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Non-adiabatic dynamics and thermodynamics in isolated out of equilibrium systems

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Non-adiabatic dynamics and thermodynamics in isolated out of equilibrium systems.

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AFOSR

* Basic facts from thermodynamics: energy, heat, work, first and second laws of thermodynamics, fundamental thermodynamic relation. Non-equilibrium work relations (Jarzyisky equality).

* Thermalization in isolated systems; eigenstate thermalization hypothesis. Heat, entropy in driven gapless systems. Consistency of laws of thermodynamics and Hamiltonian dynamics.

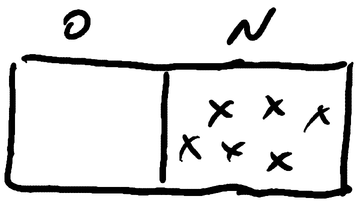
* Connection between quantum and thermodynamic adiabatic theorems.

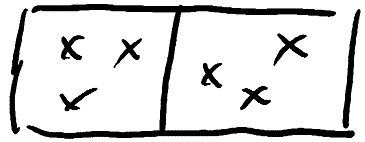
* Universal adiabatic dynamics near critical points

Basic facts from thermodynamics

Macroscopic properties of large systems are fully determined by energy (other possible conserved quantities) and external parameters: volume, magnetic field, ...

Example

a) 

b) 

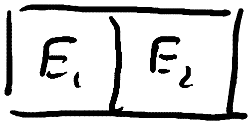
Such two microstates are equally probable. However, the number of microstates for $N/2$, $N/2$ configuration is much bigger

$$\Omega \approx \frac{N!}{(N/2)!\,(N/2)!} \sim \frac{1}{\sqrt{N}}\, 2^N$$

For large N b) macrostate is overwhelmingly more probable than a) macrostate.

Key quantity in thermodynamics - entropy

$$S(E) = \ln \Omega(E)$$



Equilibrium: most probable macrostate is the one which maximizes the number of available microstates

$$\Omega_1(E_1)\,\Omega_2(E-E_1) = \max$$

$$\ln \Omega_1(E_1) + \ln \Omega_2(E-E_1) = \max$$

$$\frac{\partial \ln \Omega_1(E_1)}{\partial E_1} = \frac{\partial \ln \Omega_2(E_2)}{\partial E_2} = \frac{1}{T} \Rightarrow \left(\frac{\partial S}{\partial E}\right)_X = \frac{1}{T}$$

So $dE\big|_X = TdS$

More generally

(*) $dE = TdS - \mathcal{F}dX$ $\quad$ $\mathcal{F}$ - generalized force

X = Volume $\Rightarrow$ $\mathcal{F}$ = pressure

X = magnetic field $\Rightarrow$ $\mathcal{F}$ = magnetization

Equation (*) is called 'fundamental thermodynamics relation. It is thought to be ALWAYS true.

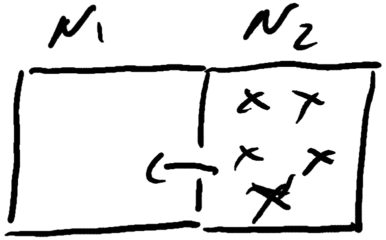
Out of equilibrium systems

$\boxed{E_1 \mid E-E_1}$ $\quad \Omega_1(E_1)\,\Omega_2(E-E_1) \leq \mathrm{MAX}$

$$S_1(E_1)+S_2(E_2) \leq S(E) = S_1(E_1^*)+S_2(E-E_1^*)$$

It is generally assumed that if the system is not in equilibrium then

$S_1(E_1)+S_2(E-E_1) \nearrow$ until the equilibrium is reached.



This is basically probabilistic statement – the system has a higher chance to end up in a more probable state.

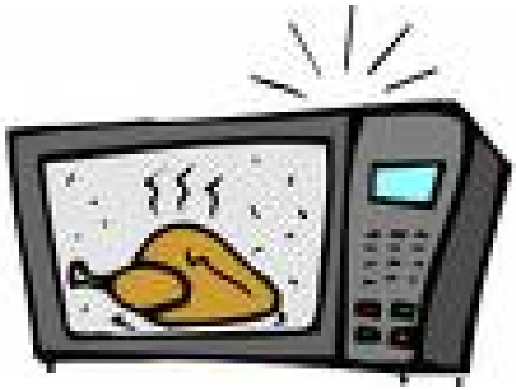
Many phenomena like friction, spontaneous emission, etc. are explained through this principle.

E.g. 

Friction is explained by the fact that the released energy can go to many different phonon configurations.

Non quasistatic processes : problems with separation of energy on heat & work

Electric oven heats food



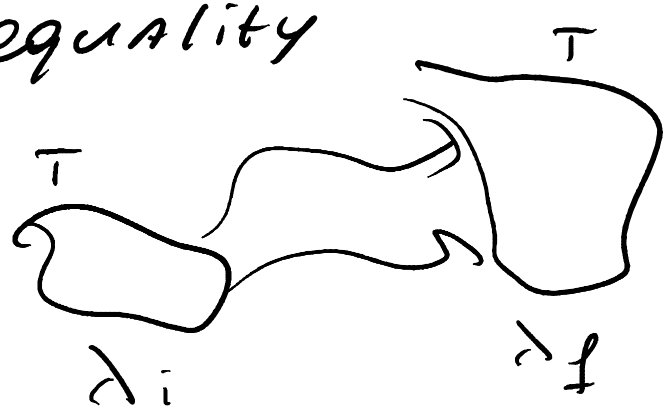
Microwave oven does work on food

Usual candidate for entropy:

classical systems Gibbs entropy

$$S = -\int d\Gamma\ \varrho(p,q) \ln \varrho(p,q)$$

A very interesting exact non-equilibrium result for open systems: Jarzinsky equality



$$\langle e^{-\beta W} \rangle_{\text{init state}} = e^{-\beta(F(\lambda_f) - F(\lambda_i))}$$

