

# Universal dynamics in thermally isolated systems.

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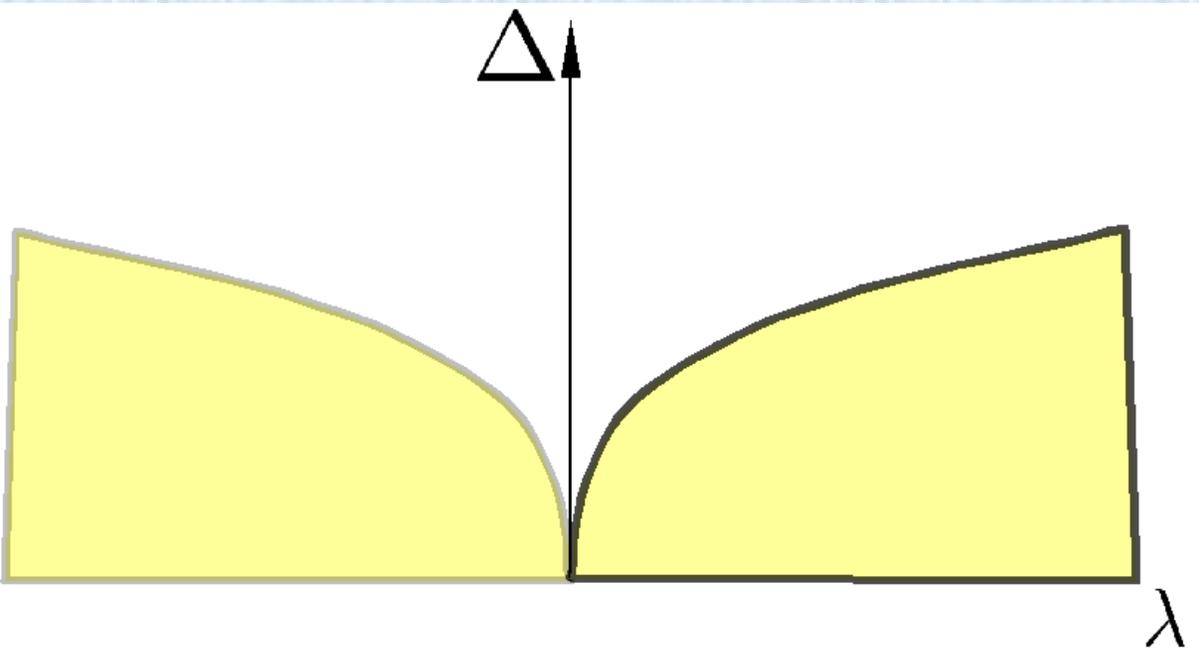
# Non-equilibrium. Set of questions to answer.

1. Is there a notion of universality in quantum dynamics?
2. If yes, can we classify perturbations according to their relevance. Is it different from equilibrium?
3. How is complexity of dynamics related to universality?
4. How can we describe relaxation in integrable, non-integrable and weakly non-integrable systems?
5. Can we think about relaxation (dynamics) as an RG process? If yes, what is it?
6. How can we reconcile quantum and classical complexity?
7. ...

# Universality of dynamics

1. Nearly adiabatic dynamics near quantum critical points. Universal scalings from adiabatic fidelity.
2. Diagonal entropy and laws of thermodynamics.
3. Relaxational dynamics as an RG process. Universal dynamics near non-equilibrium KT phase transition.
4. Universal energy distribution in externally driven systems.

## Quantum phase transitions in a nutshell.



correl. length:  $\xi \sim |\lambda|^{-\nu}$

gap:  $\Delta \sim |\lambda|^{z\nu}$

susceptibility  $\chi \sim |\lambda|^{-\alpha}$

susceptibility

Equilibrium properties of the system are universal near critical points (both classical and quantum).

What can we say about non-equilibrium dynamics?

# Quench dynamics near a quantum critical point (QCP)

Dynamics:

