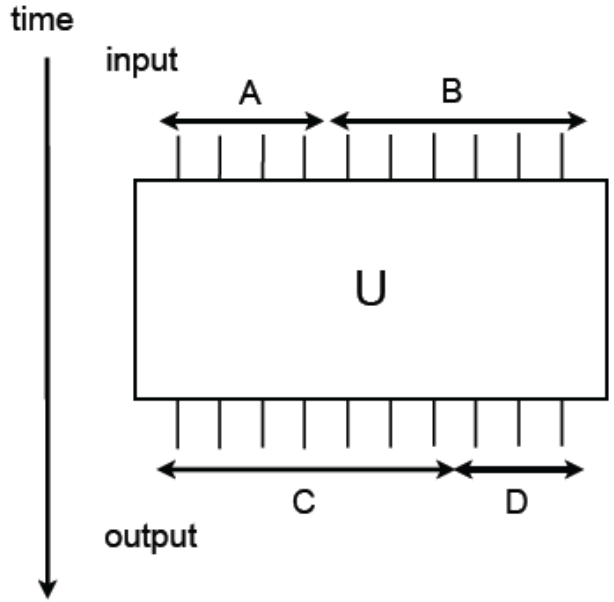
Decay of OTO correlator F(t) → mutual information between small subsystem in input and any partition of output is small (scrambling)

Unitary operator $U(t) : \mathcal{H} \to \mathcal{H}$

$$U(t) = \sum_{i,j} u_{ij}(t) \, |i\rangle\langle j|$$

mapped to vector $|U(t)\rangle \in \mathcal{H} \otimes \mathcal{H}$

$$|U(t)\rangle = \frac{1}{(\dim\mathcal{H})^{1/2}} \sum_{i,j} u_{ij}(t) \, |j\rangle_{\text{in}} \otimes |i\rangle_{\text{out}}$$



Source: Hosur et al. (2016)

Measure for scrambling:

Amount of information about A hidden non-locally over C and D

$$I(A:CD) - I(A:C) - I(A:D)$$

Tripartite information

$$\begin{aligned} I_3(A:C:D) &= I(A:C) + I(A:D) - I(A:CD) \\ &= S_A + S_C + S_D - S_{AC} - S_{AD} - S_{CD} + S_{ACD} \end{aligned}$$

must become negative with large magnitude for system to scramble

Hosur et al. (2015):

Qubits, infinite temperature, $[A_i, D_j] = 0$

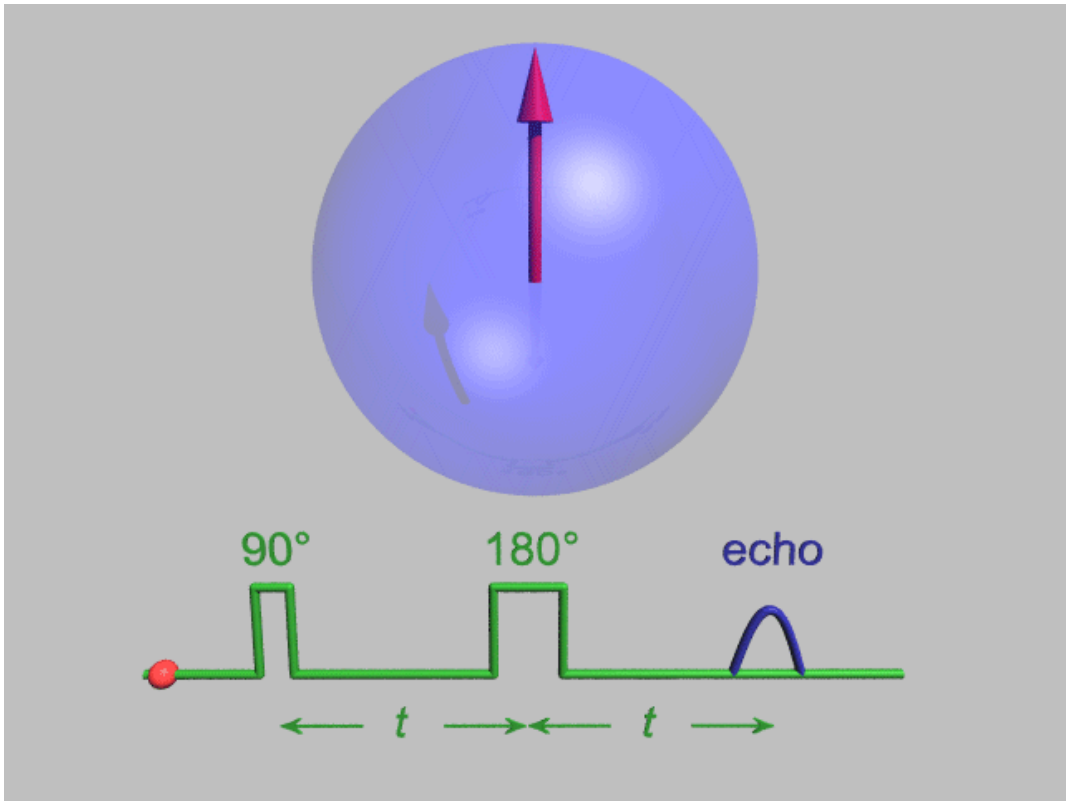
OTO average $\bar{F}(t) \xrightarrow{t\to\infty} \epsilon$