$F = E - TS$ - free energy

Proof

$$\frac{1}{Z_i} \int d\Gamma_i \, e^{-\beta (E_f(p,q) - E_i(p,q))} \, e^{-\beta E_i(p,q)} =$$

$$= \frac{1}{Z_i} \int d\Gamma_i \, e^{-\beta E_f(p,q)} = \frac{1}{Z_i} \int d\Gamma_f \, e^{-\beta E_f(p,q)} = \frac{Z_f}{Z_i}$$

$$Z = e^{-\beta F}$$

Thermalization in isolated systems. Ergodic hypothesis

STUDIES OF NON LINEAR PROBLEMS

E. FERMI, J. PASTA, and S. ULAM

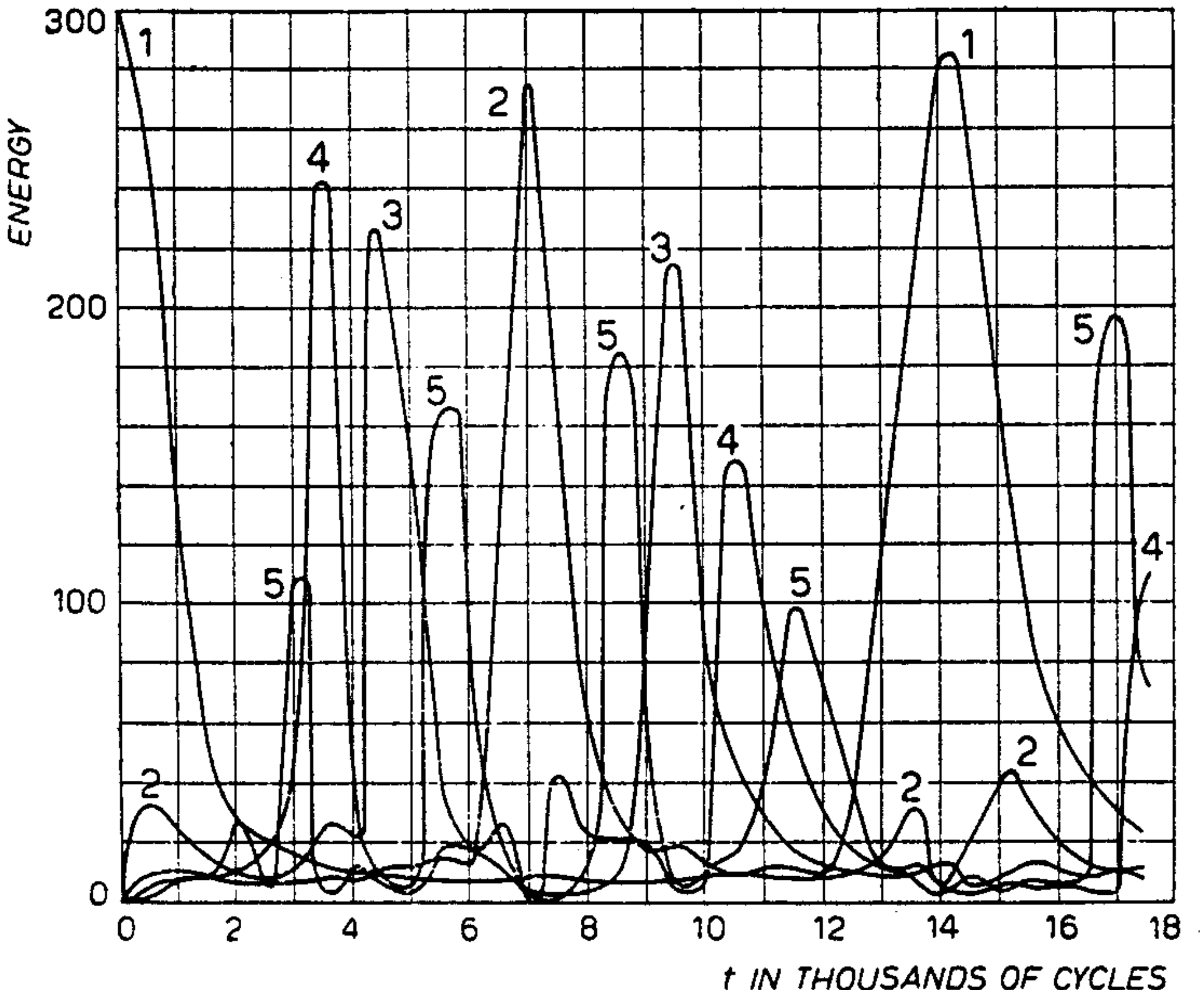
Document LA-1940 (May 1955).

A one-dimensional dynamical system of 64 particles with forces between neighbors containing nonlinear terms has been studied on the Los Alamos computer MANIAC I. The nonlinear terms considered are quadratic, cubic, and broken linear types. The results are analyzed into Fourier components and plotted as a function of time.

The results show very little, if any, tendency toward equipartition of energy among the degrees of freedom.

$$\ddot{x}_i = (x_{i+1} + x_{i-1} - 2x_i) + \alpha\left[(x_{i+1} - x_i)^2 - (x_i - x_{i-1})^2\right]$$