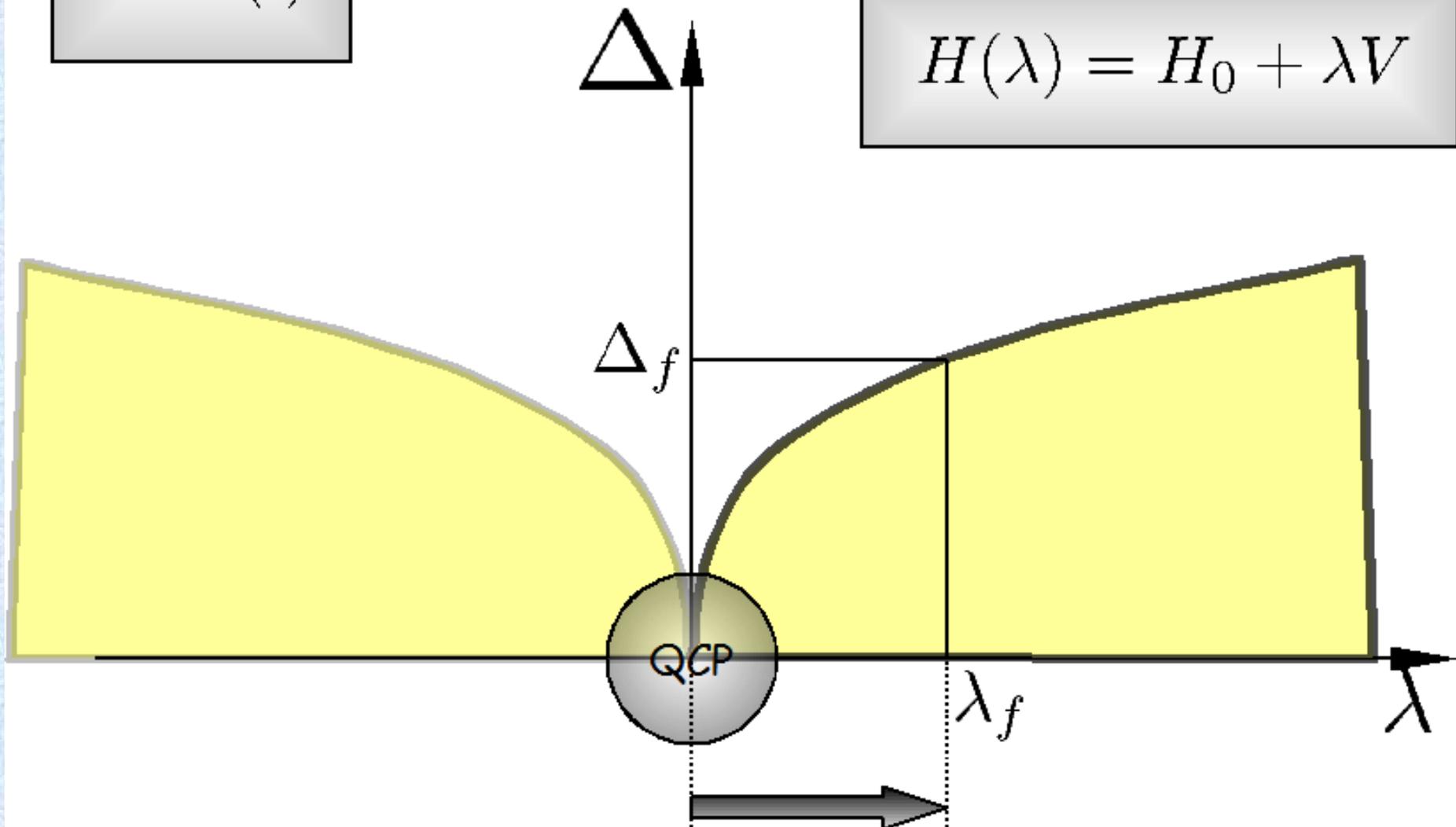
$$\lambda = \lambda(t)$$

Hamiltonian  
at the QCP

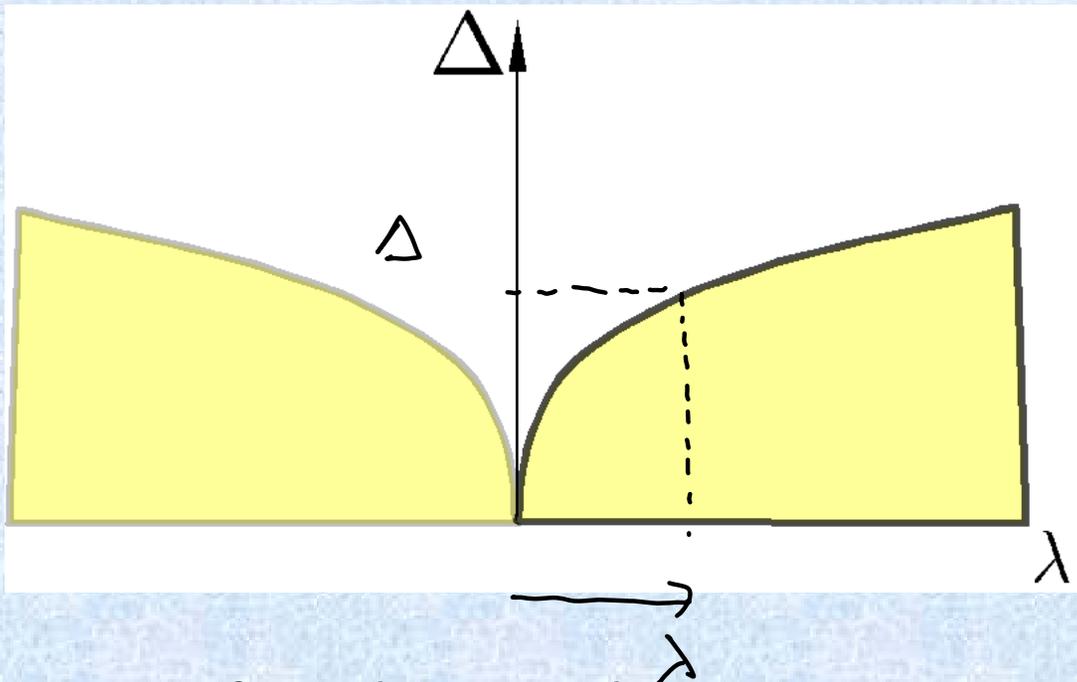
external  
parameter

relevant  
operator

$$H(\lambda) = H_0 + \lambda V$$



# Sudden quench



$$\text{gap: } \Delta \sim |\lambda|^{z\nu}$$

States with  $\epsilon \lesssim \Delta$   
are diabatic - highly excited

States with  $\epsilon \gg \Delta$   
are adiabatic - not excited

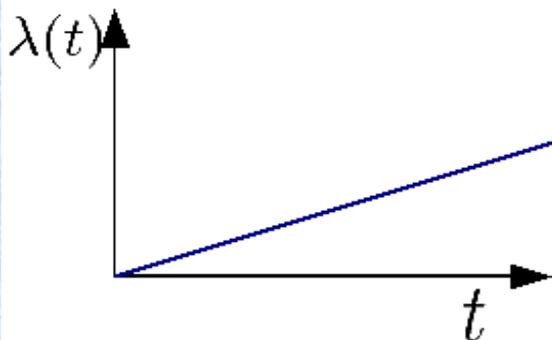
Excess energy = heat

Density of single-particle excitations

$$n_{\text{ex}} \sim 1/\xi^d \sim |\lambda|^{d\nu}$$

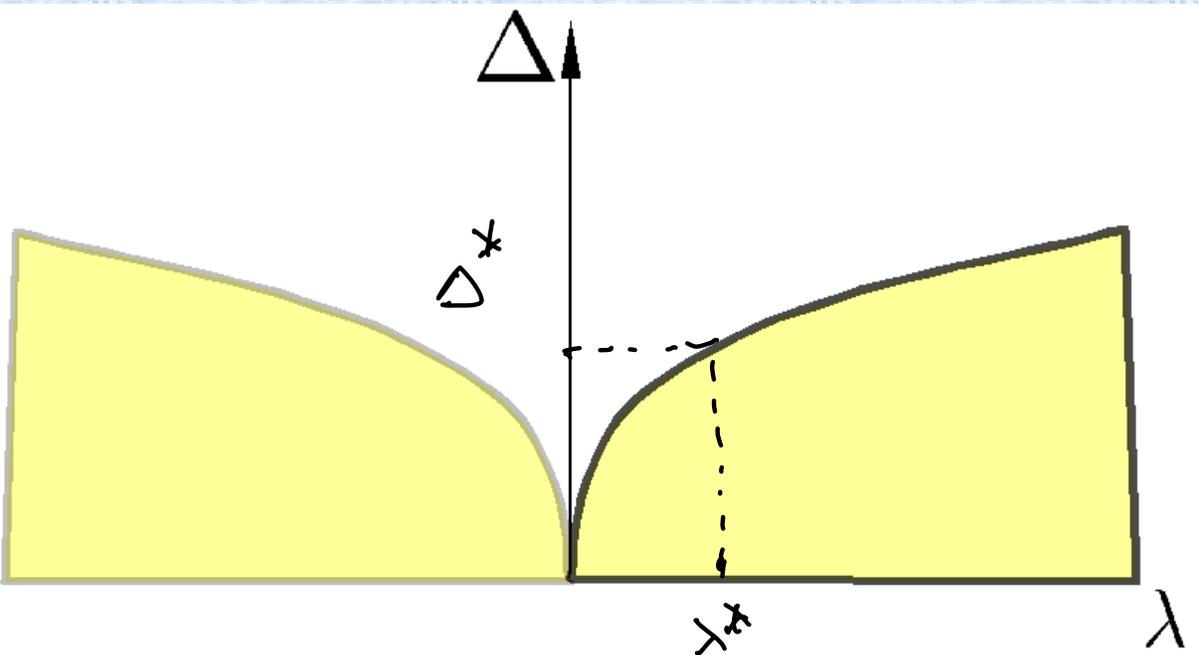
$$Q \sim |\lambda|^{z\nu} n_{\text{ex}} \sim |\lambda|^{(d+z)\nu}$$

Power law dependence in time of the external parameter  $\lambda(t)$



$$\lambda(t) = vt$$

The system is not adiabatic near QCP.



States with  $\epsilon \lesssim \Delta^*$   
are diabatic, excited.

States with  $\epsilon \gg \Delta^*$   
are adiabatic, not excited

Use Landau-Zener criterion

$$\frac{d\Delta^*}{dt} = (\Delta^*)^2, \quad \Delta^* = (vt^*)^{z\nu} \Leftrightarrow \begin{cases} t^* \sim |v|^{-z\nu/(z\nu+1)} \\ \xi^* \sim |v|^{-\nu/(z\nu+1)} \end{cases}$$

$$\Delta^* = (vt^*)^{z\nu} \sim |v|^{z\nu/(z\nu+1)}$$

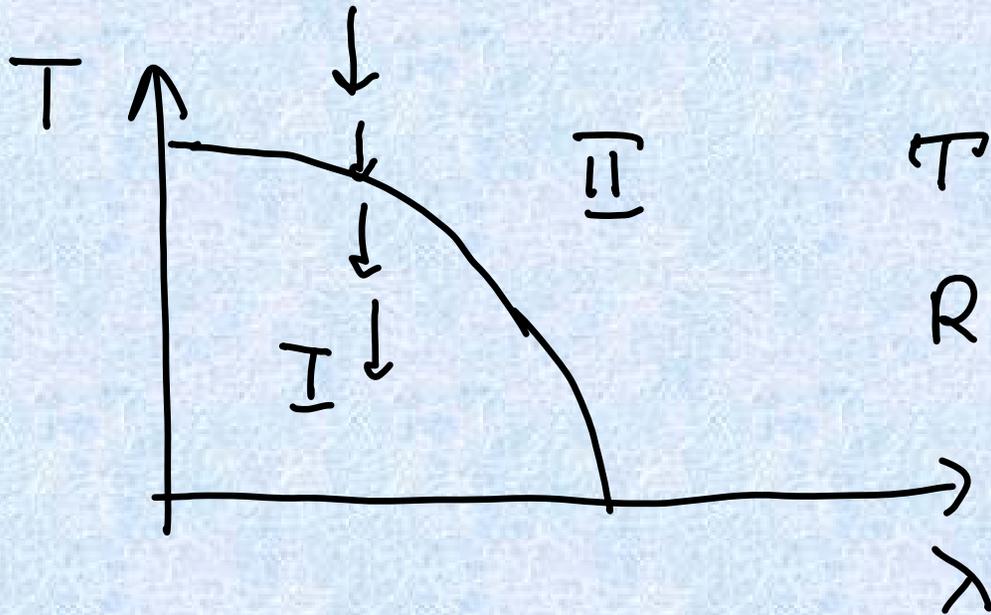
$$n_{ex} \sim (\Delta^*)^{d/z} \sim |v|^{d\nu/(z\nu+1)}$$

$$Q \sim |v|^{(d+z)\nu/(z\nu+1)}$$

A.P. 2003, Zurek, Dorner, Zoller 2005

analogue of the latent heat

# Classical Kibble-Zurek mechanism



$$T \sim T_0 - \nu t$$

$$\text{Rel. time } \tau \sim \frac{1}{|T_c - T|^{z\nu}}$$

$$\xi \sim \frac{1}{|T_c - T|^\nu}$$

Time to transition

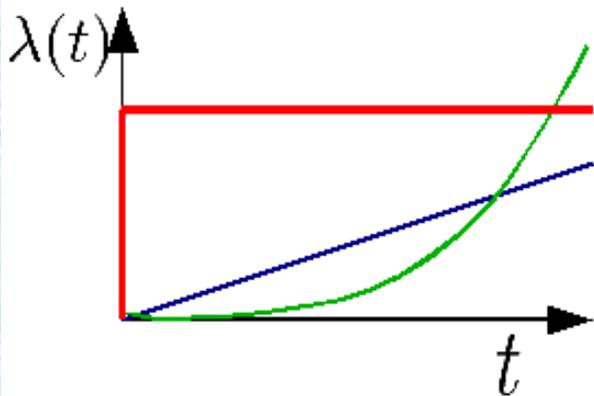
$$t^* = \frac{T - T_c}{\nu} \sim \tau = \frac{1}{(T_c - T)^{z\nu}} \Rightarrow (T - T_c) \sim \nu^{\frac{1}{1+z\nu}}$$

Adiabatic to diabatic crossover

$$\xi^* \sim |\nu|^{-\nu/(z\nu+1)} \Leftrightarrow n_{ex} \sim \frac{1}{(\xi^*)^d} \sim |\nu|^{\frac{d\nu}{z\nu+1}}$$

Arbitrary power law quench.

Power law dependence in time of the external parameter  $\lambda(t)$



$$\lambda(t) = v \frac{t^r}{r!} \Theta(t)$$

Use the same argument

$$\frac{d\Delta^*}{dt} = (\Delta^*)^2, \quad \Delta^* = (vt^r)^{z\nu} \Leftrightarrow \begin{cases} t^* \sim |v|^{-z\nu/(z\nu r+1)} \\ \xi^* \sim |v|^{-\nu/(z\nu r+1)} \end{cases}$$

$$n_{ex} \sim (\Delta^*)^{d/z} \sim |v|^{d\nu/(z\nu r+1)}$$

$$\lambda(t) = v \frac{t^r}{r!} \Theta(t)$$

$$n_{ex} \sim |v|^{d\nu/(z\nu r+1)}$$
$$Q \sim |v|^{(d+z)\nu/(z\nu r+1)}$$

$v$  is the adiabatic parameter - controls proximity to the instantaneous ground state

$r = 0$  - instantaneous quench,  $v$  is the quench amplitude.

$r = 1$  - linear quench,  $v$  is the quench rate.

$r = 2$  - quadratic quench,  $v$  is the quench acceleration.

The scalings suggest usability of the adiabatic perturbations theory: small parameter - proximity to the instantaneous ground state.

Non-analytic scalings are usually related to singularities in some susceptibilities. Need to identify the relevant adiabatic susceptibility.