→ $$I_3(A:C:D) = -2a + 2\log_2 \frac{\epsilon}{\epsilon_{\min}}$$

with $\epsilon_{\min} = 2^{-2a}$

c) Echo dynamics

NMR spin echo



Source: http://en.wikipedia.org/wiki/Spin_echo

Quantum systems

NMR spin echo (Hahn, 1950):

Time evolution of macroscopic polarization governed by

$$H = \sum_i H_i(\vec{S}_i)$$

local Hamiltonians with randomness

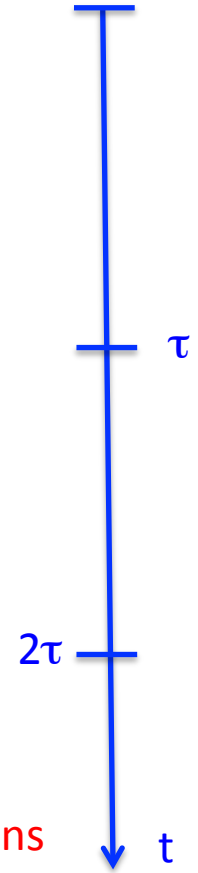
π-pulse:

Effectively $H_i \rightarrow -H_i$

Spin echo:

Measure natural linewidth

Limited by many-body interactions



VOLUME 25, NUMBER 4 PHYSICAL REVIEW LETTERS 27 JULY 1970

VIOLATION OF THE SPIN-TEMPERATURE HYPOTHESIS*

W.-K. Rhim, A. Pines,† and J. S. Waugh
Department of Chemistry and Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139
(Received 5 May 1970)

A "Loschmidt demon" is exhibited which effectively reverses the spin-spin relaxation of a system of interacting magnetic dipoles in a strong external field, thereby demonstrating that this system does not approach internal thermodynamic equilibrium in a time T_2 as was implicitly recognized by Philippot.

The coupled nuclear spins in a solid with very slow spin-lattice relaxation comprise an isolated system which for many purposes can be treated by thermodynamic methods.[1] One begins with the system in equilibrium at the lattice temperature T, performs various manipulations on the spins, waits a time T_2 characteristic of the spin-spin coupling, during which the spin system is imagined to approach internal equilibrium, and calculates a final spin temperature T_s through conservation of energy or other constants of the motion. The purpose of this Letter is to report some experiments for which this simple spin-temperature picture is not valid.

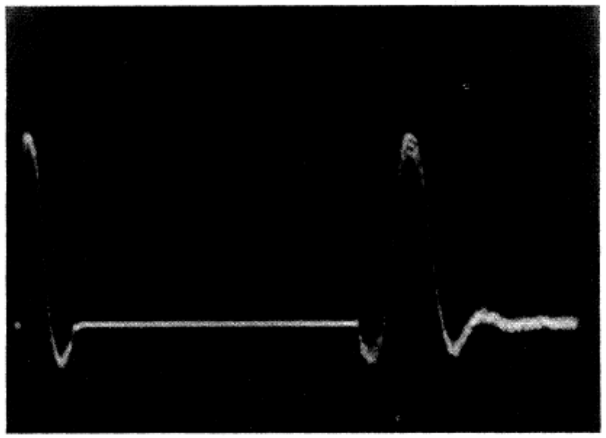


FIG. 1. Transient NMR of the ^{19}F nuclei in solid CaF_2. Following a normal Bloch decay, an rf burst of length 260 μsec with $H_1 = 95$ G (see text) was applied during the noise-free portion of the trace. Thereupon an echo occurs at a total delay of 365 μsec from the beginning of the experiment. In other experiments the initial decay was allowed to disappear fully before applying the burst.

Back to a fundamental question:

For an isolated system a pure state $|\psi_i\rangle$ remains pure $|\psi(t)\rangle$ for all times t. Can it be distinguished by some realistic protocol from a density matrix ρ even if the system "thermalizes"?

Quantum systems

NMR spin echo (Hahn, 1950):

Time evolution of macroscopic polarization governed by

$$H = \sum_i H_i(\vec{S}_i)$$

local Hamiltonians with randomn

Loschmidt daemon

π-pulse:

Effectively $H_i \rightarrow -H_i$

Spin echo:

Measure natural linewidth

Limited by many-body interactions

τ

2τ

3τ

t

Magic echo
(Rhim et al. 1970, Zhang et al. 1992):

Dipolar coupled spins

$$H_{\text{eff}} = \sum_{i,j} d_{ij} \left(2S_i^z S_j^z - \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+) \right)$$

spin diffusion

Magic echo pulse sequence:

$$H_{\text{eff}} \rightarrow -\frac{1}{2} H_{\text{eff}} - \Sigma$$

undoes spin diffusion

Spin echo

What is the effect of Σ ?