$$(i = 1, 2, \cdots, 64),$$

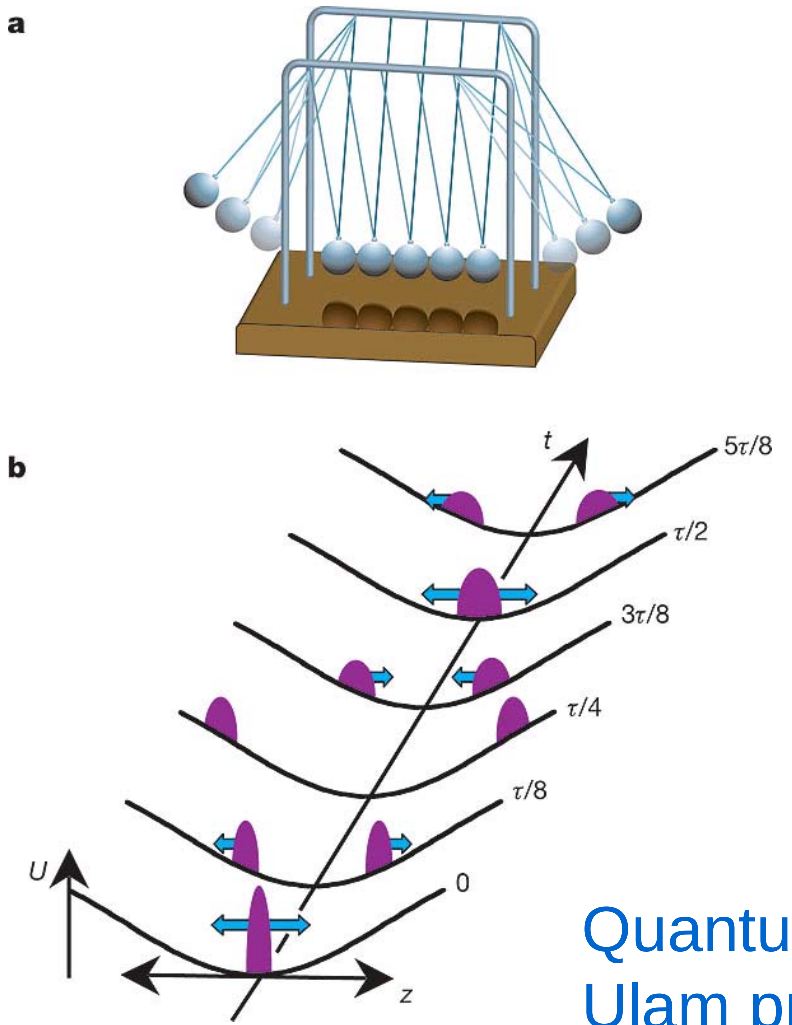


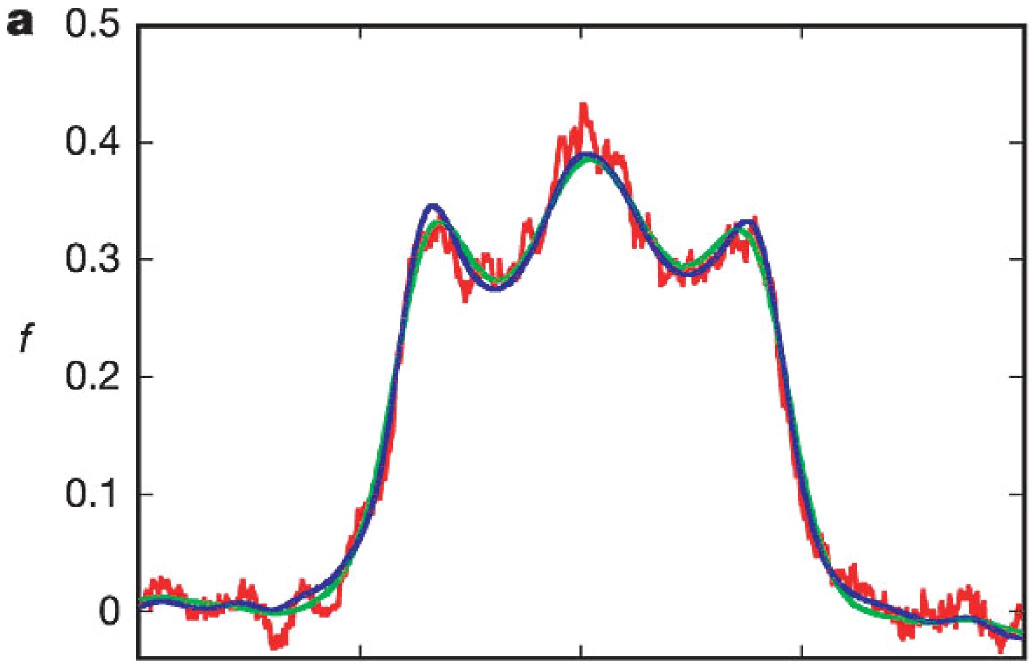
In the continuum this system is equivalent to an integrable KdV equation. The solution splits into non-thermalizing solitons Kruskal and Zabusky (1965).

Qauntum Newton Craddle.

(collisions in 1D interecating Bose gas – Lieb-Liniger model)

T. Kinoshita, T. R. Wenger and D. S. Weiss, Nature **440**, 900 – 903 (2006)





No thermalization in1D.

Fast thermalization in 3D.

Quantum analogue of the Fermi-Pasta-Ulam problem.

Thermalization in Quantum systems.

