Pure state quantum statistical mechanics - an overview

Christian Gogolin

ICFO - The Institute of Photonic Sciences

Heidelberg University
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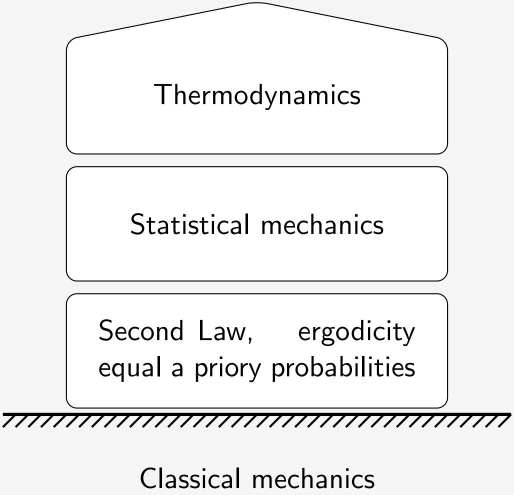
Old questions and new results

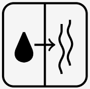
How do quantum mechanics and statistical mechanics go together?

New foundation for statistical mechanics



New foundation for statistical mechanics

Thermodynamics

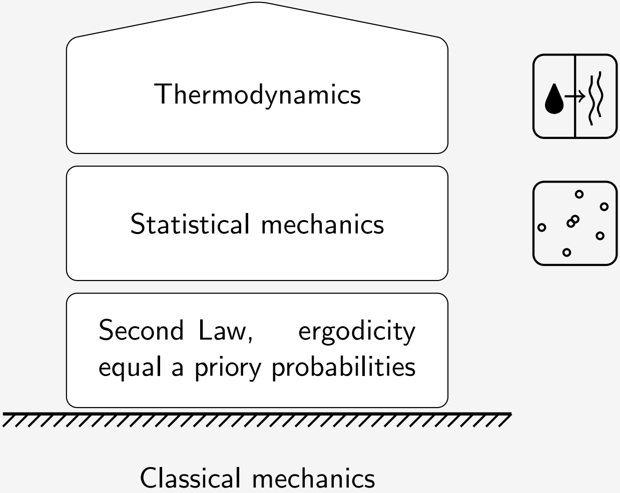


Statistical mechanics

Second Law, ergodicity
equal a priory probabilities

Classical mechanics

New foundation for statistical mechanics



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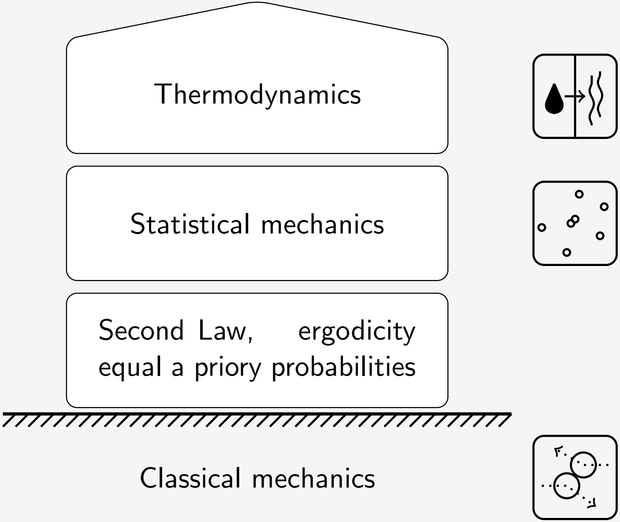

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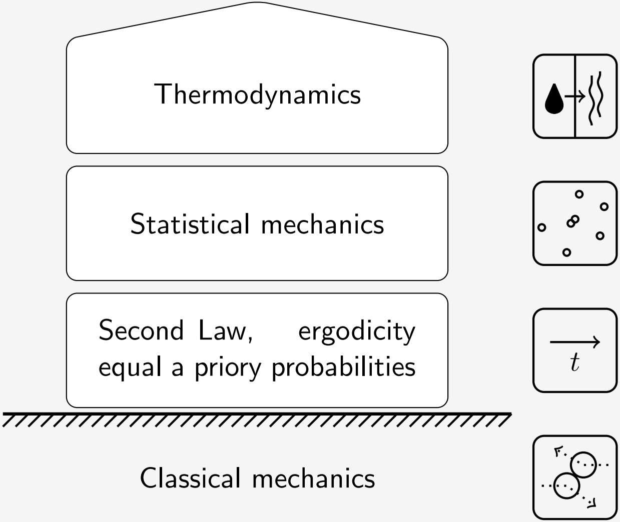

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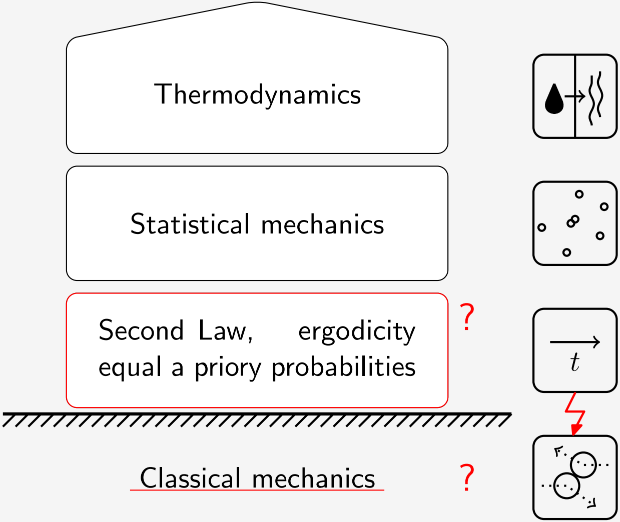


New foundation for statistical mechanics

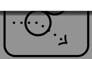
"There is no line of argument proceding from the laws of microscopic mechanics to macroscopic phenomena that is generally regarded by physicists as convincing in all respects."