Kibble-Zurek scaling through adiabatic perturbation theory.

$$i\partial_t\psi = H\psi$$

Expand wavefunction in the instantaneous energy basis

$$|\psi\rangle = \sum_n a_n(t) |\phi_n(\lambda(t))\rangle$$

$$i\dot{a}_n + \sum_m \langle n | \partial_t | m \rangle a_m = \epsilon_n a_n$$

Adiabatic limit: no transitions between levels. Expand in transition amplitudes to instantaneous excited states.

Sudden quenches  $\dot{\lambda} \rightarrow \infty$

$$a_n(\lambda) \approx \int_0^\lambda d\lambda' \frac{\langle n | V | 0 \rangle}{\epsilon_n(\lambda') - \epsilon_0(\lambda')}$$

Reduces to the symmetrized version of the ordinary perturbation theory.

Perturbative regime

Sudden quenches

$$a_n(\lambda) \approx \int_0^\lambda d\lambda' \frac{\langle n|V|0\rangle}{\epsilon_n(\lambda') - \epsilon_0(\lambda')} \approx \lambda \frac{\langle n|V|0\rangle}{\epsilon_n(0) - \epsilon_0(0)}$$

Slow quenches  $\lambda(t) = v \frac{t^r}{r!}$ . Integrating fast oscillating function

$$a_n(\lambda) \approx \int_0^\lambda d\lambda' \langle n|\partial_{\lambda'}|0\rangle e^{i \int_0^{\lambda'} \frac{E_n(\mu) - E_0(\mu)}{\dot{\mu}} d\mu} \approx v \frac{\langle n|V|0\rangle}{(\epsilon_n(0) - \epsilon_0(0))^{r+1}}$$

Define adiabatic fidelity:

$$F_a^2 = |\langle \psi(t) | \psi_{gs}(t) \rangle|^2$$

Sudden quenches: adiabatic fidelity = standard fidelity

## Probability of exciting the system

$$P_{ex} = 1 - F_a^2 = \sum_n' |a_n|^2 \approx v^2 \sum_n' \frac{\langle n|V|0\rangle^2}{(\epsilon_n - \epsilon_0)^{2r+2}} = L^d v^2 \chi_{2r+2}$$

Where

$$\chi_{2r+2} = \frac{1}{L^d} \sum_n' \frac{\langle n|V|0\rangle^2}{(\epsilon_n - \epsilon_0)^{2r+2}}$$

is the generalized adiabatic susceptibility of order  $2r + 2$ ;  
 $\chi_2$  is the fidelity susceptibility.

Two (qualitative) contributions to susceptibility:

UV (high energy) – analytic, cutoff-dependent,

IR (low energy) - universal, non-analytic, cutoff-independent.

Smother protocols suppress high-energy contributions.

“Fluctuation-dissipation” relation for the fidelity

$$\chi_{2r+2} = \frac{1}{L^d} \sum'_n \frac{\langle n|V|0\rangle^2}{(\epsilon_n - \epsilon_0)^{2r+2}}$$

$$V = \int d^d x u(x)$$

$$\chi_{2r+2} = \int_0^\infty d\tau \frac{\tau^{2r+1}}{(2r+1)!} [\langle 0|V(\tau)V(0)|0\rangle - \langle 0|V(0)|0\rangle^2]$$

Relevant (marginal) operators:

$$\dim[\chi_{2r+2}] = -\frac{2}{\nu} + d - z2r$$

If the scaling dimension of  $\chi$  is negative then universal contribution to the scaling is the leading one,

# General scaling results

Scaling for the number of excitations  $n_{\text{ex}}$  :

$$n_{\text{ex}} \sim \begin{cases} v^2 L^{2/\nu - d + 2zr} & \text{for } |v| \ll 1/L^{1/\nu + zr} \text{ i)} \\ |v|^{d\nu/(z\nu r + 1)} & \text{for } |v| \gg 1/L^{1/\nu + zr} \text{ ii)} \end{cases}$$

Heat:  $d \rightarrow d + z$

**Main conclusion: quantum Kibble-Zurek scaling and its generalizations are associated with singularities in the adiabatic susceptibilities describing adiabatic fidelity.**

# Non-critical gapless phases (send $\nu$ to $\infty$ )

$$\dim[\chi_{2r+2}] = -\frac{2}{\nu} + d - z2r \rightarrow d - 2zr$$

Negative for  $d < 2zr$

(A.P., V. Gritsev (2008))

$$n_{ex} \sim \begin{cases} |\nu|^{d/zr} & 2zr > d \\ \nu^2 & 2zr < d \end{cases}$$

What is important for adiabaticity only quench time or shape?

(Martin Eckstein, Marcus Kollar, 2008)

$$\lambda(t) \sim \nu t^r$$

$$\Rightarrow \nu \sim 1/T^r$$

$$n_{ex} \sim \begin{cases} |T|^{-d/z} & 2zr > d \\ T^{-2r} & 2zr < d \end{cases}$$

For  $r > d/2z$  shape is unimportant.

$$r_{opt} \approx d/(2z),$$

For QPT  $r_{opt} \approx 1/(z\nu) \ln(CT \ln(CT))$ , A.P., R. Barankov, PRL (2008)

Thermalization in quantum systems (EoM are linear in time – no chaos?)

Consider time average of a certain observable  $\mathbf{A}$  in an isolated system after a quench.

$$\langle A(t) \rangle = \sum_{n,m} \rho_{n,m}(t) A_{m,n} = \sum_{n,m} \rho_{n,m}(0) e^{i(E_m - E_n)t} A_{m,n}$$

$$\overline{\langle A \rangle} = \frac{1}{T} \int_0^T \langle A(t) \rangle dt = \sum_{n,m} \rho_{n,n} A_{n,n}$$

Eigenstate thermalization hypothesis (*Srednicki 1994; M. Rigol, V. Dunjko & M. Olshanii, Nature 452, 854, 2008.*):  $A_{n,n} \sim \text{const}(n)$  so there is no dependence on  $\rho_{nn}$ .

**Information about steady state is fully contained in the diagonal elements of the density matrix.**

True for all thermodynamic observables: energy, pressure, magnetization, .... (pick your favorite). They all are linear in  $\rho$ .

Not true about von Neumann entropy!

$$S_n = -\text{Tr}(\rho \ln \rho)$$

Off-diagonal elements do not average to zero.

Von Neumann's entropy: conserved in time (in thermally isolated systems).

Thermodynamics: entropy is conserved only for adiabatic (slow, reversible) processes. Otherwise it increases.

Quantum mechanics: for adiabatic processes there are no transitions between energy levels:  $\rho_{nn}(t) = \text{const}(t)$

If these two adiabatic theorems are related then the entropy should only depend on  $\rho_{nn}$ . Simple resolution:

$$S_d = -\sum_n \rho_{nn} \ln \rho_{nn}$$

The sum is taken over the instantaneous energy states.

Initial stationary density matrix, closed systems

$$S_d(t) \geq S_n(t) = S_n(0) = S_d(0),$$

$$S_{d1}(t) + S_{d2}(t) \geq S_{d1}(0) + S_{d2}(0) \quad \text{Boltzmann's h-theorem}$$

(thanks to C. Gogolin)

$$\Delta E \cong \sum_n \Delta \varepsilon_n \rho_n^0 + \varepsilon_n^0 \Delta \rho_{nn}$$

$$\Delta S_d \cong - \sum_n \Delta \rho_{nn} (\ln \rho_n^0 + 1) = \frac{1}{T} \sum_n \varepsilon_n^0 \Delta \rho_n$$

$$\Delta E = \left( \frac{\partial E}{\partial \lambda} \right)_{S_d} \Delta \lambda + T \Delta S_d$$

If  $\lambda$  stands for the  
volume the we find

$$\Delta E = -P \Delta V + T \Delta S_d$$

## Diagonal entropy and the energy distribution

$$S_d = - \sum_n \rho_{nn} \ln \rho_{nn} = - \int d\epsilon \rho(\epsilon) N(\epsilon) \ln \rho(\epsilon)$$

$$\rho(\epsilon) N(\epsilon) = W(\epsilon) \quad \text{energy distribution}$$

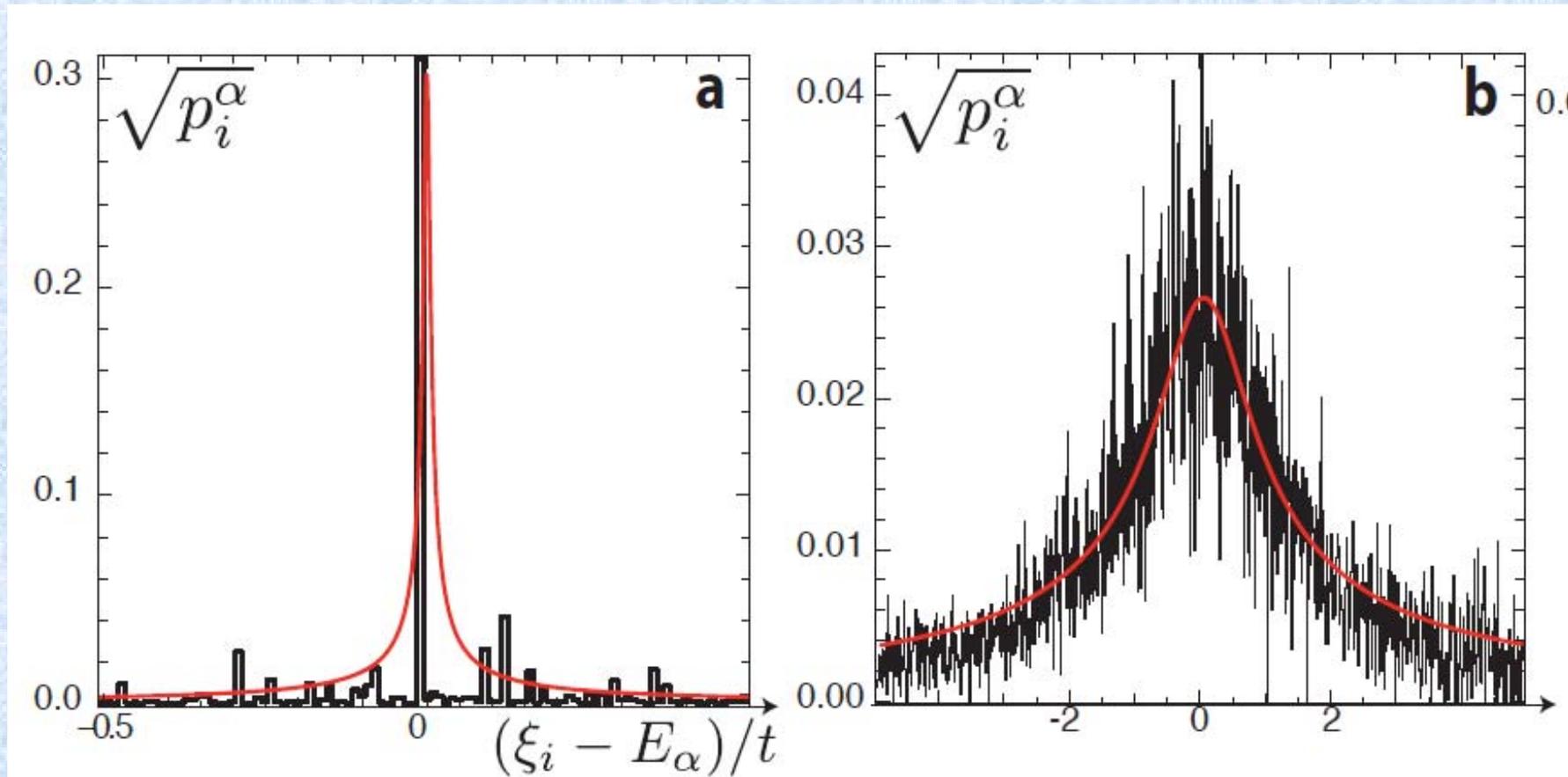
$$\ln N(\epsilon) = S_{\text{micro}}(\epsilon)$$