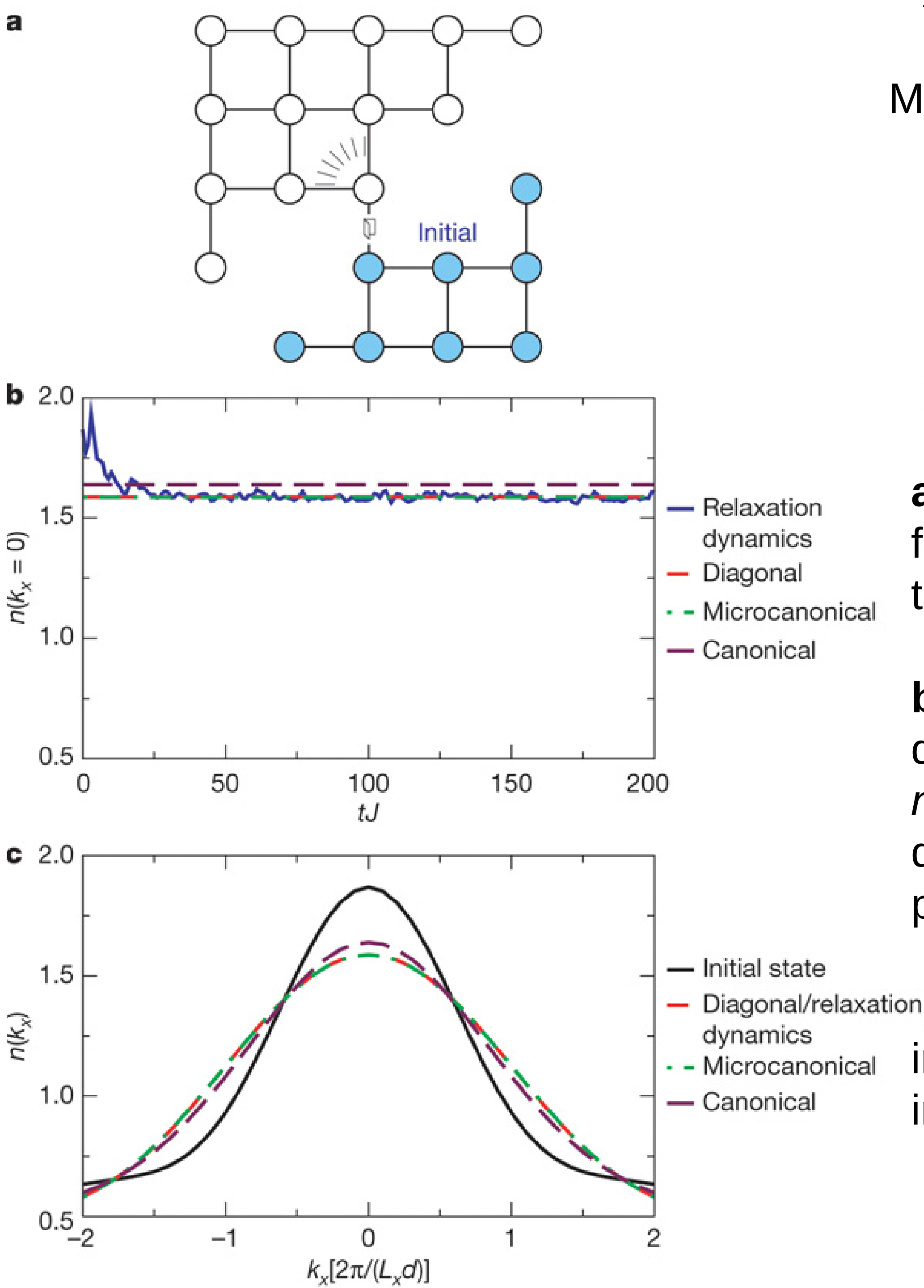
Consider the time average of a certain observable ***A*** in an isolated system after a quench.

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

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

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

Necessary assumption: $A_{m,n} \to 0, \quad |E_n - E_m| << 1/\tau$



M. Rigol, V. Dunjko & M. Olshanii, Nature **452**, 854 (2008)

a, Two-dimensional lattice on which five hard-core bosons propagate in time.

b, The corresponding relaxation dynamics of the central component $n(k_x = 0)$ of the marginal momentum distribution, compared with the predictions of the three ensembles

c, Full momentum distribution function in the initial state, after relaxation, and in the different ensembles.

Information about equilibrium is fully contained in diagonal elements of the density matrix.

This is true for all thermodynamic observables: energy, pressure, magnetization, …. (pick your favorite). They all are linear in ρ.

This is not true about von Neumann entropy!

$$S_n = -Tr(\rho \ln \rho)$$

Off-diagonal elements do not average to zero.

The usual way around: coarse-grain density matrix (remove by hand fast oscillating off-diagonal elements of ρ.

Problem: not a unique procedure, explicitly violates time reversibility and Hamiltonian dynamics.

Von Neumann entropy: always conserved in time (in isolated systems). More generally it is invariant under arbitrary unitary transfomations

$$-S_n(t) = Tr\rho(t)\ln\rho(t) = TrU^+\rho U\ln U^+\rho U = Tr\rho\ln\rho$$

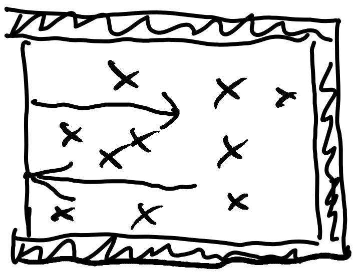
Thermodynamics: entropy is conserved only for adiabatic (slow, reversible) processes. Otherwise it increases.

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

If these two adiabatic theorems are related then the entropy should only depend on ρ_{nn}.

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)

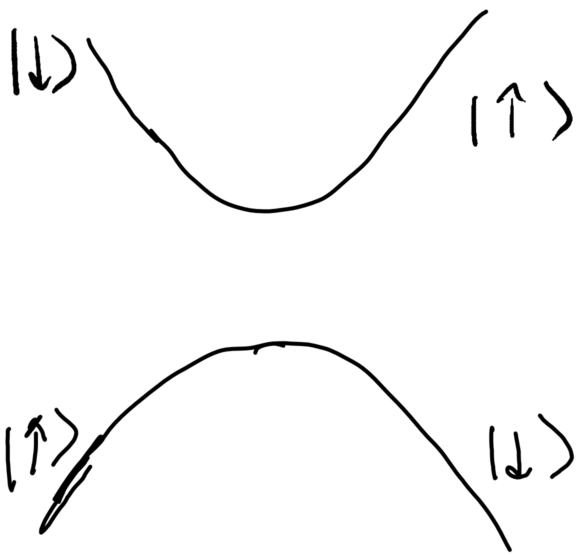
General expectation:

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

$\dot{\lambda}$ - 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

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

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

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

Three regimes of response to the slow linear 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

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

C. Non-adiabatic – low dimensions, bosonic excitations

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

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).

$$E(\lambda_t, t) = \sum_n \varepsilon_n(\lambda_t)\rho_{nn}(t) = \sum_n \varepsilon_n(\lambda_t)\rho_{nn}(0)$$

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

- 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.