— E. T. Jaynes [1] (1957)

"Statistical physics [...] has not yet developed a set of generally accepted formal axioms [...]"

— Jos Uffink [2] (2006)

Classical mechanics ?



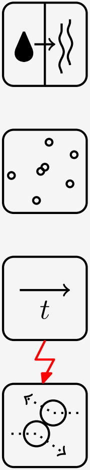
New foundation for statistical mechanics

Thermodynamics

Statistical mechanics

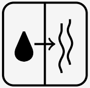
Second Law, ergodicity equal a priory probabilities ?

Classical mechanics ?

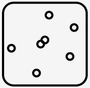


New foundation for statistical mechanics

Thermodynamics



Statistical mechanics



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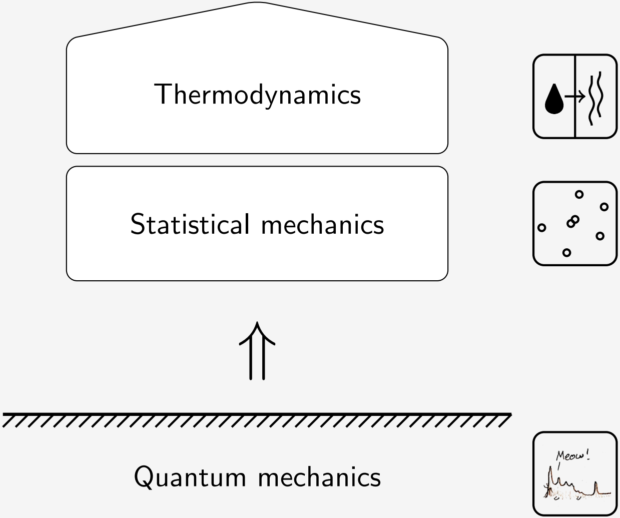

Recent experiments and numerical simulations

Science 337, 1318 (2012):

Relaxation and Prethermalization in an Isolated Quantum System

M. Gring,[1] M. Kuhnert,[1] T. Langen,[1] T. Kitagawa,[2] B. Rauer,[1] M. Schreitl,[1] I. Mazets,[1,3] D. Adu Smith,[1] E. Demler,[2] J. Schmiedmayer[1,4*]

Understanding relaxation processes is an important unsolved problem in many areas of physics. A key challenge is the scarcity of experimental tools for the characterization of complex transient states. We used measurements of full quantum mechanical probability distributions of a coherently split one-dimensional ...

this occurs. In situations in which conservation laws inhibit efficient relaxation, many-body systems are expected to display a complex behavior. An intriguing phenomenon that has been suggested in this context is prethermalization (4), a general concept that is predicted to be applicable to a large variety of physical systems (5–9). In the present understanding, prethermalization is characterized by the rapid establishment of a quasi-stationary state that already exhibits some equilibrium-like properties. Full relaxation to the

LETTERS
PUBLISHED ONLINE: 8 SEPTEMBER 2013 | DOI: 10.1038/NPHYS2739
nature physics

Local emergence of thermal correlations in an isolated quantum many-body system

T. Langen*, R. Geiger, M. Kuhnert, B. Rauer and J. Schmiedmayer*

Understanding the dynamics of isolated quantum many-body systems is a central open problem at the intersection between statistical physics and quantum physics. Despite important theoretical effort[1], no generic framework exists yet to understand when and how an isolated quantum ...

well, thereby realizing the matter-wave analogue of a coherent beamsplitter[18] (see Methods). The system is allowed to evolve in the double well for a variable time t, before the gases are released ...

LETTER nature
doi:10.1038/nature10...

Light-cone-like spreading of correlations in a quantum many-body system

Marc Cheneau[1], Peter Barmettler[2], Dario Poletti[2], Manuel Endres[1], Peter Schauß[1], Takeshi Fukuhara[1], Christian Gross[1], Immanuel Bloch[1,3], Corinna Kollath[2,4] & Stefan Kuhr[1,5]

In relativistic quantum field theory, information propagation is bounded by the speed of light. No such limit exists in the non-relativistic case, although in real physical systems, short-range interactions may be expected to restrict the propagation of information to finite velocities. The question of how fast correlations can spread in quantum many-body systems has been long studied[1]. The existence of a maximal velocity, known as the Lieb–Robinson bound, has been shown theoretically to exist in several interacting many-body systems (for example, spins on a lattice[2–5])—such systems can be regarded as exhibiting an effective light cone that bounds the propagation speed of correlations. The existence of such a 'speed of light' has profound implications for condensed matter physics and quantum information, but has not been observed experimentally. Here we report the time-resolved detection of propagating correlations in an interacting quantum many-body system. By quenching a one-dimensional quantum gas in an optical lattice, we reveal how quasiparticle pairs transport correlations with a finite velocity across the system, resulting in an effective light cone for the quantum dynamics. Our results open perspectives for understanding the relaxation of closed quantum systems far from equilibrium[6], and for engineering the efficient quantum channels necessary for fast quantum computations[7].