$$S_d(\epsilon) = \int d\epsilon W(\epsilon) S_{\text{micro}}(\epsilon) - \int d\epsilon W(\epsilon) \ln(W(\epsilon))$$

Entropy is a unique function of energy (in the thermodynamic limit) if the Hamiltonian is local and density matrix is not (exponentially) sparse

# Sparseness of the density matrix(after quench) is related to integrability

C. Neuenhahn, F. Marquardt, arXiv:1007.5306; G. Biroli, C. Kollath, A. Laeuchli, arXiv:0907.3731

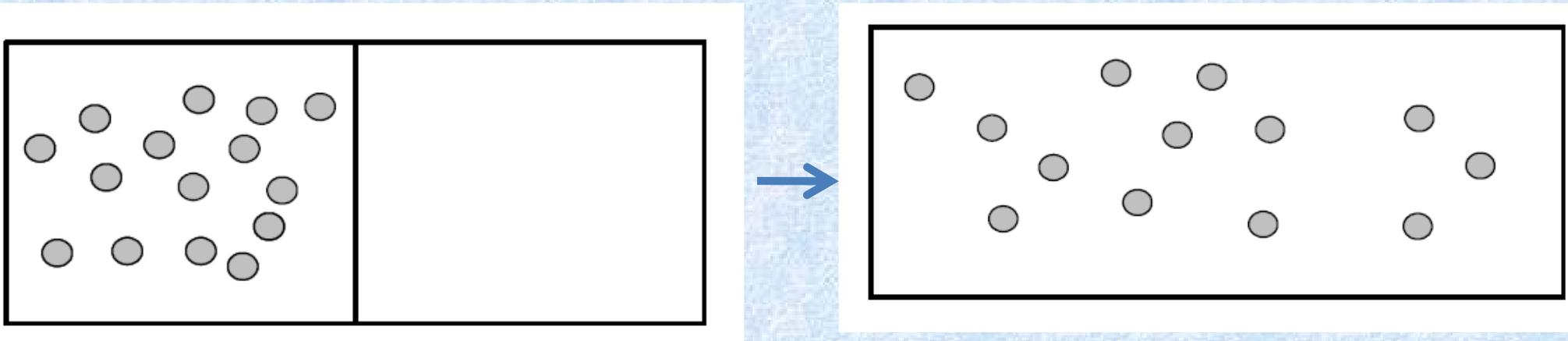


nearly integrable

nonintegrable

Thermalization  $\leftrightarrow$  delocalization of the initial state in the basis of the eigenstates (cf. many-body Anderson localization transition, Basko, Aleiner, Altshuler 06)

Examples for diagonal entropy.



Distribution remains thermal.  $S_n = \text{const}$

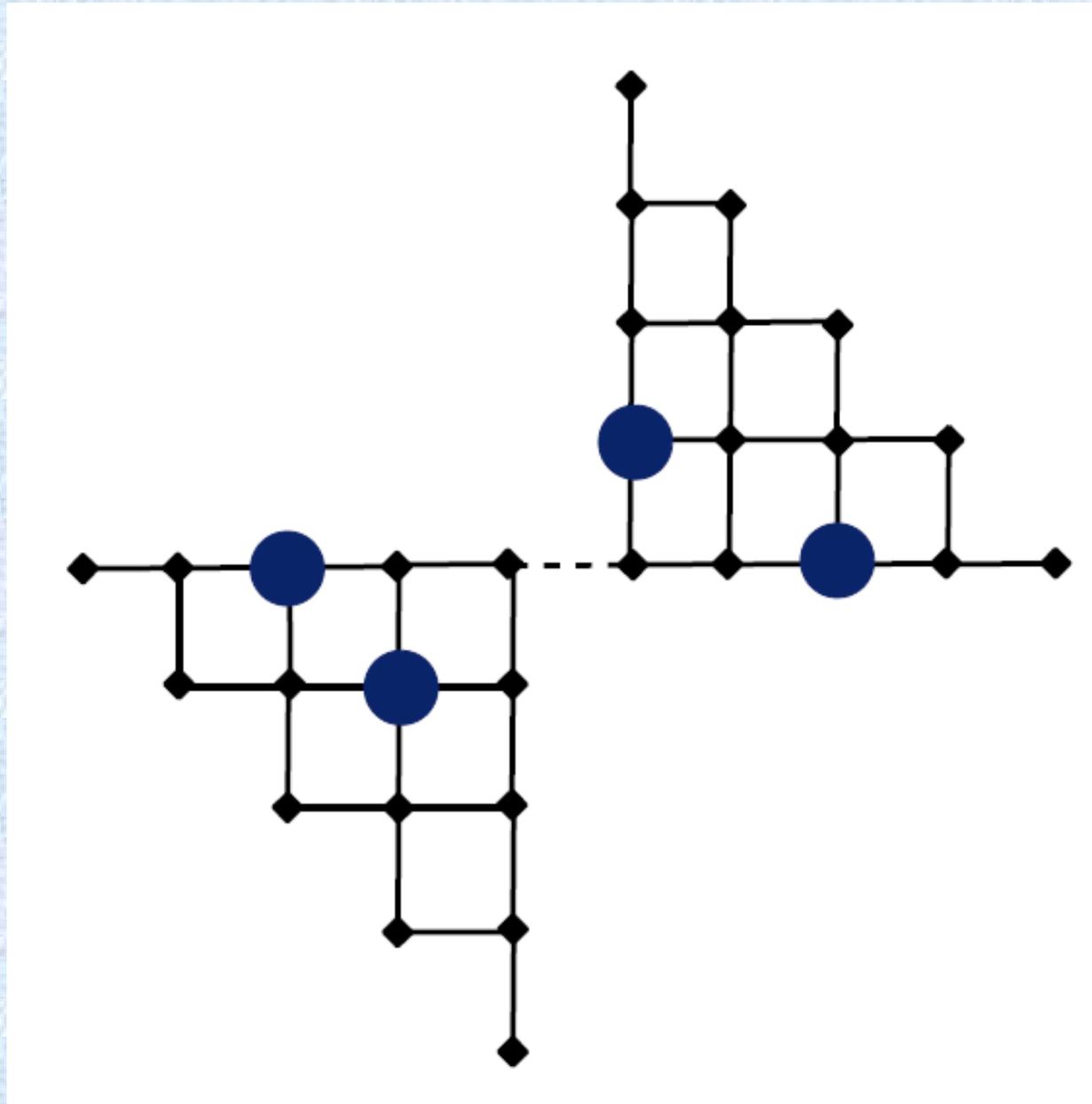
$$\rho_{nn} \rightarrow \frac{1}{2} \rho_{nn}$$