Other recent application of echo dynamics:

- Identification of many-body localized phases [Serbyn et al., PRL (2014)]

Definition of irreversibility:

Echos in physical observables decay exponentially or faster as function of waiting time τ for realistic echo protocols

Note: Depends on observables, protocol & initial state (similar to def. of thermalization)

Forward time evolution $$|\psi(\tau)\rangle = U(\tau)\,|\psi_{\rm ini}\rangle$$

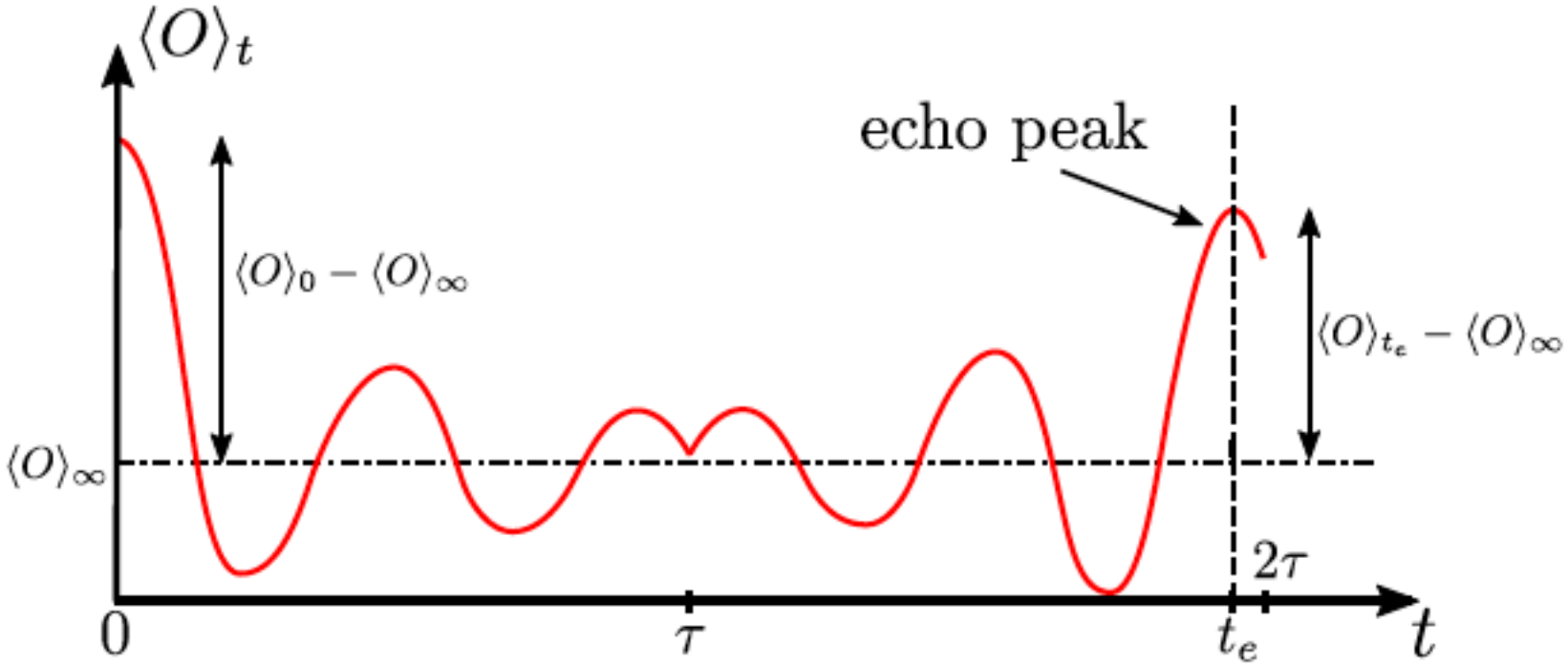
Backward time evolution (t>τ) $$|\psi(t)\rangle = V(t-\tau)\,U(\tau)\,|\psi_{\rm ini}\rangle$$

Expectation value of observable $$O_s \stackrel{\rm def}{=} \langle\psi(s)\,|\,O\,|\,\psi(s)\rangle$$

Normalised echo peak height $$E^*_\tau[O] = \max_{t>\tau}\left|\frac{O_t - O_\infty}{O_0 - O_\infty}\right|$$

echo peak at t≈2τ
(and usually not exactly at t=2τ)

contrast



$$E^*_\tau[O] = \max_{t>\tau} \left| \frac{O_t - O_\infty}{O_0 - O_\infty} \right|$$

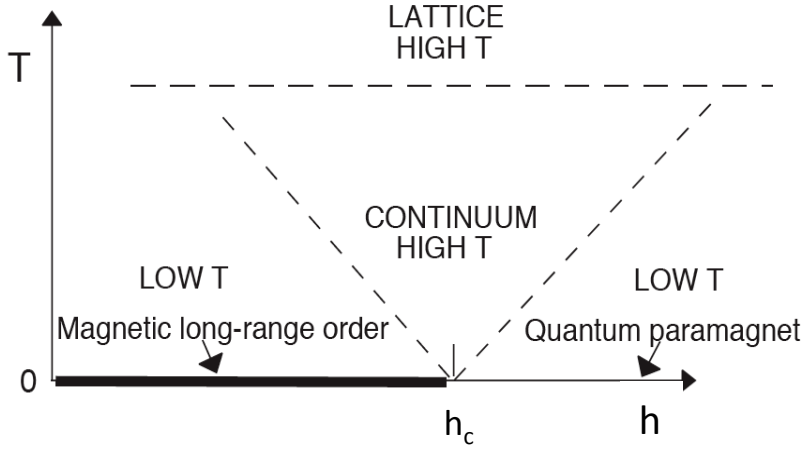
Irreversible dynamics means $E_\tau^*[O]$ decays exponentially or faster, otherwise the dynamics is reversible.