Lieb–Robinson bounds have already found a number of fundamental applications[8,9]. For example, they enable a rigorous proof of a long-standing conjecture that linked the presence of a spectral gap in a lattice system to the exponential decay of correlations in the ground state[10,11]. They also provide fundamental scaling laws for entanglement entropy, which is an indicator of the computational cost of simulating strongly interacting systems[12]. Despite intensive theoretical work, the extent to which Lieb–Robinson bounds for interacting spins on a lattice[2–5] can be generalized remains however an open question[13–16].

In the context of quantum many-body systems, the existence of a Lieb–Robinson bound can be probed by recording the dynamics following a sudden parameter change (a quench) in the Hamiltonian. In that case, a simple picture has been suggested: quantum-entangled quasiparticles emerge from the initially highly excited state and propagate ballistically[5], carrying correlations across the system. Ultracold atomic gases offer an ideal test bed for exploring such quantum dynamics owing to their almost perfect decoupling from the environment and their fast tunability[17]. In addition, the recently demonstrated technique of single-site imaging in an optical lattice[18,19]

the one-dimensional geometry considered here, the critical point of this transition is located at $(U/J)_c \approx 3.4$ (ref. 22). We observed the ti... evolution of spatial correlations after a fast decrease of the effecti... interaction strength U/J, from an initial value deep in the Mo... insulating regime, with filling $n=1$, to a final value closer to the criti... point (Fig. 1a). After such a quench, the initial many-body state $|\Psi_0\rangle$ ... highly excited and acts as a source of quasiparticles. In order ... elucidate the nature and the dynamics of these quasiparticles, we ha... developed an analytical model in which the occupancy of each latti... site is restricted to $n=0$, 1 or 2 (Supplementary Information). F... large interaction strengths, the quasiparticles consist of either an exce... particle ('doublon') or a hole ('holon') on top of the unity-filling bac... ground. The quasiparticles inherit the bosonic nature of the atoms, b... they can be turned into fermions (fermionized) using a Jorda... Wigner transformation. This allows us to partially eliminate ... non-physical states in which a lattice site would be occupied by tw... quasiparticles. To first order in J/U, we then find that the many-bo... state at time t after the quench reads:

$$|\psi(t)\rangle \simeq |\psi_0\rangle + i\sqrt{8}\frac{J}{U}\sum_k \sin(ka_{\text{lat}}) \left[1-e^{-i(\epsilon_d(k)+\epsilon_h(-k))t/\hbar}\right]\hat{d}_k^\dagger \hat{h}_{-k}^\dagger|\psi_0\rangle$$

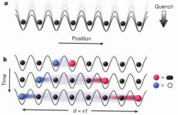

Figure 1 | Spreading of correlations in ...

nature physics
ARTICLES
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Probing the relaxation towards equilibrium in an isolated strongly correlated one-dimensional Bose gas

S. Trotzky[1,2,3]*, Y-A. Chen[1,2,3], A. Flesch[4]*, I. P. McCulloch[5], U. Schollwöck[1,6], J. Eisert[6,7,8] and I. Bloch[1,2,3]

The problem of how complex quantum systems eventually come to rest lies at the heart of statistical mechanics. The maximum-entropy principle describes which quantum states can be expected in equilibrium, but not how closed quantum many-body systems dynamically equilibrate. Here, we report the experimental observation of the non-equilibrium dynamics of a density wave of ultracold bosonic atoms in an optical lattice in the regime of strong correlations. Using an optical superlattice, we follow its dynamics in terms of quasi-local densities, currents and coherences—all showing a fast relaxation towards equilibrium values. Numerical calculations based on matrix-product states are in an excellent quantitative agreement with the experimental data. The system fulfills the promise of being a dynamical quantum simulator, in that the controlled dynamics runs for longer times than present classical algorithms can keep track of.

Ultracold atoms in optical lattices provide highly controllable quantum systems allowing one to experimentally probe various quantum many-body phenomena. In this way, ground state properties of Hamiltonians that play a fundamental role in the condensed matter context have been investigated under precisely tunable conditions[1–3]. Features that are even harder to probe in actual condensed matter materials or to simulate in numerical studies are dynamical ones, including dynamical properties emerging in adiabatic sweeps[4] and in systems far from equilibrium[5–11]. In this respect, for example, the quench from a shallow to a deep optical lattice[6–8] and the phase dynamics emerging after splitting a one-dimensional Bose liquid[12] have previously been studied experimentally.

Here, we report on the direct observation of relaxation dynamics in an interacting many-body system using ultracold atoms in an optical lattice. Starting with a patterned density with alternating empty and occupied sites in isolated Hubbard

see refs 15,16 and references therein) of the Hamiltonian dynamics without free parameters, further developing the ideas of previous numerical studies[17,18].