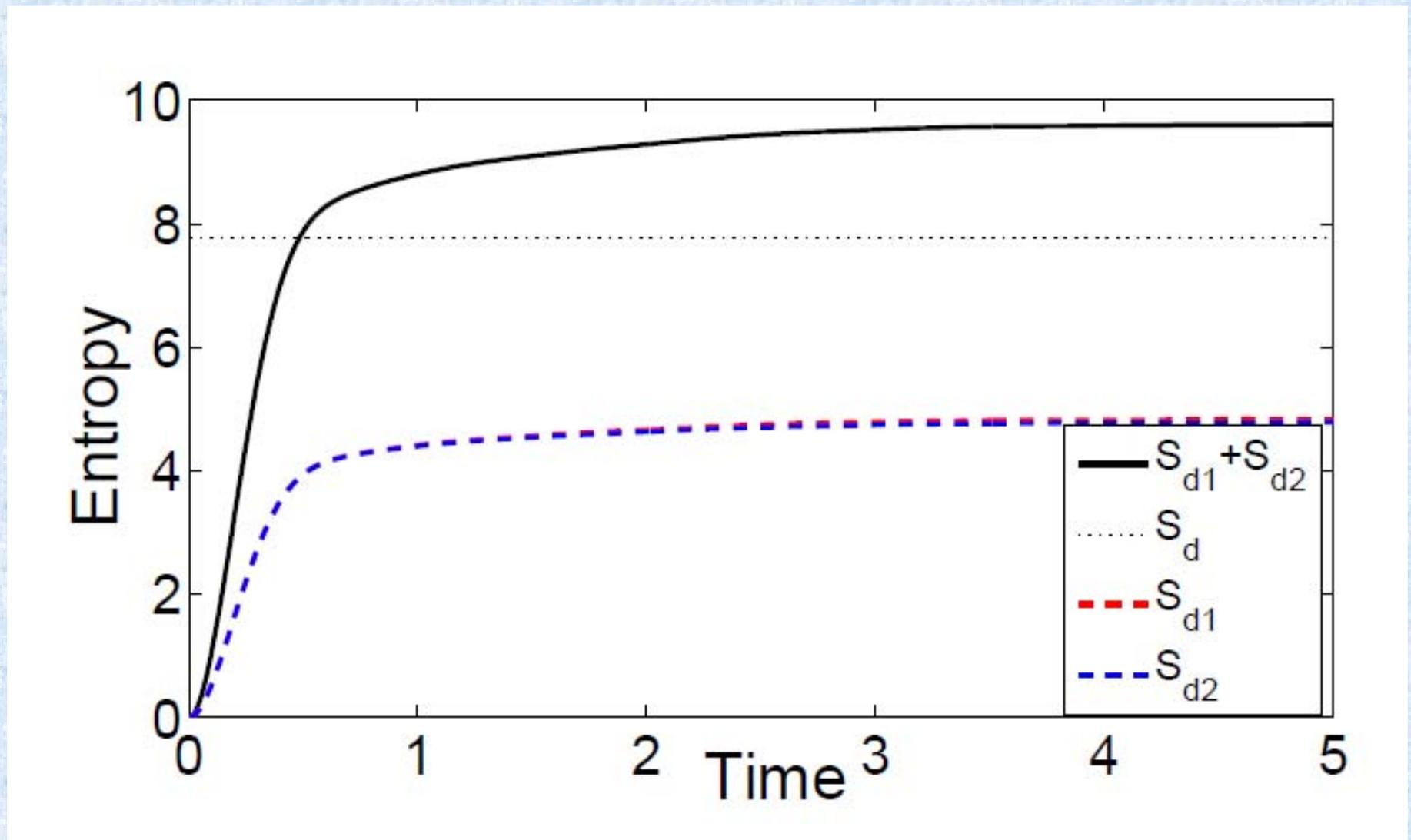
$$\Delta S_d = N \ln(2)$$

Diagonal entropy changes suddenly after the quench

# Hard core bosons in two dimensions

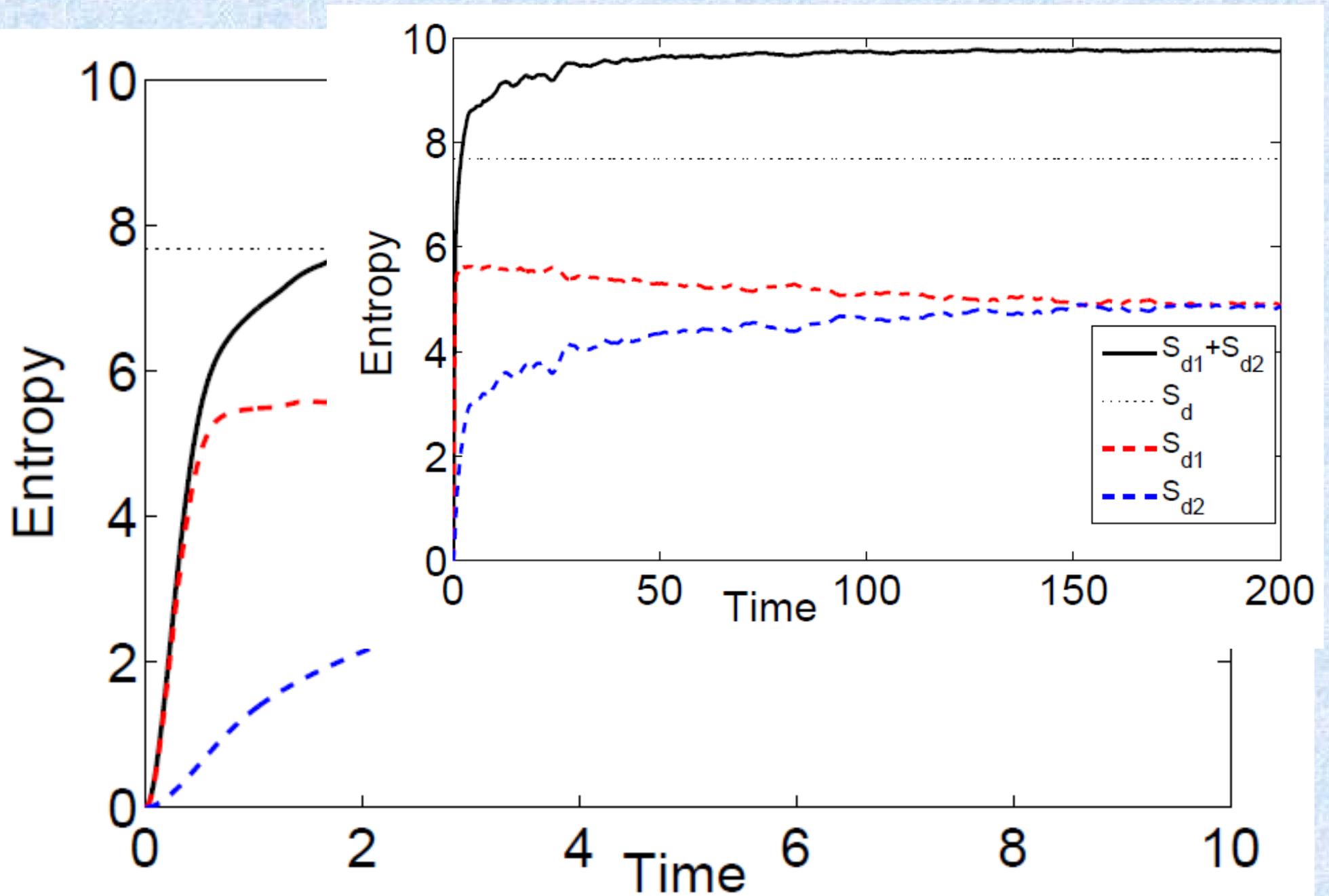


## Local diagonal entropies after the quench

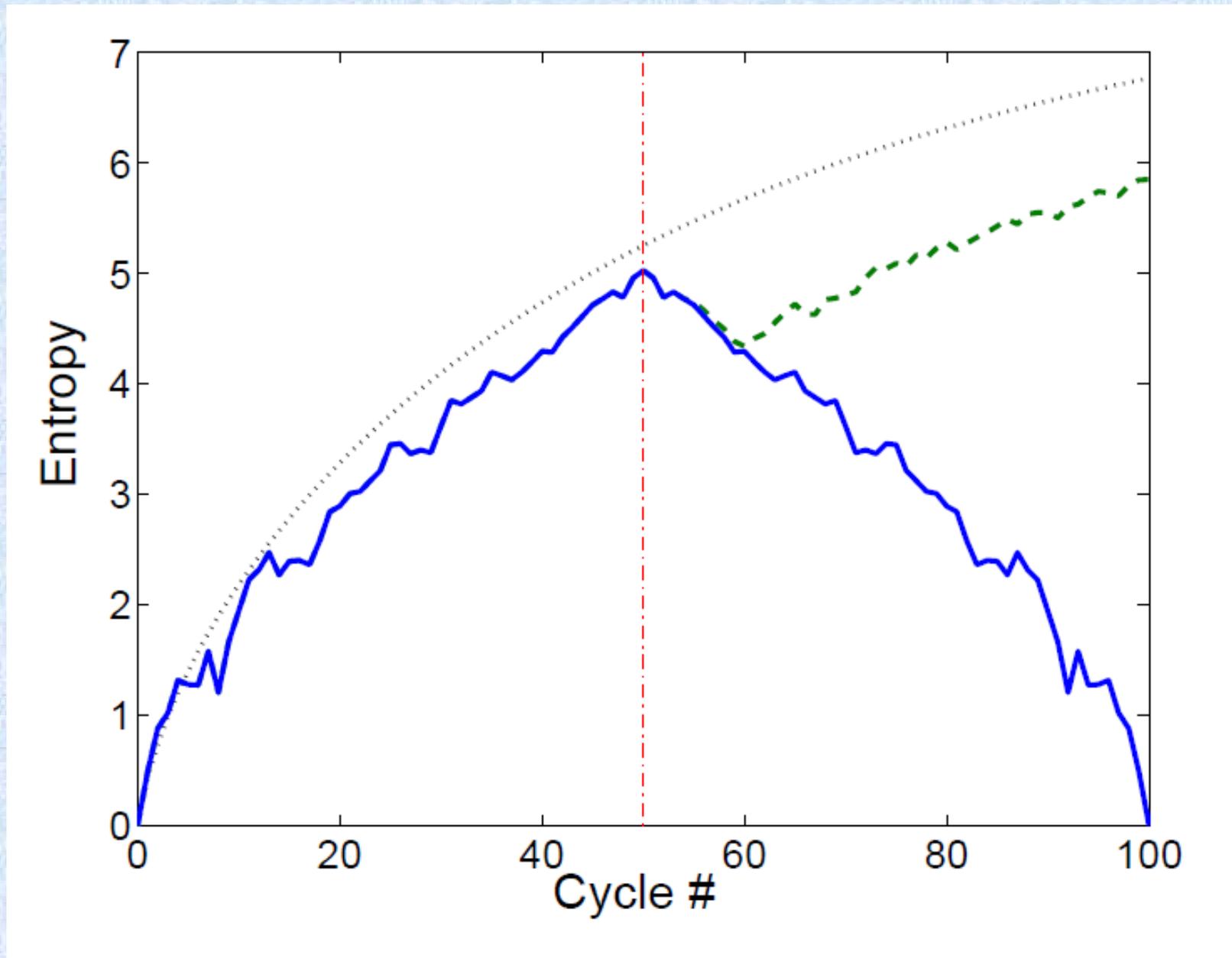


$$\log D \approx 8.49 < \log(D_1 * D_2) \approx 11.91$$

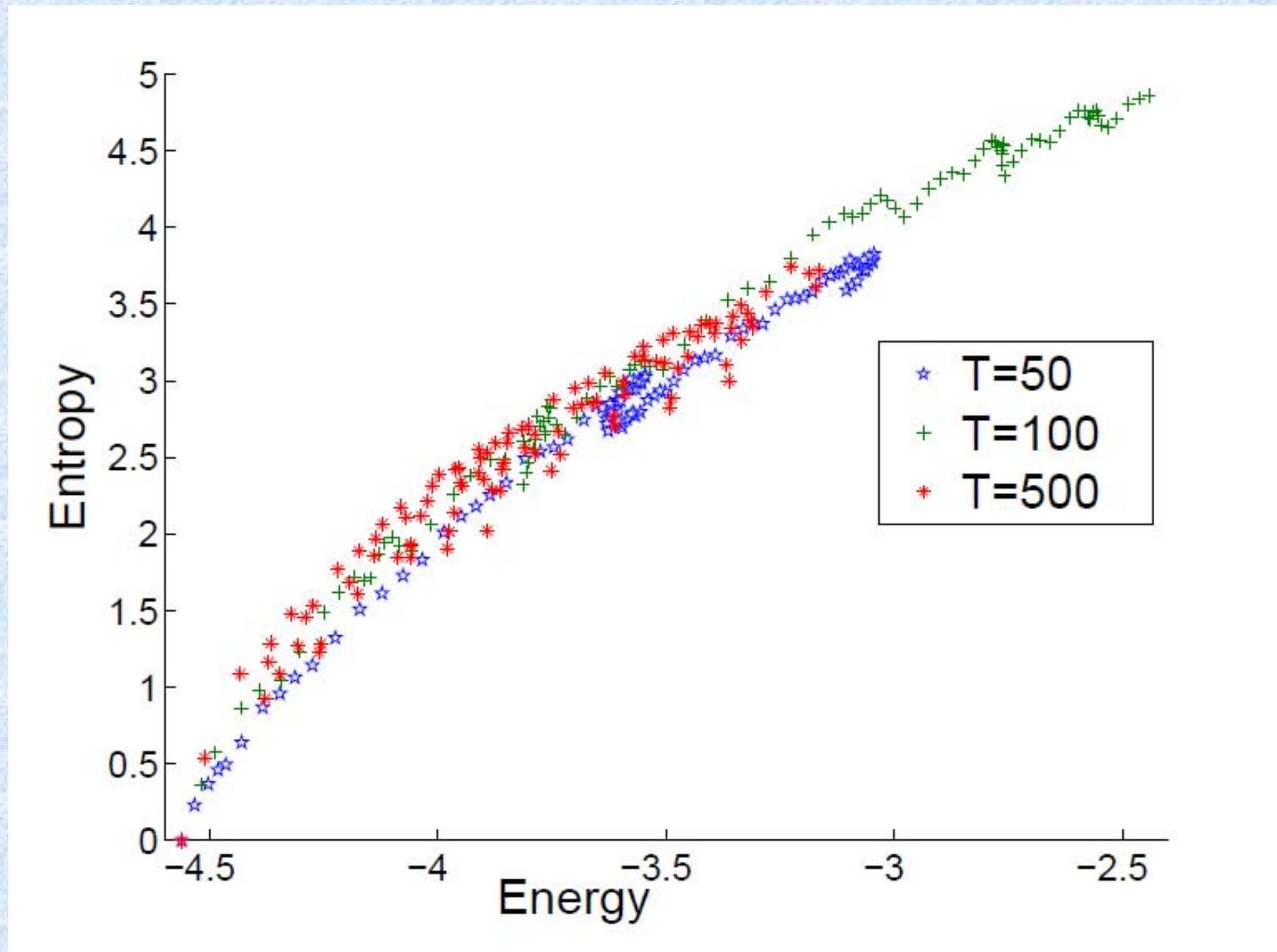
# Initial non-equal populations



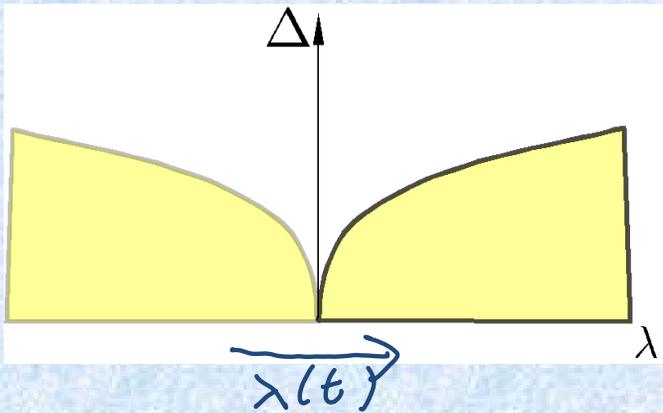
# Diagonal entropy and reversibility (periodic modulation of the weak link)



# Uniqueness of $S(E)$ for different periods of modulation



## Entropy as a measure of non-adiabaticity



### Probability of excitation

$$P_{ex} = - \sum'_n |\alpha_n|^2 \sim |\nu|^2 L^{2/\nu+2zr}$$

Universal. Not dependent on the choice of observable. **Not intensive. Unity unless rate vanishes in the thermodynamic limit.**

$$\text{Density of excitations } n_{ex} \sim |\nu|^{d\nu/(z\nu r+1)}$$

Universal. Intensive: well defined in thermodynamic limit. **Depends on knowing structure of excitations. Ill defined in non-integrable systems.**

$$\text{Heat } Q \sim |\nu|^{(d+z)\nu/(z\nu r+1)}$$