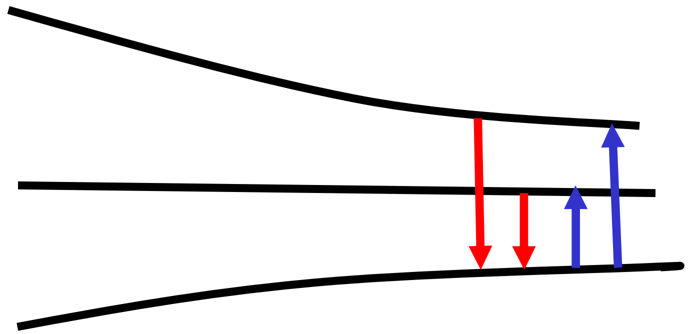
$$\rho_{nm}(0) = \rho_n^0 \delta_{nm}$$

Unitarity of the evolution:

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

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

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



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

What about entropy?

- Entropy should be related to heat (energy), which knows only about ρ_{nn}.
- Entropy does not change in the adiabatic limit, so it should depend only on ρ_{nn}.
- Ergodic hypothesis requires that all thermodynamic quantities (including entropy) should depend only on ρ_{nn}.
- In thermal equilibrium the statistical entropy should coincide with the von Neumann's entropy:

$$S_n = -Tr(\rho \ln \rho) = -\sum_n \rho_n \ln \rho_n, \quad \rho_n = \frac{1}{Z}\exp[-\beta E_n]$$

Simple resolution: diagonal entropy

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

the sum is taken in the instantaneous energy basis.

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

Jensen's inequality:

$$Tr(-\rho \ln \rho + \rho_d \ln \rho_d) \le Tr[(\rho - \rho_d) \ln \rho_d] = 0$$

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

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

Now assume that the initial state is thermal equilibrium

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

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

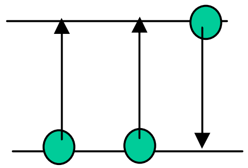
$$\rho_{nn}(t) = \rho_n^0 + \sum_m p_{m\to n}(t)(\rho_m^0 - \rho_n^0)$$

yields

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

If there is a detailed balance then

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



Heat is non-negative for cyclic processes if the initial density matrix is passive $(\varepsilon_n - \varepsilon_m)(\rho_m^0 - \rho_n^0) \geq 0$. Second law of thermodynamics in Thompson (Kelvin's form).

The statement is also true without the detailed balance but the proof is more complicated (Thirring, Quantum Mathematical Physics, Springer 1999).

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

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

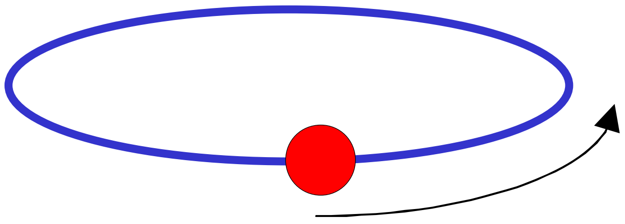
Recover the first law of thermodynamics (Fundamental Relation).

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

If λ stands for the volume the we find

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

Classical systems.



Instead of energy levels we have orbits.

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

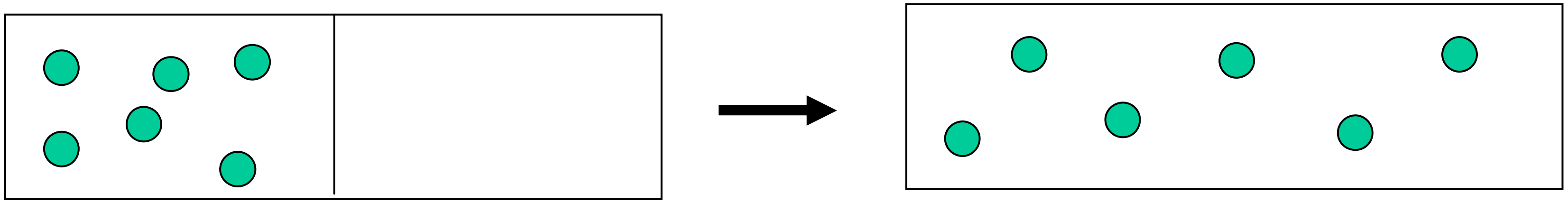
$\rho_{nm} \propto \exp[i(\varepsilon_n - \varepsilon_m)t] \quad \leftrightarrow \quad$ describes the motion on this orbits.

Classical d-entropy

$$\boxed{S_d = -\int N(\varepsilon)\, \rho(\varepsilon) \ln \rho(\varepsilon) d\varepsilon} \qquad \rho(\varepsilon) = \int d\Gamma \rho(p,q) \delta(\varepsilon - \varepsilon(p,q))$$

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

Classic example: freely expanding gas



Suddenly remove the wall

$$\Delta S_{Gibbs} = 0$$ by Liouville theorem

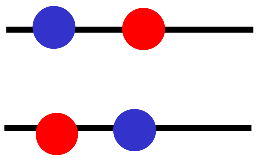
$$\rho_{nn}(0+) = \frac{1}{2}\rho_{nn}(0-)$$ double number of occupied states

$$\boxed{\Delta S_d = N \ln 2}$$ result of Hamiltonian dynamics!

Example

Cartoon BCS model:

$$H = \sum_k \varepsilon_k c^+_{k\uparrow} c_{k\downarrow} - \frac{g}{2N} \sum_{k,p} c^+_{k\uparrow} c^+_{-k\downarrow} c_{-p\downarrow} c_{p\uparrow}$$