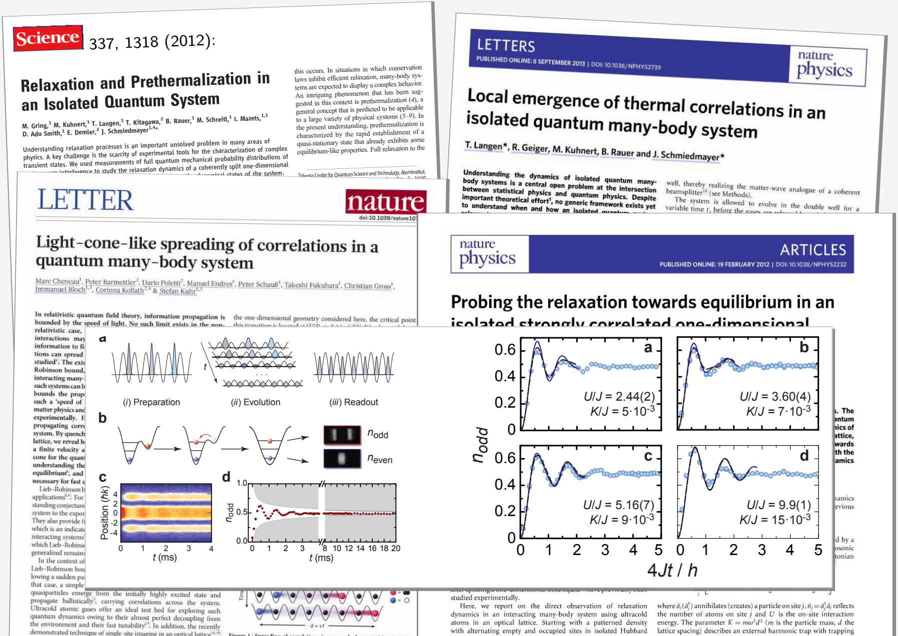
Concept of the experiments

We consider a one-dimensional chain of lattice sites coupled by a tunnel coupling J and filled with repulsively interacting bosonic particles. In the tight-binding approximation, the Hamiltonian takes the form of a one-dimensional Bose–Hubbard model[5,19]

$$\hat{H} = \sum_j \left[-J(\hat{a}_j^\dagger \hat{a}_{j+1} + \text{h.c.}) + \frac{U}{2}\hat{n}_j(\hat{n}_j - 1) + \frac{K}{2}\hat{n}_j j^2 \right]$$

where $\hat{a}_j$ ($\hat{a}_j^\dagger$) annihilates (creates) a particle on site j, $\hat{n}_j = \hat{a}_j^\dagger \hat{a}_j$ reflects the number of atoms on site j and U is the on-site interaction energy. The parameter $K = m\omega^2 d^2$ (m is the particle mass, d the lattice spacing) describes an external harmonic trap with trapping

Recent experiments and numerical simulations



What is wrong with the canonical foundations?

Thermodynamics

Statistical mechanics

Second Law, ergodicity
equal a priory probabilities ?

Classical mechanics ?

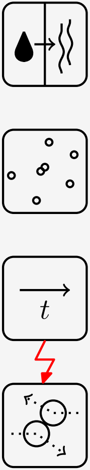


Table of contents

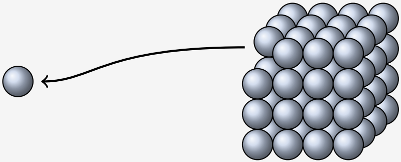
Setting

Subsystem, H_S

d_S

Bath, H_B

$d_B \gg d_S$



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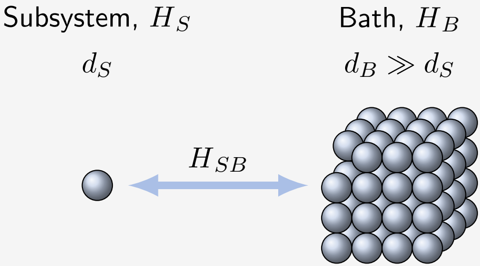


Setting

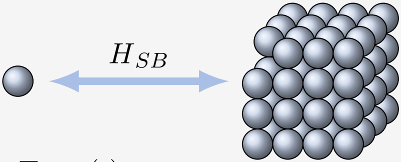
$$H = H_S + H_B + H_{SB} \qquad \rho(t) = |\psi(t)\rangle\langle\psi(t)|$$

Subsystem, H_S

d_S

Bath, H_B

$d_B \gg d_S$



$$\rho^S(t) = \mathrm{Tr}_B\, \rho(t)$$

Equilibration

Equilibration

Theorem (Equilibration on average [9])

If H has non-degenerate energy gaps, then for every $\rho(0) = |\psi_0\rangle\langle\psi_0|$ there exists a ω^S such that:

$$\overline{\mathcal{D}\left(\rho^S(t), \omega^S\right)} \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\mathrm{eff}}}}$$

[7] M Cramer, C. M. Dawson, J Eisert, and T. J. Osborne, Physical Review Letters, 100.3 (2008), 30602
[8] P. Reimann, Physical Review Letters, 101.19 (2008), 190403
[9] N. Linden, S. Popescu, A. Short, and A. Winter, Physical Review E, 79.6 (2009), 61103
[10] A. J. Short and T. C. Farrelly, New Journal of Physics, 14.1 (2012), 013063
[11] P. Reimann and M. Kastner, New Journal of Physics, 14.4 (2012), 43020

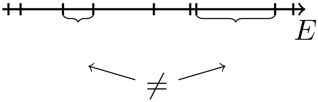
Equilibration

Non-degenerate energy gaps

H has non–degenerate energy gaps iff:

$$E_k - E_l = E_m - E_n$$

$$\implies k = l \wedge m = n \quad \vee \quad k = m \wedge l = n$$



Intuition: Sufficient for H to be fully interactive

$$H \neq H_1 \otimes \mathbb{1} + \mathbb{1} \otimes H_2$$

Theorem

If H has ... $\rangle\langle\psi_0|$

there exis...