4) Echos in the transverse field Ising model

M. Schmitt, S. Kehrein, arXiv: 1607.02272

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

Ising interaction — transverse magnetic field



S. Sachdev, Quantum Phase Transitions (Cambridge Univ. Press, 2011)

- Quantum phase transition at $h_c = 1$
- Integrable model:
  Quadratic in fermions after Jordan-Wigner transformation

Thermalization to "generalized Gibbs ensemble" (GGE) for all quenches $h_0 \rightarrow h$

Fagotti and Essler, Phys. Rev. B 87 (2013)

Reduced density matrix for n spin subsystem from time evolved initial state

$$\lim_{t\to\infty} |\psi_i(t)\rangle\langle\psi_i(t)|_n = \rho_{\mathrm{GGE},n}$$

Echo protocols:

a) Initial state: Ground state of $H(h_0)$

b) Forward time evolution (quench dynamics $h \neq h_0$): $U(\tau) = e^{-iH(h)\tau}$

c) Backward time evolution:

1) Sign change with perturbation $V(s) = e^{iH(h+\delta h)s}$

2) Loschmidt pulse $V(s) = U_P^\dagger \, e^{-iH(h)s} \, U_P$

3) Generalised Hahn echo $V(s) = e^{-iH(-h)s}$

approx. particle-hole trf. (equiv. to velocity reversal)

d) Observables:

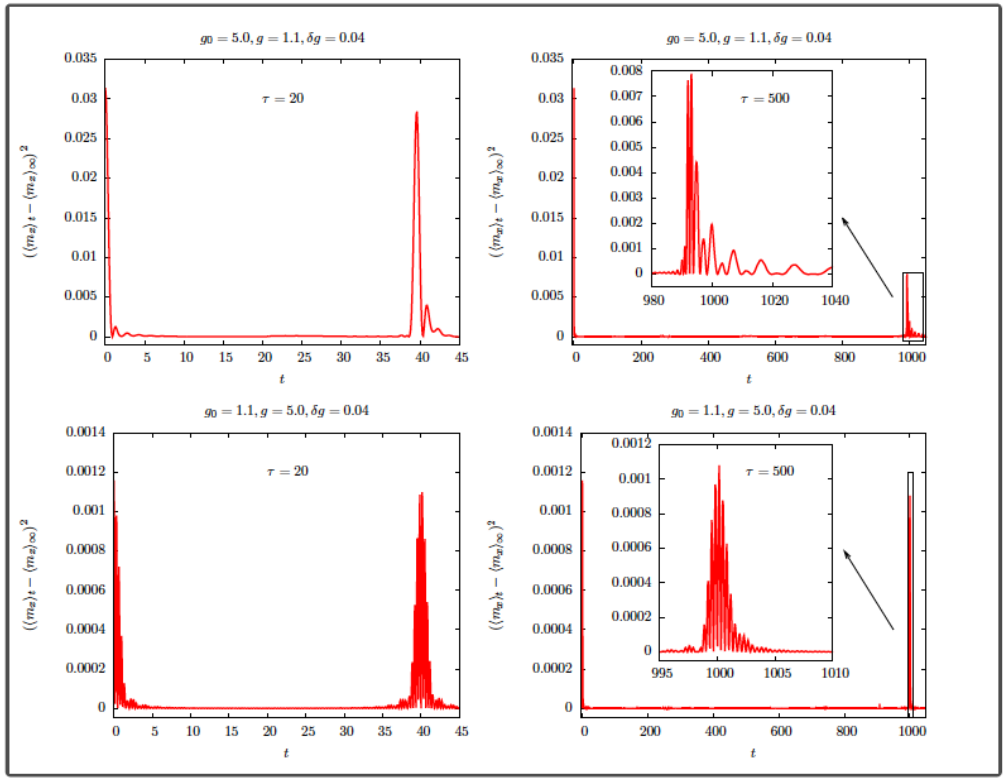
transverse magnetization σ_i^x

longitudinal spin-spin correlation function (distance d) $\sigma_i^z \, \sigma_{i+d}^z$

Methods:

- Numerical evaluation of Toeplitz determinants in the thermodynamic limit
- Stationary phase approximation for large waiting times (analytical result)