$\varepsilon_k = 1$

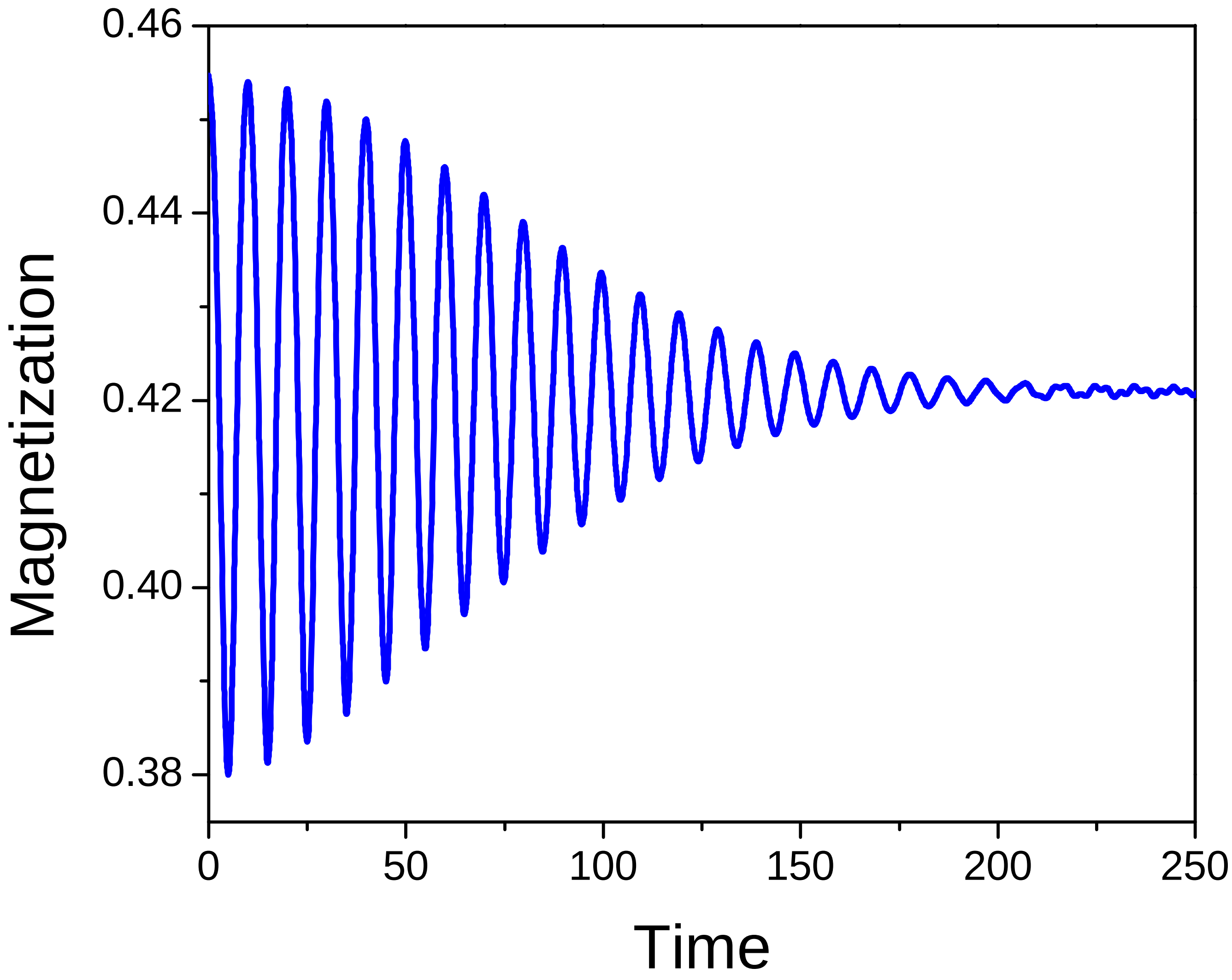
$\varepsilon_k = -1$

Mapping to spin model (Anderson, 1958)

$$H = (S_{1z} - S_{2z}) - \frac{g}{2N}\left(S_1^+ S_2^- + S_2^+ S_1^-\right)$$

In the thermodynamic limit this model has a transition to superconductor (XY-ferromagnet) at $g = 1$.

Change g from g_1 to g_2.