[7] M Cramer, C. ...
[8] P. Reimann, P...
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Effective dimension

$$d^{\mathrm{eff}} := \frac{1}{\sum_k |\langle E_k|\psi_0\rangle|^4}$$

Intuition: Dimension of supporting energy subspace

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$$\overline{\mathcal{D}\left(\rho^S(t), \omega^S\right)} \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\mathrm{eff}}}}$$

$\Longrightarrow$ If $d^{\mathrm{eff}} \gg d_S^2$ then $\rho^S(t)$ equilibrates on average.

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Maximum entropy principle

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Theorem (Maximum entropy principle [12])

If $\mathrm{Tr}[A\,\rho(t)]$ equilibrates on average, it equilibrates towards its time average

$$\overline{\mathrm{Tr}[A\,\rho(t)]} = \mathrm{Tr}[A\,\overline{\rho(t)}] = \mathrm{Tr}[A\,\omega],$$

and ω is the state that maximizes the von Neumann entropy, given all conserved quantities.

[12] C. Gogolin, M. P. Müller, and J. Eisert, Physical Review Letters, 106.4 (2011), 40401

Maximu

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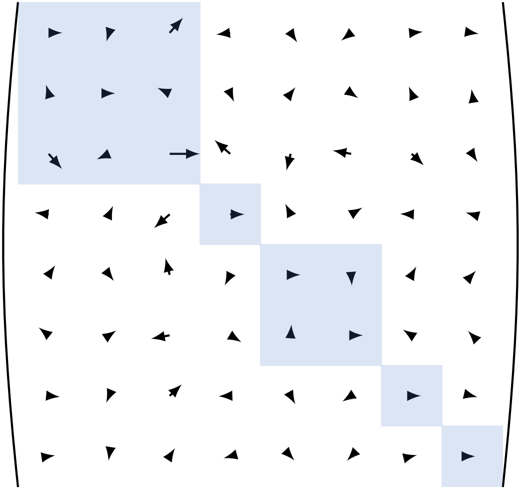
Time averaging

$\rho(0) =$ 

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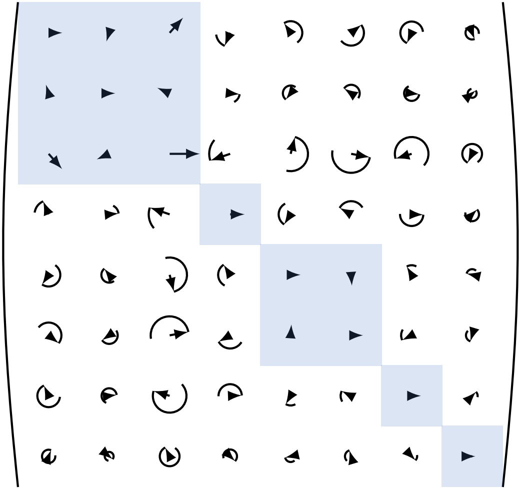

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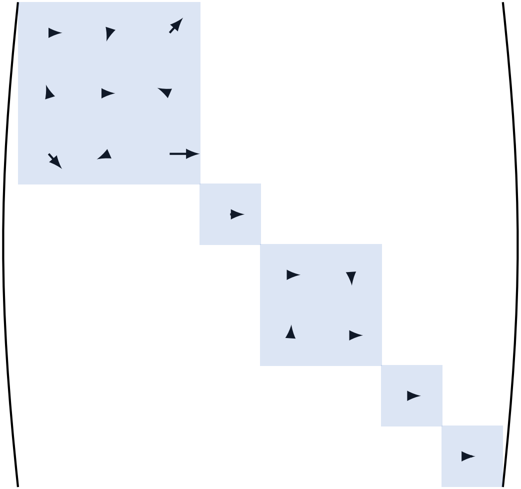

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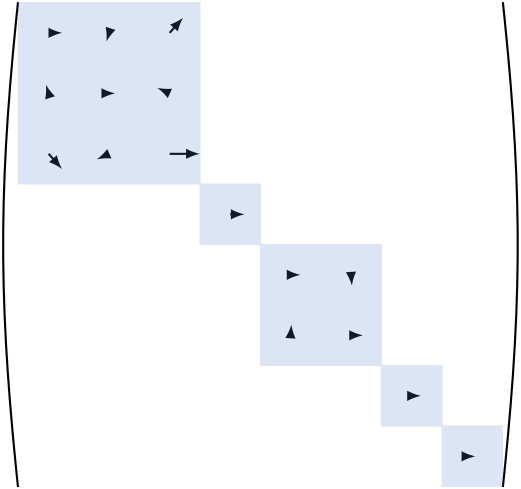
$\omega =$ 

$\rho(0) \mapsto \omega$ is a pinching $\Rightarrow \omega$ maximizes entropy

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$\Rightarrow$ Maximum entropy principle from pure quantum dynamics.