Sign change with perturbation, transverse magnetization



Different protocols

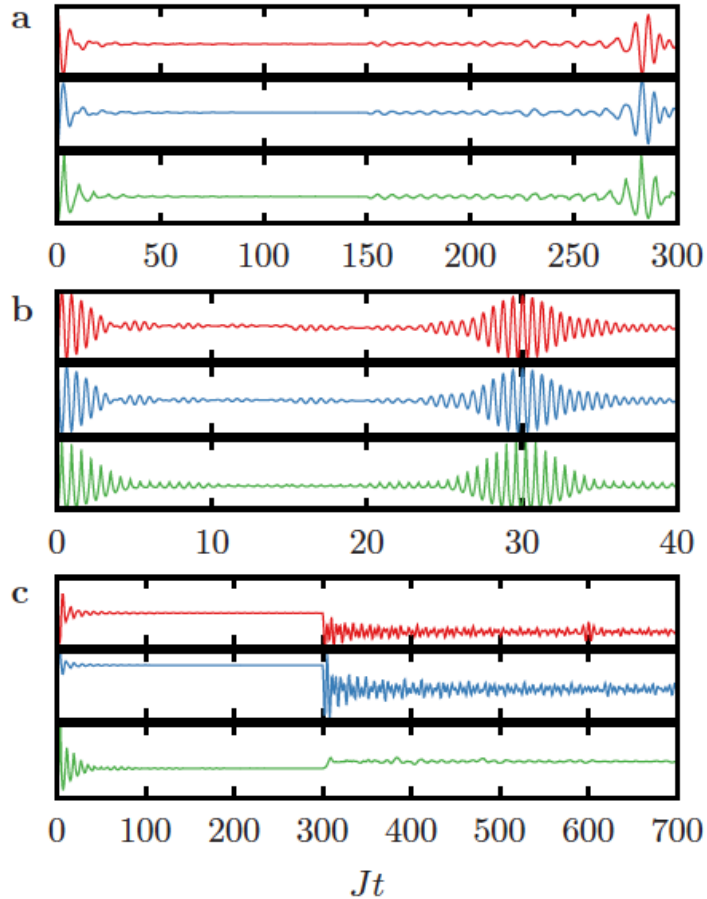


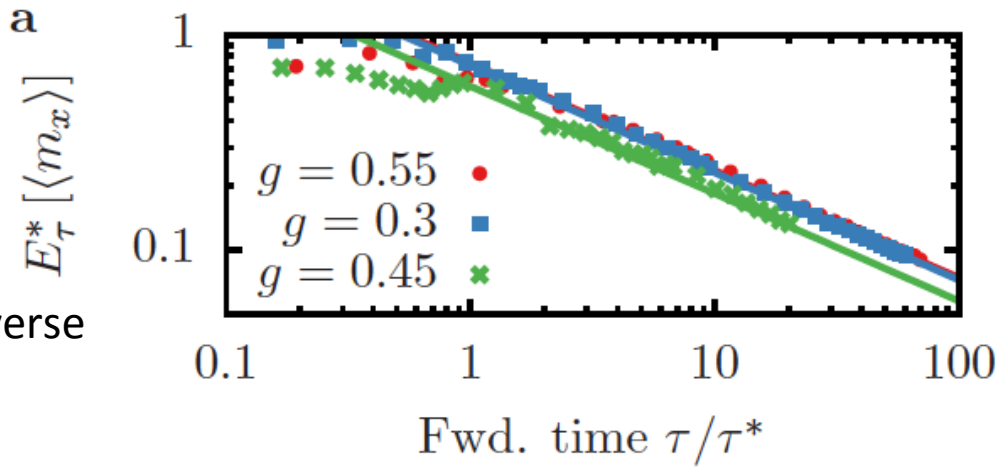
Fig. 1: Time evolution of the transverse magnetisation $\langle m_x \rangle_t$ (red curves), the longitudinal spin-spin correlation $\langle S_i^z S_{i+1}^z \rangle_t$ (blue curves), and the rate function of the fidelity $l(t) = \lim_{N\to\infty} \ln(\langle \psi_0 | \psi(t) \rangle)/N$ (green curves) for the three different echo protocols: (a) by explicit sign change, (b) generalised Hahn echo, (c) by pulse.

Decay of normalised echo peak height $E^*_\tau[O] = \max_{t>\tau} \left| \frac{O_t - O_\infty}{O_0 - O_\infty} \right|$

Stationary phase approximation predicts algebraic decay for all protocols

$$E^*_\tau[O] \propto \tau^{-1/2}$$

- with known prefactor (for transverse magnetization and protocol sign change with perturbation)