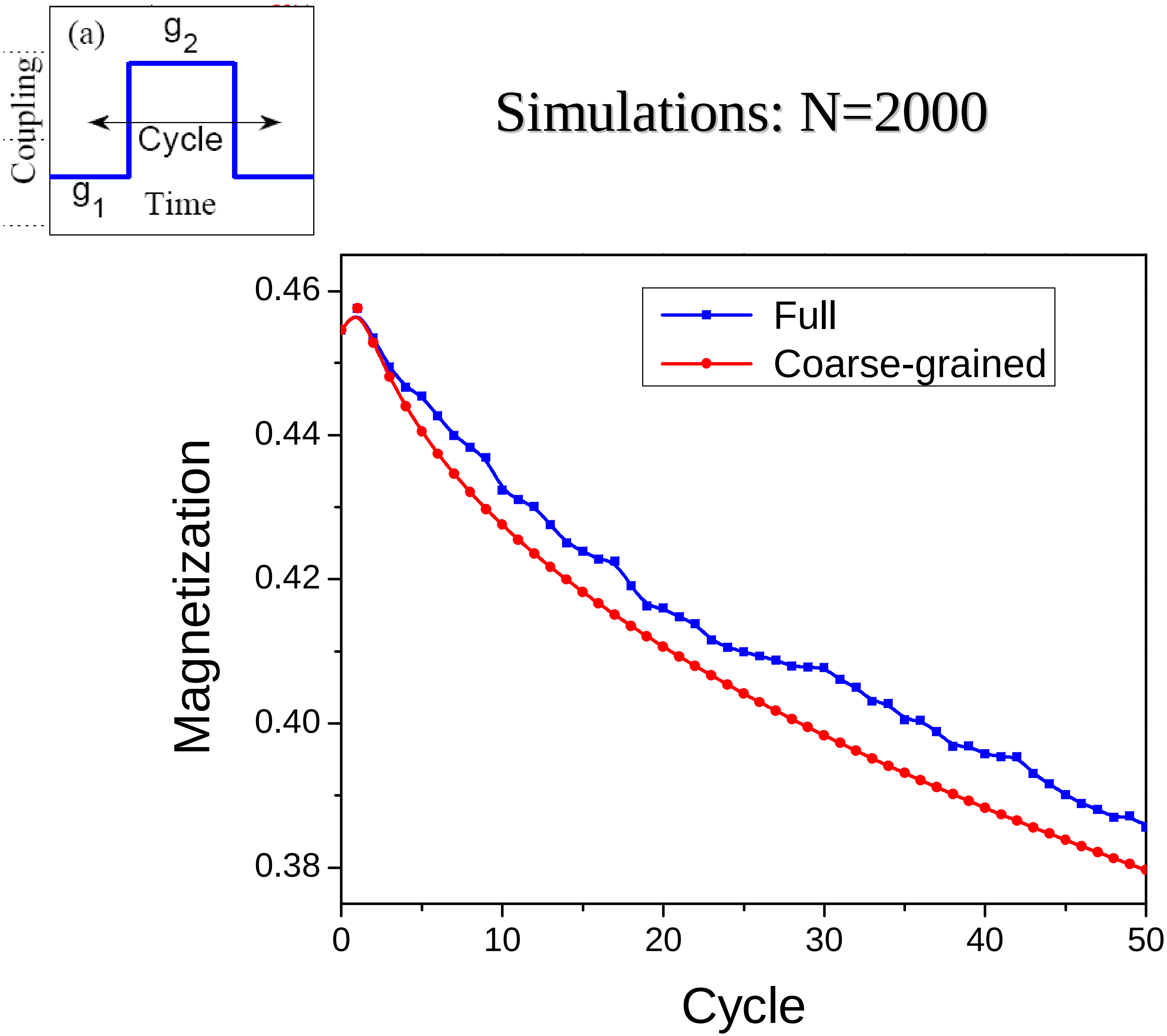


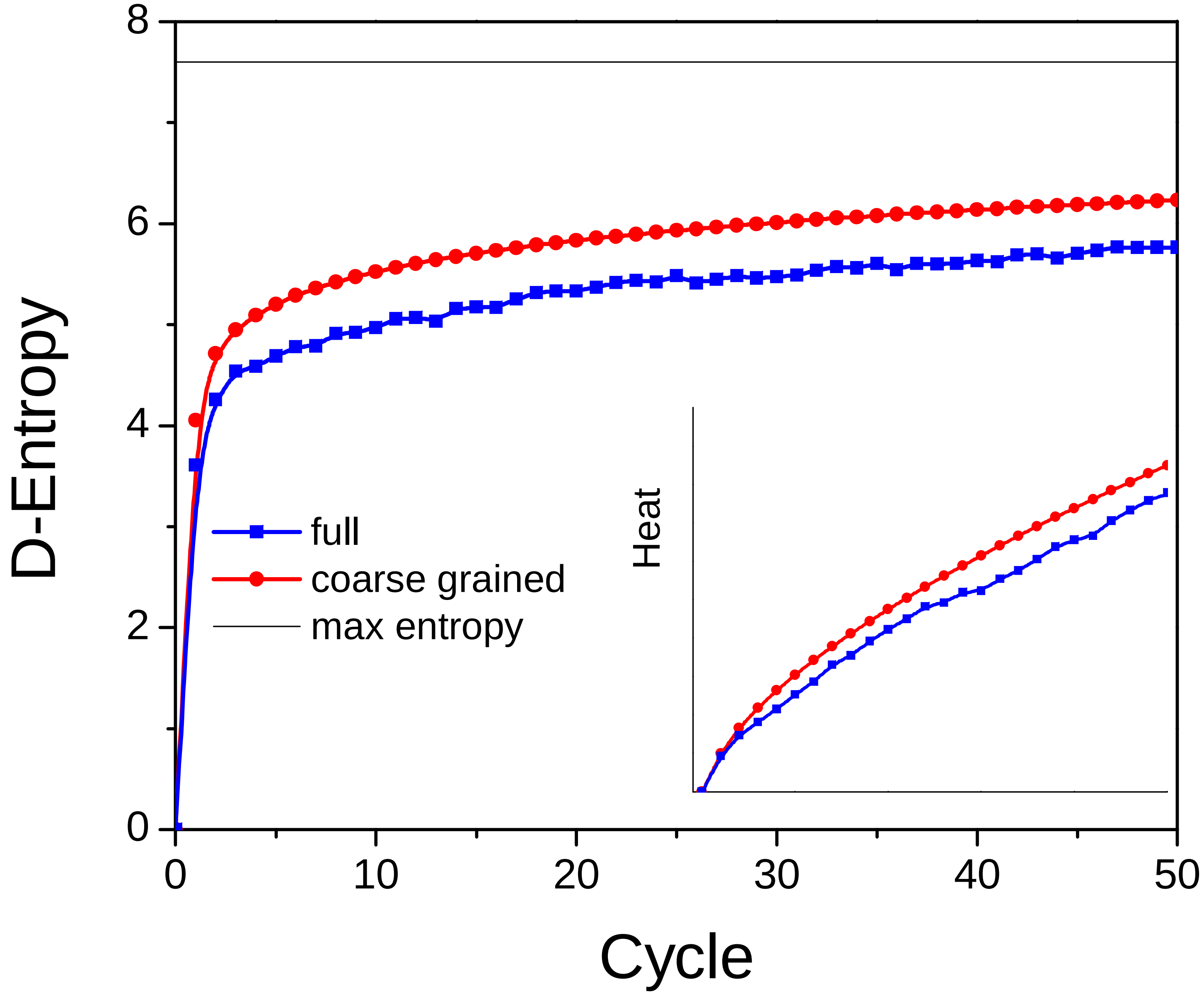
$$\tau \propto \sqrt{N}$$

$$T_r \propto N$$

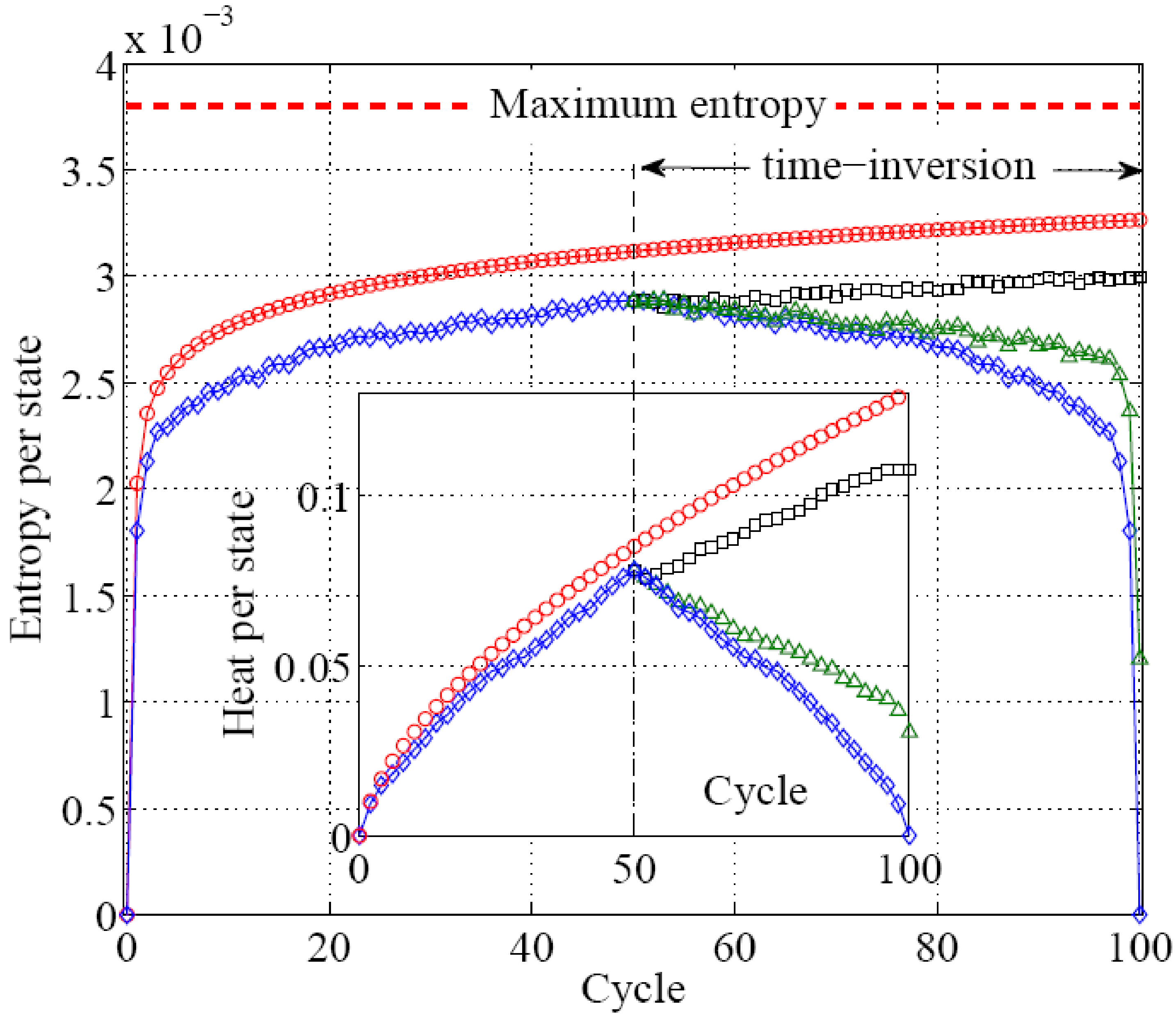
Work with large N.

Simulations: N=2000




D-Entropy
Cycle
0
2
4
6
8
0
10
20
30
40
50
full
coarse grained
max entropy
Heat

Entropy and reversibility.



$\delta g = 10^{-4}$

$\delta g = 10^{-5}$

Simple picture

$\uparrow \; \downarrow \; \uparrow \; \uparrow \; \uparrow \; \uparrow \; \downarrow \qquad \uparrow h$

Two sources of energy change:

1) change external parameters without transitions between microstates (flipping spins)

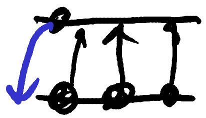
→ adiabatic change, conserves entropy, can be reversed

2) introduce transitions (either due to contact with external environment or due to changing external parameters)

leads to entropy increase, heat generation, irreversible.

3) $\rho_{nn} = \text{const}$ is a natural attractor of the Hamiltonian dynamics.

A simple reason is that one can introduce transition probabilities

 It is more likely to occupy empty states.

Hamiltonian dynamics is presumably sufficient but not necessary condition for this.

Nearly adiabatic dynamics in many-particle systems