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⇒ Maximum entropy principle from pure quantum dynamics.

Interesting open questions:

- Do we really need all (exponentially many) conserved quantities?
- If not, then which?
- Does this depend on integrability of the model?
- What is the relation to the GGE?

[12] C. Gogolin, M. P. Müller, and J. Eisert, Physical Review Letters, 106.4 (2011), 40401

Decoherence and the speed of fluctuations

Speed of the fluctuations around equilibrium

$$v_S(t) \coloneqq \frac{1}{2} \left\| \frac{d\rho^S(t)}{dt} \right\|_1$$

[13] N. Linden, S. Popescu, A. J. Short, and A. Winter, New Journal of Physics, 12.5 (2010), 055021

Speed of the fluctuations around equilibrium

$$v_S(t) := \frac{1}{2}\left\|\frac{d\rho^S(t)}{dt}\right\|_1 \qquad \frac{d\rho^S(t)}{dt} = \mathrm{i}\ \mathrm{Tr}_B[\psi(t), H]$$

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Theorem (states are slow most of the time [13])

For every $\rho(0) = |\psi_0\rangle\langle\psi_0|$

$$\overline{v_S(t)} \leq \| H_S \otimes \mathbb{1} + H_{SB} \|_\infty \sqrt{\frac{d_S^3}{d^{\mathrm{eff}}(\omega)}}.$$

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$\Longrightarrow$ If $d^{\text{eff}}(\omega) \gg d_S^3$ then $\rho^S(t)$ is slow most of the time.

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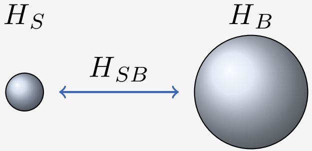
When can a subsystem be slow?

When can a subsystem be slow?

Given the interaction is weak

$$\| H_{SB} \|_\infty \ll \| H_S \|_\infty,$$



When can a subsystem be slow?

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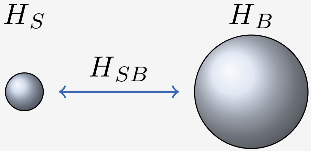

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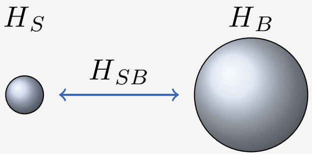

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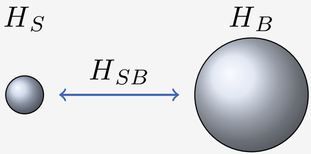

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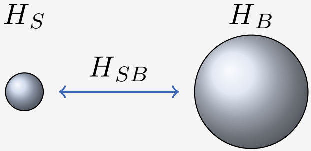

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Two competing forces

$$\frac{d\rho^S(t)}{dt} = \mathrm{i}\,[\rho^S(t), H_S] + \mathrm{i}\ \mathrm{Tr}_B[\rho(t), H_{SB}]$$

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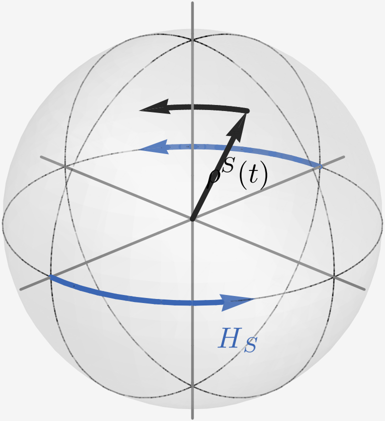

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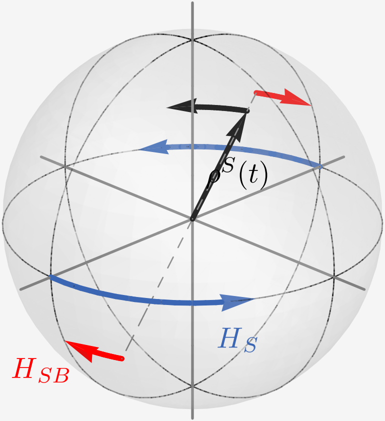

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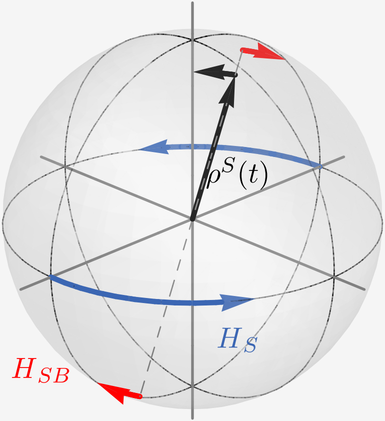

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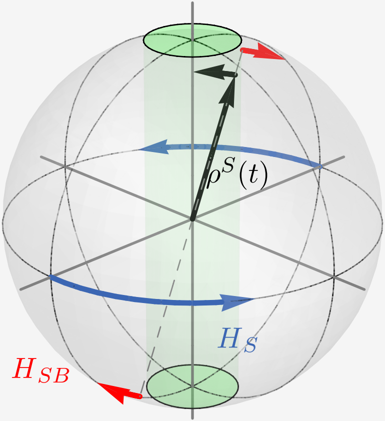

