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

5. Echos in interacting models

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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


Goal: Understand irreversibility in quantum many-body systems
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?

\[ \rho = \frac{1}{Z} e^{-\beta H} \]
The Fermi-Pasta-Ulam-Tsingou problem


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

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

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

Initial state: Mode k=1 excited

⇒ Recurrences
⇒ Violation of equipartition theorem
⇒ No thermalization (?!)

Graph showing energy vs. time in thousands of cycles.
Basic issues in closed quantum systems

- A pure state always remains pure:
  \[ |\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle \text{ never becomes a Gibbs state} \]

\[ \rho = \frac{1}{Z} e^{-\beta H} \]

- Definition of thermalization:
  For “all” physically relevant observables O:
  \[ \lim_{t \to \infty} \langle \psi(t)|O|\psi(t)\rangle = \text{Tr}(\rho O) \]

\[ \Rightarrow \text{time evolved pure state in practise indistinguishable from thermal or generalized Gibbs state} \]

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

- Quantum quench:
  - Prepare system in ground state of \( H_0 \):
    \[ H_0 |\psi(0)\rangle = E_{GS} |\psi(0)\rangle \]
  - Time evolve with H:
    \[ [H_0, H] \neq 0 \]
Eigenstate thermalization hypothesis (ETH)

Time evolution:

\[ |\psi(t)\rangle = e^{-iHt} |\psi_0\rangle = \sum_n e^{-iE_n t} c_n |E_n\rangle \text{ with } c_n \overset{\text{def}}{=} \langle E_n | \psi_0 \rangle \]

\[ \Rightarrow A(t) = \langle \psi(t) | A | \psi(t) \rangle = \sum_{n,m} c_n^* c_m e^{-i(E_n - E_m)t} \langle E_m | A | E_n \rangle \]

Thermalization: Initial states with the same total energy

\[ E_{\text{tot}} + O(\text{many-body level spacing}) \]

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

\[ \lim_{t \to \infty} A(t) = A_{E_{\text{tot}}} \]

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

Eigenstate thermalization hypothesis (ETH):

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

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

\[
= 1 \times A_{E_{tot}} \quad \forall |\psi_0\rangle
\]


In a non-integrable quantum many-body system the expectation value of physically relevant observables does not depend on the specific eigenstate with energy \( E \) of the Hamiltonian

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

\( \rightarrow \) physical observables (few body operators) cannot distinguish nearby many-body eigenstates
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 $I_k$

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

$\rightarrow$ 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 $\lambda_k$

\[\langle I_k(0) \rangle = \text{Tr}(\rho I_k)\]

• 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)

\[
L(t) = \left| \langle \psi_i | e^{i(H+\Sigma)t} e^{-iHt} | \psi_i \rangle \right|^2
\]

Few-body systems: (classically chaotic)

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

\[
\alpha e^{-\lambda t} + e^{-\Gamma t}
\]

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

Chaotic Dephasing dynamics
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 $$\langle \psi_0 | \psi_1 \rangle = 0$$

$\Rightarrow$ Orthogonality of states no useful criterion for “physically different”

$\Rightarrow$ Loschmidt echo not useful for characterizing irreversibility

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

$\Rightarrow$ generic exponential decay
b) Out-of-time-order (OTO) correlators

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


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) ]
\( \rightarrow \) 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 \( \frac{F(t)}{2\langle B^2 \rangle \langle A^2 \rangle} = g_0 - g_1 e^{\lambda_L t} \)

- For large-N CFT holographically described by Einstein gravity (t>>\beta)
  \( g_0 = O(1) \), \( g_1 \propto \frac{1}{N^2} \), \( \lambda_L = \frac{2\pi}{\beta} \) [Shenker, Stanford (2014)]

- Conjecture [Maldacena et al. (2015)]:
  Universal bound \( \lambda_L \leq \frac{2\pi}{\beta} \)
Quantum information [Hosur et al. (2016)]

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

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

$U(t) = \sum_{i,j} u_{ij}(t) \ket{i} \bra{j}$

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

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

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

\[ I_3(A : C : D) = I(A : C) + I(A : D) - I(A : CD) = S_A + S_C + S_D - S_{AC} - S_{AD} - S_{CD} + S_{ACD} \]

must become negative with large magnitude for system to scramble

Hosur et al. (2015):
Qubits, infinite temperature, \([A_i, D_j] = 0\)

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

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

with \( \epsilon_{\text{min}} = 2^{-2a} \)
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

\( \pi \)-pulse:

Effectively \( H_i \rightarrow -H_i \)

Spin echo:

Measure natural linewidth

Limited by many-body interactions
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 $\rho$ 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 randomness

$\pi$-pulse:

Effectively $H_i \rightarrow -H_i$

Spin echo:

Measure natural linewidth

Limited by many-body interactions

Magic echo


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

Loschmidt daemon

What is the effect of $\Sigma$?
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 $\tau$ for realistic echo protocols

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

Forward time evolution

$$\langle \psi(\tau) \rangle = U(\tau) \langle \psi_{ini} \rangle$$

Backward time evolution

$$\langle \psi(t) \rangle = V(t - \tau) U(\tau) \langle \psi_{ini} \rangle$$

Expectation value of observable

$$O_s \overset{\text{def}}{=} \langle \psi(s) | O | \psi(s) \rangle$$

Normalised echo peak height

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

echo peak at $t \approx 2\tau$
(and usually not exactly at $t=2\tau$)
Irreversible dynamics means $E_t^*[O]$ decays exponentially or faster, otherwise the dynamics is reversible.
4) Echos in the transverse field Ising model


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

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

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

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

\[
\text{Reduced density matrix for } n \text{ spin subsystem from time evolved initial state } \lim_{t \to \infty} |\psi_i(t)\rangle \langle \psi_i(t)|_n = \rho_{\text{GGE},n}
\]

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 $\sigma_z^x$

   longitudinal spin-spin correlation function (distance d) $\sigma_z^x \sigma_z^{i+d}$

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 $\langle m_y \rangle_t$ (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 $\delta h$

- Measure entanglement entropy $S_{\text{ent}}^d(t)$ for subsystem with $d$ spins

Algebraic decay of normalised echo peak height of the entanglement entropy

$$E^*_\tau[S_{\text{ent}}^d] \propto \tau^{-1/2}$$
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
\[ H = -J \sum_t S_t^x S_{t+1}^x - h_x \sum_t S_t^x - h_z \sum_t S_t^z \]

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