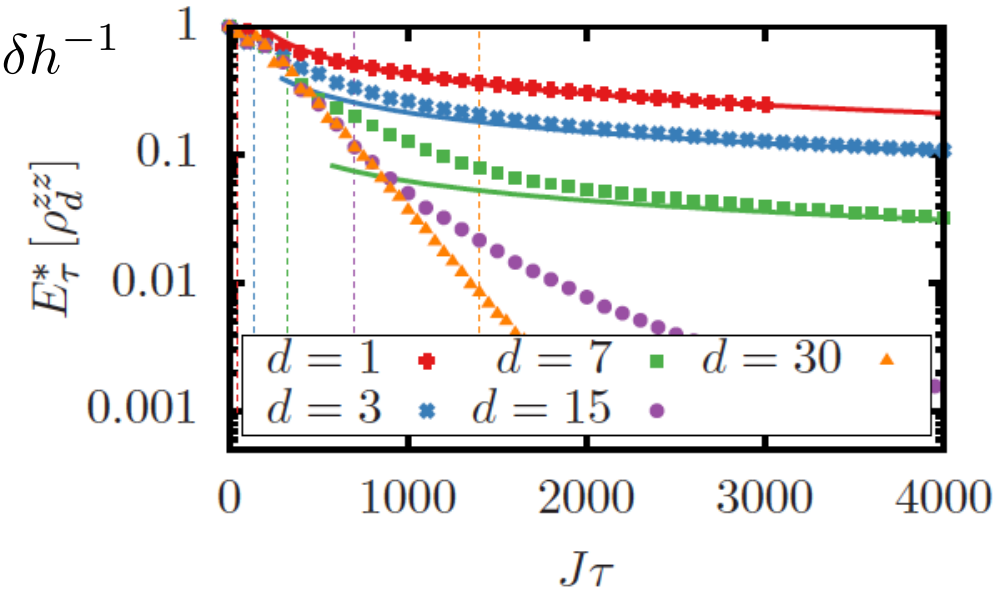


$$E^*_\tau[\sigma^x] \approx \delta h^{-1/2} \tau^{-1/2} \quad \text{for } \tau \gtrsim \delta h^{-1}$$

- full lines show predictions

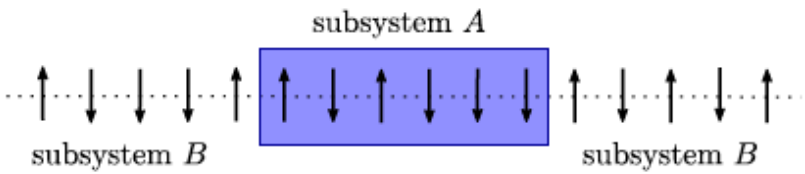
- Exception Loschmidt pulse: the transverse magnetization does not decay

- essentially dephasing dynamics



Entanglement entropy

- Analytical calculation of the entanglement entropy after quenches in the transverse field Ising model: Calabrese, Cardy (2005)

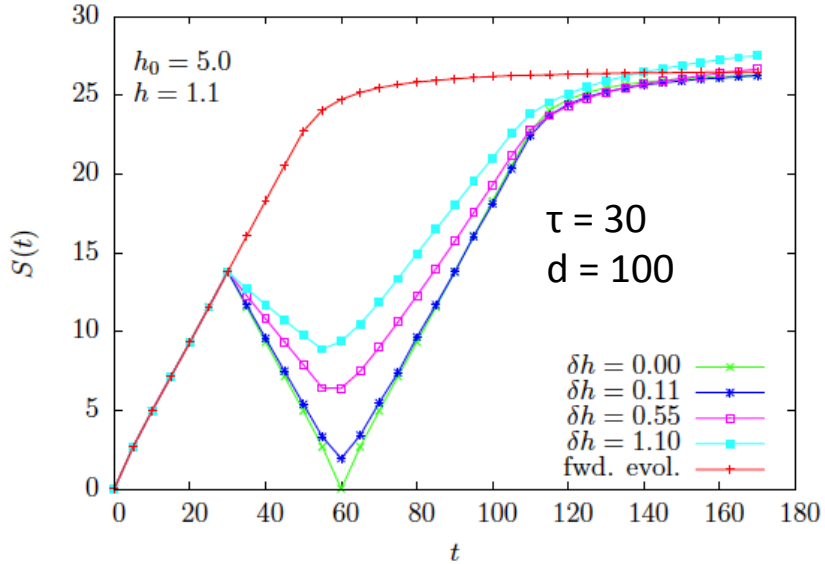


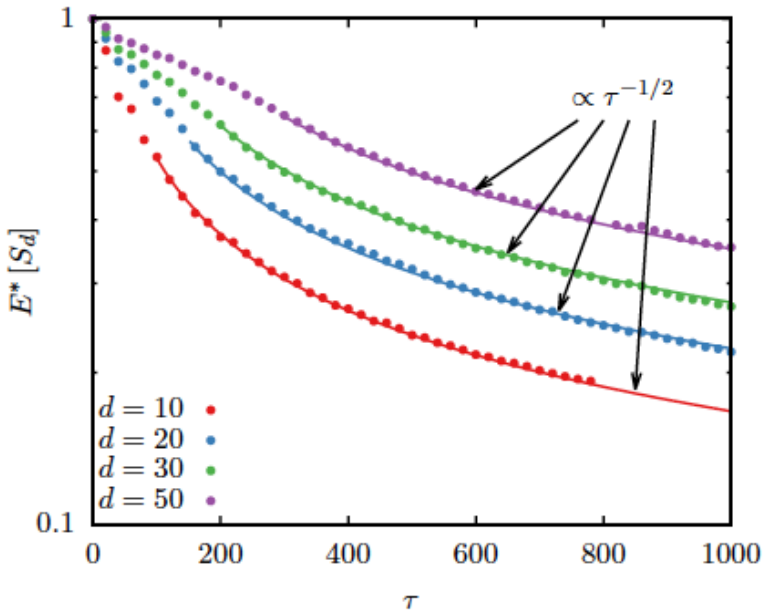
- Echo protocol:
  Sign change with perturbation δh