Decoherence through weak interaction

Theorem

$$\max_{\{(k,l)\}} \sum_{(k,l)} 2\,|E_k^S - E_l^S|\,|\rho_{kl}^S| \leq 2\,\|\,H_{SB}\,\|_\infty + \left\| \frac{d\rho^S(t)}{dt} \right\|_1$$

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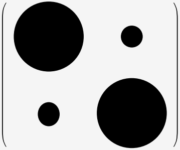

Decoherence in the H_S eigenbasis

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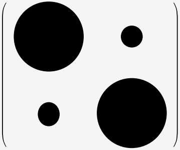
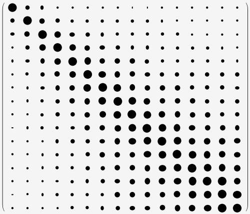


Decoherence in the H_S eigenbasis



No Schrödinger's cat states

Justification of ensembles

Typicality of expectation values

Theorem (most pure states look like microcanonical states [14])

Let $\mathcal{K} \subseteq \mathcal{H}$, $d := \dim(\mathcal{K})$ and $\Pi_{\mathcal{K}}$ the projector onto $\mathcal{K}$.
For randomly chosen pure states $|\psi\rangle \in \mathcal{K}$ and every $\epsilon > 0$

$$\Pr\left\{ \left| \operatorname{Tr}(A\,\psi) - \operatorname{Tr}(A \frac{\Pi_{\mathcal{K}}}{d_{\mathcal{K}}}) \right| \geq \epsilon \right\} \leq 2\, \mathrm{e}^{-\frac{C\,d\,\epsilon^2}{\|A\|_\infty^2}},$$

with $C = (36\,\pi^3)^{-1}$.

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$\Longrightarrow$ Can be thought of as a justification of the equal a priory probability postulate

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Thermalization

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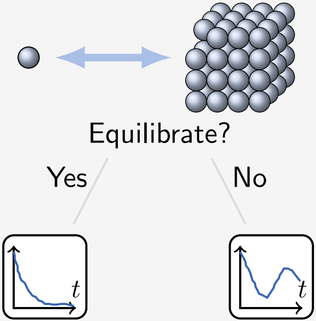

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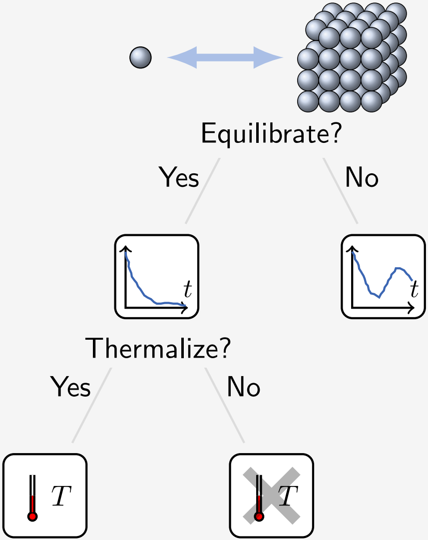

Thermalization is a complicated process

Thermalization implies:

1. Equilibration [7–11, 15]
2. Subsystem initial state independence [12, 16]
3. Weak bath state dependence [17]
4. Diagonal form of the subsystem equilibrium state [18]
5. ...
6. Thermal state $\omega^S = \mathrm{Tr}_B[\omega] \approx g^S_{H_S}(\beta) \propto \mathrm{e}^{-\beta\, H_S}$ [17, 19]

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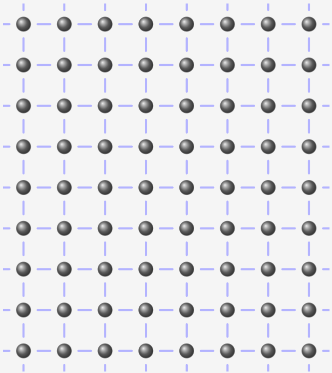
...

Locality of temperature

The setting

- Local Hamiltonian (spins or fermions)

$$H := \sum_{\lambda \in \mathcal{E}} h_\lambda$$



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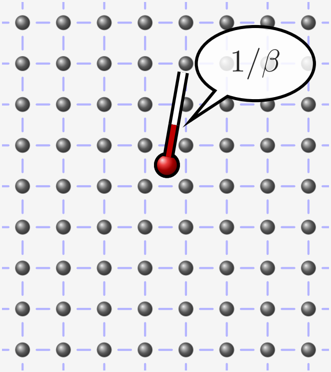

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- Thermal state

$$g(\beta) := \frac{\mathrm{e}^{-\beta H}}{\mathrm{Tr}\left[\mathrm{e}^{-\beta H}\right]}$$

The setting

- Local Hamiltonian truncated to $S \subset V$

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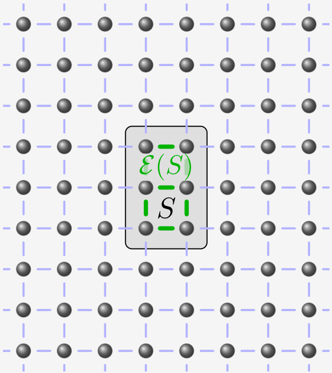