Universal. Intensive. Measurable. **Not easy to separate from adiabatic energy. Not-universal unless end exactly at the critical point.**

$$(d) \text{ Entropy } S_d \sim |\nu|^{d\nu/(z\nu r+1)}$$

Universal. Intensive. Sensitive only to crossing QCP (not where we start (end) the quench). ~~(not) Measurable~~. **Measurable.**

Time evolution as an RG process. Universal dynamics near non-equilibrium KT phase transition. (with L. Mathey, PRA 2010).

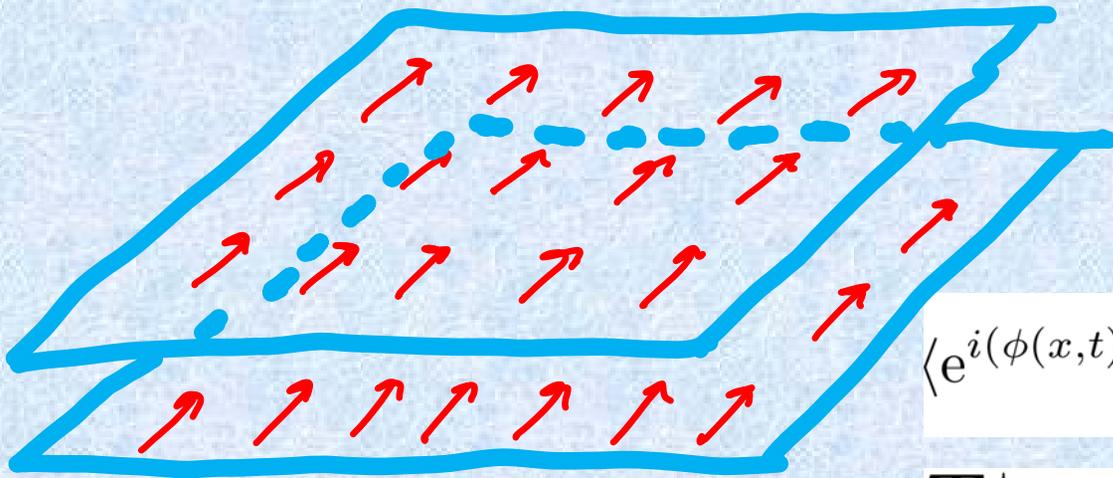
$$\langle A(t) \rangle = \sum_{n,m} \rho_{n,m}(t) A_{m,n} = \sum_{n,m} \rho_{n,m}(0) e^{i(E_m - E_n)t} A_{m,n}$$

$$\overline{\langle A \rangle} = \frac{1}{T} \int_0^T \langle A(t) \rangle dt \cong \sum_{\substack{n,m \\ |E_n - E_m|t < \pi}} \rho_{n,m} A_{m,n}$$

In quantum mechanics relaxation is like an RG process where high frequency modes are gradually eliminated.

Idea: gradually average over high momentum non-interacting modes and follow time evolution of the remaining low energy modes.

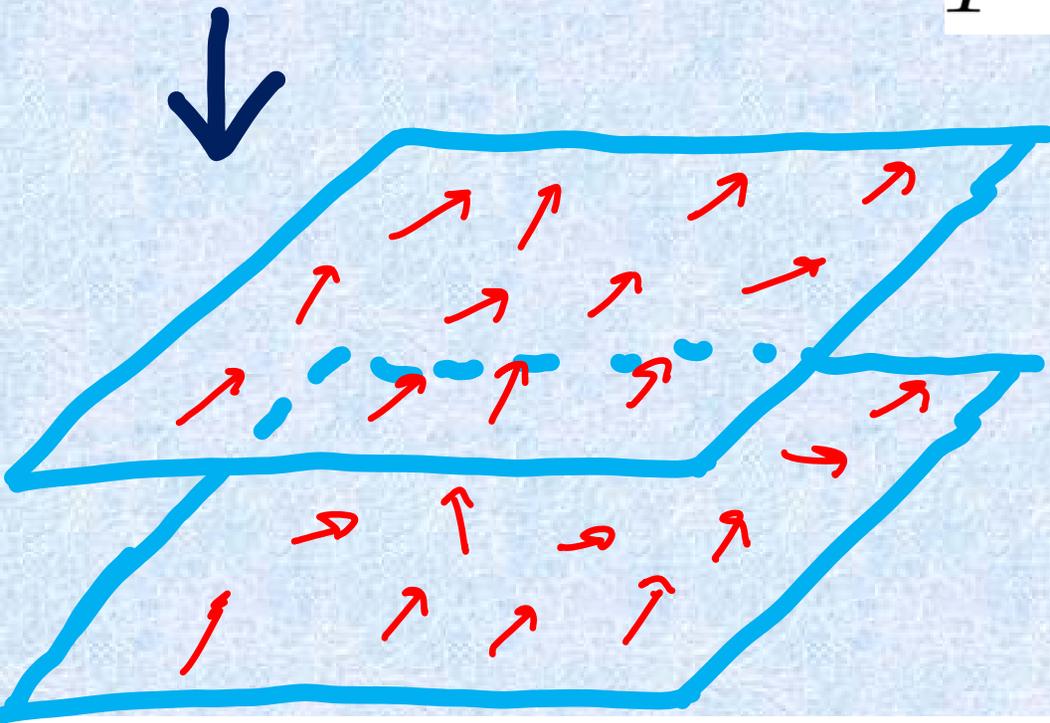
# Decoupling of two 2D superfluids (with L. Mathey, PRA 2010)