- Measure entanglement entropy $S^d_{ent}(t)$ for subsystem with d spins

Algebraic decay of normalised echo peak height of the entanglement entropy

$$E^*_\tau[S^d_{\rm ent}] \propto \tau^{-1/2}$$





Conclusion

Based on our definition the transverse field Ising model shows reversible dynamics (algebraic decay of echo peaks)

Note: The transverse field Ising model is

- integrable
- quadratic in suitable degrees of freedom

Question

What about models that are

- integrable but not quadratic?
- non-integrable?

5. Echos in interacting models

Coll.: Markus Schmitt

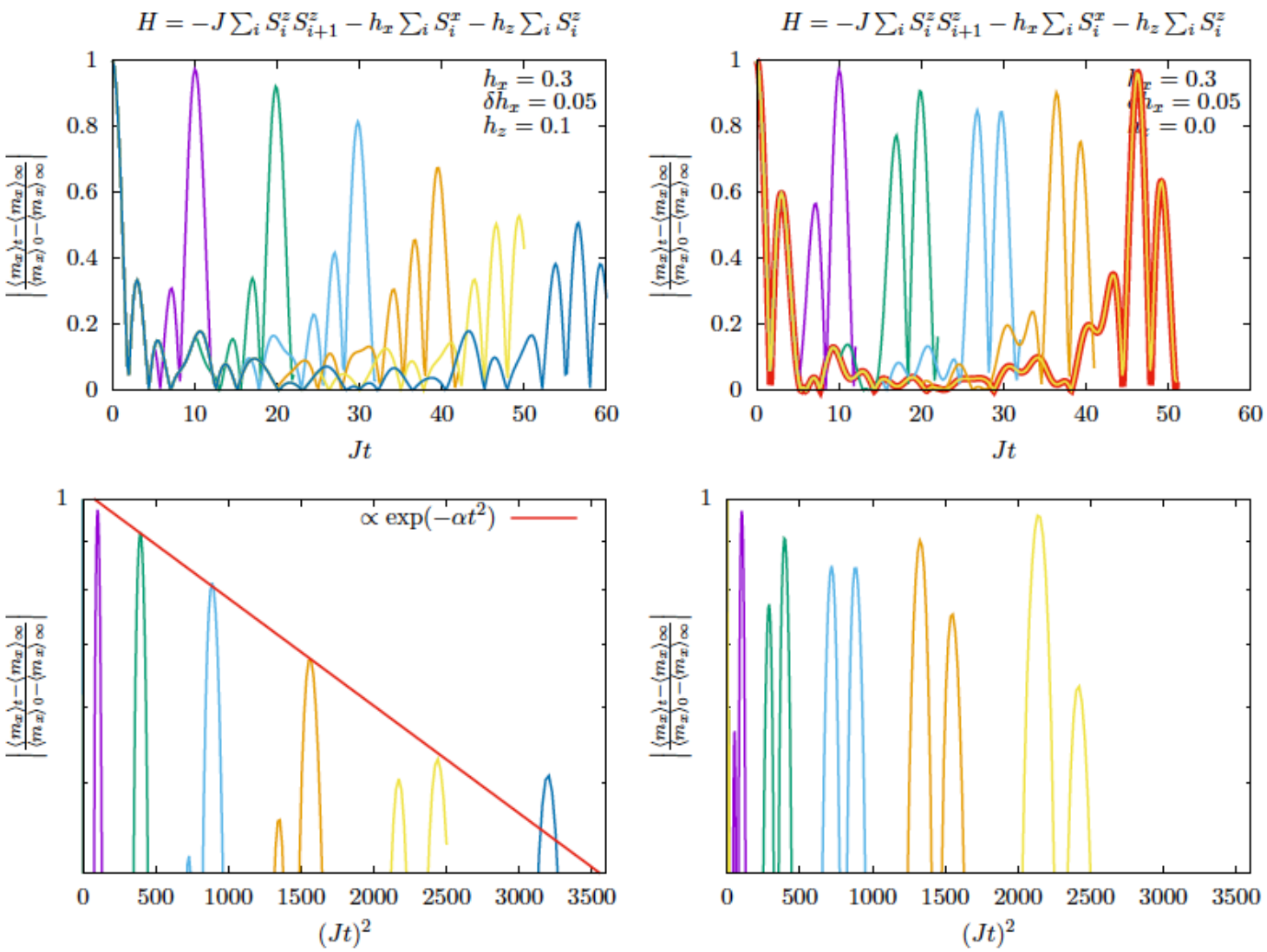
Ising model with transverse and longitudinal fields:

$$H(h_x, h_z) = -\sum \sigma_i^z \sigma_{i+1}^z + h_x \sum \sigma_i^x + h_z \sum \sigma_i^z$$

Non-integrable for h_x, $h_z \neq 0$ (Wigner-Dyson level statistics)