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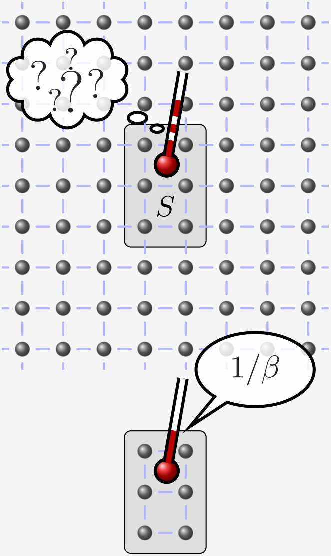

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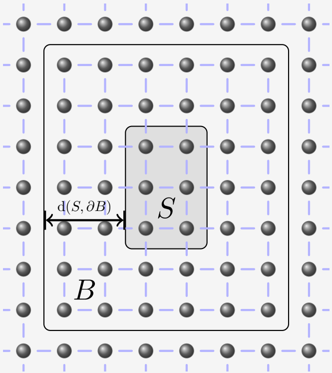
$$g_B(\beta) := \frac{\mathrm{e}^{-\beta\, H_B}}{\mathrm{Tr}\left[\mathrm{e}^{-\beta\, H_B}\right]}$$

- Introduce buffer region

$$\mathrm{Tr}_{S^c}[g_B(\beta)] \approx \mathrm{Tr}_{S^c}[g(\beta)]\ ?$$



This can be made rigorous:

Generalized covariance

$$\mathrm{cov}_\rho^\tau(A, A') := \mathrm{Tr}[\rho^\tau A\, \rho^{1-\tau} A'] - \mathrm{Tr}[\rho\, A]\, \mathrm{Tr}[\rho\, A']$$

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Theorem (Truncation formula [20])

For any observable $A = A_S \otimes \mathbb{1}$

$$\mathrm{Tr}[A\, g_B(\beta)] - \mathrm{Tr}[A\, g(\beta)] = \beta \int_0^1 \int_0^1 \operatorname{cov}^\tau_{g(s,\beta)}(H_{\partial B}, A)\, \mathrm{d}\tau\, \mathrm{d}s\,,$$

where $g(s, \beta)$ is thermal state of $H(s) := H - (1 - s)\; H_{\partial B}$.

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exactly captures the response of local expectation values.

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Let $J := \max_\lambda \|h_\lambda\|_\infty$, then for every $\tau \in [0,1]$ and $\beta < \beta^*(J,\alpha)$

$$\left|\mathrm{cov}^{\tau}_{g(\beta)}(A, A')\right| \leq C\ \mathrm{e}^{-\,\mathrm{d}(A,A')\,/\,\xi(\beta\, J,\alpha)}$$

with $\alpha = \alpha(\mathcal{E})$ the lattice animal constant.

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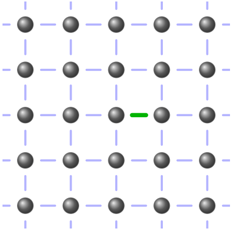

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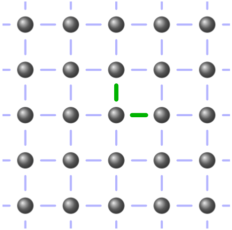

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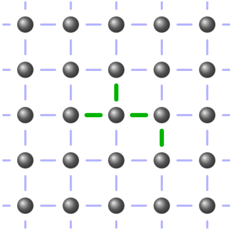

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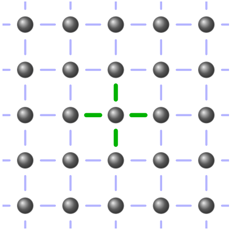

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Implications

$$\boxed{\beta < \beta^*(J,\alpha) \implies \mathcal{D}\left(g^S(\beta), {g_B}^S(\beta)\right) \leq C' \, \mathrm{e}^{-\mathrm{d}(S,\partial B)/\xi(\beta\, J,\alpha)}}$$

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Local stability of thermal states

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Classical simulability with cost independent of total system size

Local expectation values can be calculates with cost independent of the total system size.

A universal bound on phase transitions

Universal critical temperature

The critical temperature

$$\frac{1}{\beta^* J} = \frac{2}{\ln\left((1+\sqrt{1+4/\alpha})/2\right)}$$

upper bounds the physical critical temperatures of all possible models.

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upper bounds the physical critical temperatures of all possible models.

Example: 2D square lattice ($\alpha \leq 4\,\mathrm{e}$)

- The bound:
  $1/(\beta^*\, J) = 2/\ln((1+\sqrt{1+1/\mathrm{e}})/2) \approx 24.58$
- Ising model (ferromagnetic, isotropic) phase transition at:
  $1/(\beta_c\, J) = 2/\ln(1+\sqrt{2}) \approx 2.27$

Summary

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And there is more. . .

- Shallow but broad overview:
  J. Eisert, M. Friesdorf, and C. Gogolin, Nature Physics, 11.2 (2015), 124–130
- In-depth review:
  C. Gogolin and J. Eisert, Reports on Progress in Physics, 79.5 (2016), 56001

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Thank you for your attention!

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