Short times: system relaxes to a steady state with algebraic order.

$$\langle e^{i(\phi(x,t) - \phi(0,t))} \rangle \approx \begin{cases} C_1 |x|^{-T^*/4} & x \lesssim 2vt \\ C_2 |t|^{-T^*/4} & x \gtrsim 2vt \end{cases}$$

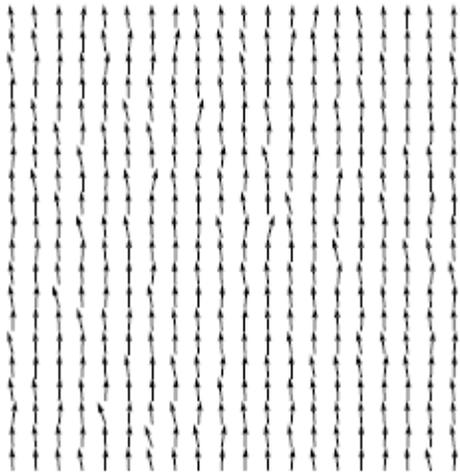
$$T^* \sim U/J,$$



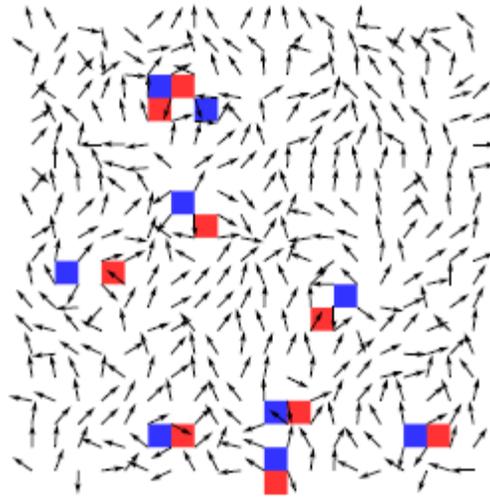
Long times – vortex anti-vortex pairs start to emerge and can unbind.

Equilibrium: KT transition is expected when  $T^* \sim 1$ .

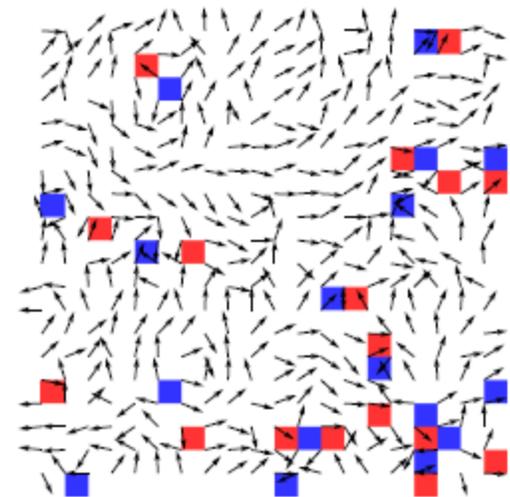
$t = 0$



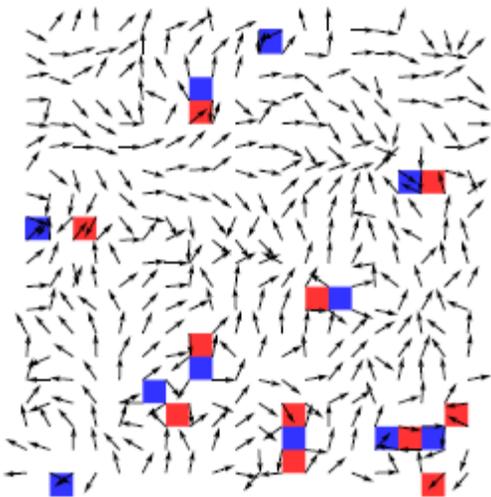
$t = 5$



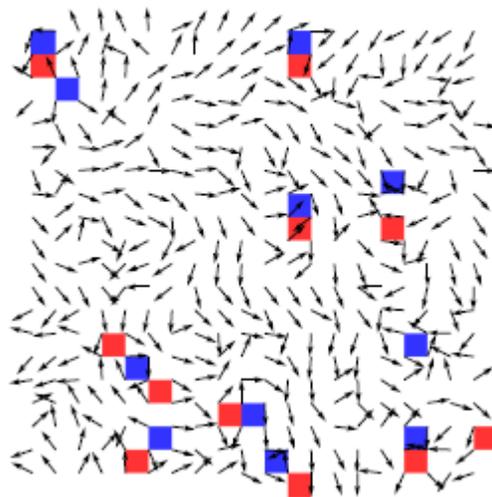
$t = 10$



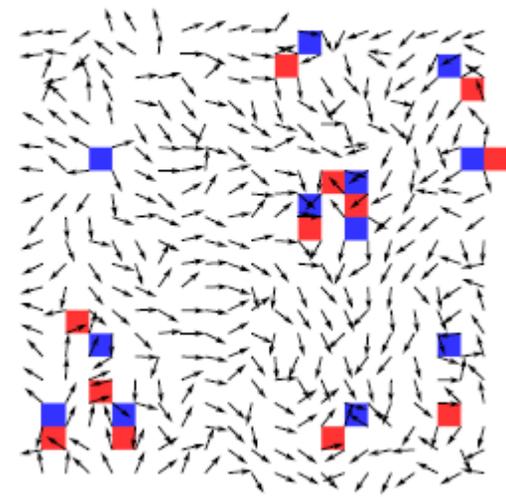
$t = 20$



$t = 40$



$t = 100$



Looks like KT transition in real time. How do we describe it analytically?

Need to solve nonlinear Hamiltonian equations of motion:

$$\frac{1}{\mu} \frac{d^2 \theta}{dt^2} = \lambda \Delta \theta + g \sin(\theta)$$

Idea: split  $\theta$  into low-momentum and high momentum sectors

$$\theta = \theta^> + \theta^<$$

$$\frac{1}{\mu} \frac{d^2 \theta^<}{dt^2} \approx \lambda \Delta \theta^< + g \sin(\theta^<) \left( 1 - \frac{(\theta^>)^2}{2} \right) + g \cos(\theta^<) \theta^>$$

Use perturbation theory in  $g$  to treat  $\theta^>$

Time average equation for  $\theta^<$  over fast oscillating modes

Rescale coordinates and time and follow the evolution of couplings and energy.

Overall formalism is similar to the adiabatic perturbation theory.

Result: flow equations for couplings, very similar to usual KT form

$$\frac{dg}{dl} = \left(2 - \frac{1}{4\pi\lambda}\right)g$$

$$\frac{d\lambda}{dl} = \alpha \frac{g^2}{\lambda}$$

Flow parameter  $l$  is the real time!

Recover for this problem two scenarios of relevant (normal) and irrelevant (superfluid) vortices with exponentially divergent time scale.

For this problem equilibrium = thermodynamics emerges as a result of the renormalization group process.

RG is a semigroup transformation (no inverse). Lost information in the time averaging of fast modes.

# Universal energy distribution in thermally isolated driven systems

(with L. D'Alessio, G. Bunin, Y. Kafri)

## Conventional heating

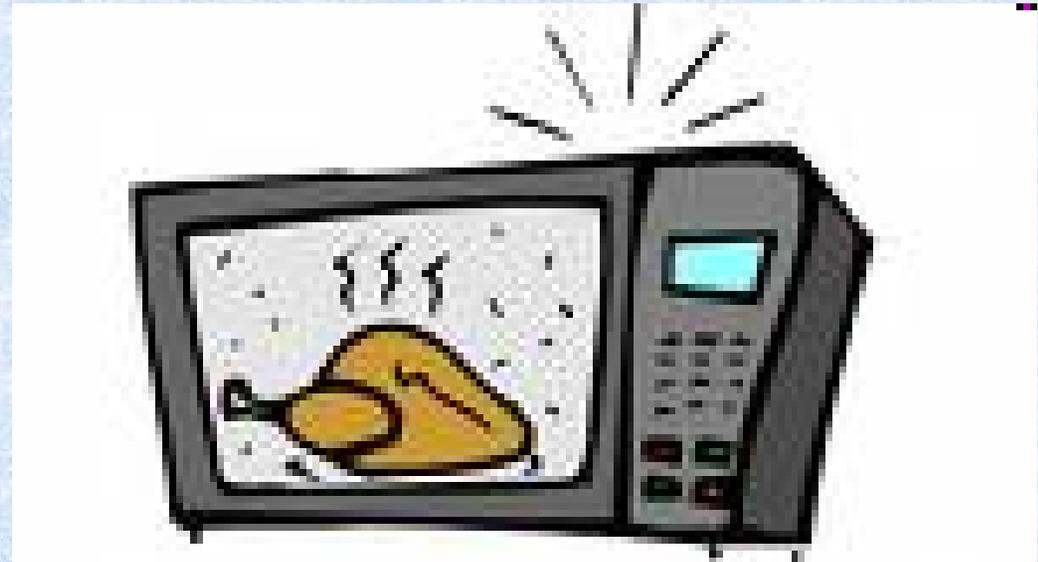


Gibbs distribution

fluctuation-dissipation relations

universal width:  $\delta E^2 = T^2 C_v$

## Nonadiabatic heating



Gibbs distribution???

fluctuation-dissipation relations???

universal width???