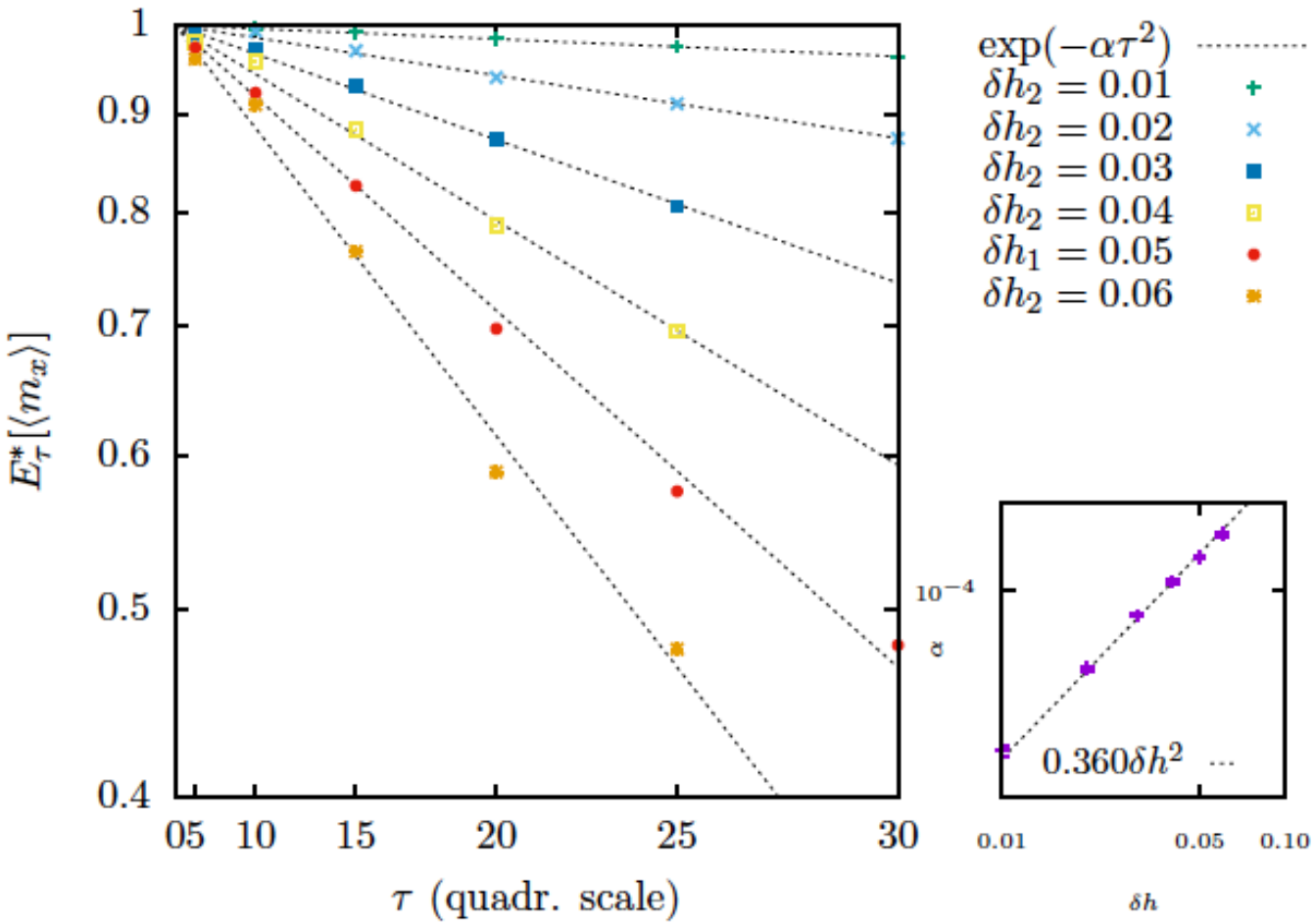
Method: infinite time-evolving block decimation (iTEBD)

Note: Numerically challenging problem since entanglement entropy also decreases during time evolution



Interacting model $h_z = 0.1$
(Gaussian decay)

Non-interacting model $h_z = 0$
(Slow algebraic decay)



Decay law well approximated by Gaussian: $e^{-\alpha\tau^2}$

Prefactor $\alpha \propto \delta h^2$

→ not independent from perturbation like Lyapunov exponent in classical chaos

6. Conclusions & Outlook

- Definition of irreversibility for quantum many-body systems based on decay of echoes in observables

- Non-interacting model (transverse field Ising model):

  Algebraic decay of echoes due to dephasing
  → Reversible dynamics

- Non-integrable model (transverse field Ising model with longitudinal field):

  Exponential decay of echoes
  → Irreversible dynamics

- Integrable interacting models (XXZ spin chain):
  Decay faster than algebraic, but not clearly Gaussian

Outlook:

- Prefactor of Gaussian decay law determined by unperturbed Hamiltonian (like Lyapunov exponent) or by perturbation
- Analytical understanding of irreversibility
- Connection to OTO-correlator definition of quantum chaos