## Approach:

Fokker-Planck equation (quasi-static process)

$$\partial_t P(E, t) = -\partial_E (AP) + \frac{1}{2} \partial_{EE}^2 (BP)$$

$$A = \partial_t \langle W \rangle |_{t=0}, \quad B = \partial_t \langle W^2 \rangle |_{t=0}$$

Unitarity of the evolution (fluctuation theorems)

$P(E) = \Omega(E)$  is a stationary solution  $\Rightarrow$

$$B = \frac{2A}{\beta} - \frac{1}{\beta} \partial_E B \approx \frac{2A}{\beta}$$

Dynamics is highly constrained by the unitarity

# Results

$$\sigma^2(E) \rightarrow A^2(E) \int_{E_0}^E dE' \frac{2T(E')}{A^2(E')} \quad T(E) \sim E^\alpha, \quad A(E) \sim E^\eta$$

Two universal regimes

$$\eta < \frac{1 + \alpha}{2} \quad \Rightarrow \quad \sigma^2(E) = \sigma_{\text{eq}}^2(E) \frac{2\alpha}{\alpha + 1 - 2\eta} \quad \text{modified thermal}$$
$$\eta > \frac{1 + \alpha}{2} \quad \Rightarrow \quad \sigma^2(E) = C \sigma_{\text{eq}}^2(E) E^{2\eta - \alpha - 1} \quad \text{runaway}$$

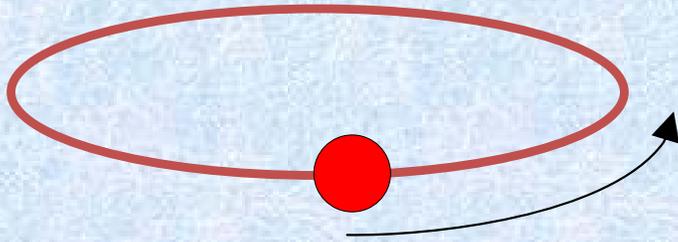
Transition:  $\eta = \frac{1 + \alpha}{2} \quad \Rightarrow \quad S(t) \propto t^2$

If the entropy grows slower than square of time then expect canonical-like distribution.

## Summary and outlook.

- Universal non-adiabatic response of various quantities near quantum critical point. Can be understood through IR divergencies of fidelity susceptibility and its generalizations.
  - Dependence of dissipation on quench time and shape?
  - Role of non-integrability (relaxation)?
  - UV singularities.
- Diagonal entropy and heat can be defined microscopically. Laws of thermodynamics follow from many-body delocalization between eigenstates.
- Thermalization (time evolution) as an RG process in real time.
  - Generality of this statement. Role of integrability.
  - Universal energy fluctuations in thermally isolated driven systems.
    - Experiments.

## Classical systems.



Instead of energy levels we have orbits.

$\rho_{nm} \leftrightarrow$  probability to occupy an orbit with energy  $E$ .

$\rho_{nm} \propto \exp[i(\varepsilon_n - \varepsilon_m)t] \leftrightarrow$  describes the motion on this orbits.

## Classical d-entropy

$$S_d = -\int N(\varepsilon) \rho(\varepsilon) \ln \rho(\varepsilon) d\varepsilon \quad \rho(\varepsilon) = \int d\Gamma \rho(p, q) \delta(\varepsilon - \varepsilon(p, q))$$

The entropy “knows” only about conserved quantities, everything else is irrelevant for thermodynamics!  $S_d$  satisfies laws of thermodynamics, unlike the usually defined  $S = \ln \Gamma$ .

## Properties of d-entropy (A. Polkovnikov, *arXiv:0806.2862* ).

Jensen's inequality:

$$\text{Tr}(-\rho \ln \rho + \rho_d \ln \rho_d) \leq \text{Tr}[(\rho - \rho_d) \ln \rho_d] = 0$$

Therefore if the initial density matrix is stationary (diagonal) then

$$S_d(t) \geq S_n(t) = S_n(0) = S_d(0)$$

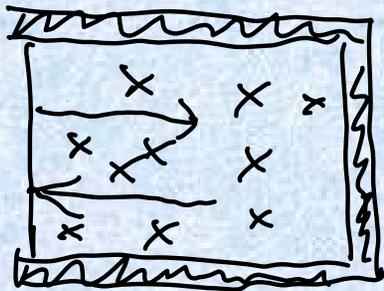
Now assume that the initial state is thermal equilibrium

$$\rho_n^0 = \frac{1}{Z} \exp[-\beta \epsilon_n]$$

Let us consider an infinitesimal change of the system and compute energy and entropy change.

# Thermodynamic adiabatic theorem.

In a cyclic adiabatic process the energy of the system *does not change*: no work done on the system, no heating, and no entropy is generated .



move fast - heat system (increase energy)  
move slow - do not heat the system  
(energy does not change)

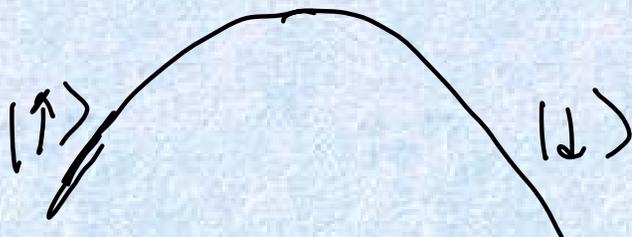
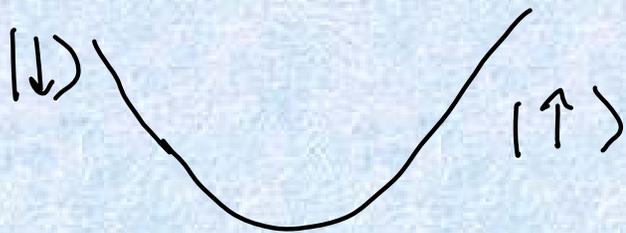
General expectation:

$$E(\dot{\lambda}) = E(0) + \beta \dot{\lambda}^2, \quad S(\dot{\lambda}) = S(0) + \alpha \dot{\lambda}^2$$

$\dot{\lambda}$  - is the rate of change of external parameter.

# Adiabatic theorem in quantum mechanics

Landau Zener process:



$$\hat{H} = \delta t \cdot \sigma_z + \Delta \sigma_x$$

$$P_{\uparrow}(\infty) = e^{-\frac{\pi \Delta^2}{\delta \hbar}}$$

In the limit  $\delta \rightarrow 0$  transitions between different energy levels are suppressed.

This, for example, implies reversibility (no work done) in a cyclic process.

## *Adiabatic theorem in QM **suggests** adiabatic theorem in thermodynamics:*

1. Transitions are unavoidable in large gapless systems.
2. Phase space available for these transitions decreases with the rate. Hence expect

$$E(\dot{\lambda}) = E(0) + \beta \dot{\lambda}^2, \quad S(\dot{\lambda}) = S(0) + \alpha \dot{\lambda}^2$$

Low dimensions: high density of low energy states, breakdown of mean-field approaches in equilibrium

**Breakdown of the Taylor expansion in low dimensions, especially near singularities (phase transitions).**

# Three regimes of response to the slow ramp:

A.P. and V.Gritsev, Nature Physics 4, 477 (2008)

A. Mean field (analytic) – high dimensions:

$$E(\dot{\lambda}) = E(0) + \beta \dot{\lambda}^2$$

B. Non-analytic – low dimensions

$$E(\dot{\lambda}) = E(0) + \beta |\dot{\lambda}|^r, \quad r \leq 2$$

C. Non-adiabatic – low dimensions, bosonic excitations

$$E(\dot{\lambda}) = E(0) + \beta |\dot{\lambda}|^r L^\eta, \quad r \leq 2, \eta > 0$$

In all three situations quantum and thermodynamic adiabatic theorem are smoothly connected.

The adiabatic theorem in thermodynamics does follow from the adiabatic theorem in quantum mechanics.

Connection between two adiabatic theorems allows us to define **heat** (A.P., *Phys. Rev. Lett.* **101**, 220402, 2008).

Consider an arbitrary dynamical process and work in the instantaneous energy basis (adiabatic basis).

$$E(\lambda_t, t) = \sum_n \varepsilon_n(\lambda_t) \rho_{nn}(t) = \sum_n \varepsilon_n(\lambda_t) \rho_{nn}(0) + \sum_n \varepsilon_n(\lambda_t) [\rho_{nn}(t) - \rho_{nn}(0)] = E_{ad}(\lambda_t) + Q(\lambda_t, t)$$

- Adiabatic energy is the function of the state.
- Heat is the function of the process.
- Heat vanishes in the adiabatic limit. *Now this is not the postulate, this is a consequence of the Hamiltonian dynamics!*

## Isolated systems. Initial stationary state.

$$\rho_{nm}(0) = \rho_n^0 \delta_{nm}$$

Unitarity of the evolution:

$$\rho_{nm}(t) = \rho_n^0 + \sum_m p_{m \rightarrow n}(t) (\rho_m^0 - \rho_n^0)$$

$$p_{m,n} = \left| (I - U_A^\dagger U)^m \right|_{m,n}^2$$

Transition probabilities  $p_{m \rightarrow n}$  are non-negative numbers satisfying

$$\sum_m p_{m \rightarrow n}(t) = \sum_n p_{n \rightarrow m}(t)$$

In general there is no detailed balance even for cyclic processes (but within the Fermi-Golden rule there is).

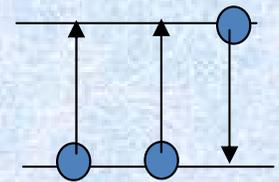
$$\rho_{nn}(t) = \rho_n^0 + \sum_m P_{m \rightarrow n}(t)(\rho_m^0 - \rho_n^0)$$

yields

$$Q(t) = \sum_n \varepsilon_n \Delta \rho_{nn}(t) = \sum_n \varepsilon_n (\rho_m^0 - \rho_n^0) P_{m \rightarrow n}(t)$$

If there is a detailed balance then

$$Q(t) = \frac{1}{2} \sum_n (\varepsilon_n - \varepsilon_m)(\rho_m^0 - \rho_n^0) P_{m \rightarrow n}(t)$$



Heat is non-negative for cyclic processes if the initial density matrix is passive

**.Second law of thermodynamics in Thompson (Kelvin's form).**

$$(\varepsilon_n - \varepsilon_m)(\rho_m^0 - \rho_n^0) \geq 0$$

The statement is also true without the detailed balance (Thirring, Quantum Mathematical Physics, Springer 1999, A. E. Allahverdyan, Th. M. Nieuwenhuizen, Physica A **305**, 542 (2002).).