Let us assume we are hanging some external parameter in time according to the protocol

$$\lambda(t) = \begin{cases} \lambda_i & t < 0 \\ \lambda_i + t\delta(\lambda_f - \lambda_i) & 0 \le t \le 1/\delta \\ \lambda_f & t > 1/\delta. \end{cases}$$

Can we say anything about system response in the limit $\delta \to 0$?

Assume (for now) that we start in the ground state.

Need to solve

$$i\hbar\partial_t|\psi\rangle = \mathcal{H}(t)|\psi\rangle$$

Convenient to work in the adiabatic (co-moving, instantaneous) basis

$$|\psi(t)\rangle = \sum_n a_n(t)|\phi_n(t)\rangle \quad \mathcal{H}(t)|\phi_n(t)\rangle = E_n(t)|\phi_n(t)\rangle$$

$$i\hbar\partial_t a_m(t) + i\hbar\sum_n a_n(t)\langle\phi_m|\partial_t|\phi_n\rangle = E_m(t)a_m(t)$$

$$a_n(t) = \alpha_n(t)\exp\left[-i\Theta_n(t)\right] \qquad \Theta_n(t) = \int_{t_i}^{t} E_n(\tau)d\tau$$

$$\dot{\alpha}_n(t) = -\sum_m \alpha_m(t)\langle n|\partial_t|m\rangle \exp\left[i(\Theta_n(t) - \Theta_m(t))\right]$$

$$\alpha_n(t) = -\int_{t_i}^{t} dt' \sum_m \alpha_m(t')\langle n|\partial_{t'}|m\rangle \mathrm{e}^{i(\Theta_n(t') - \Theta_m(t'))}$$

$$\alpha_n(\lambda) = -\int_{\lambda_i}^{\lambda} d\lambda' \sum_m \alpha_m(\lambda')\langle n|\partial_{\lambda'}|m\rangle \mathrm{e}^{i(\Theta_n(\lambda')-\Theta_m(\lambda'))}$$

$$\Theta_n(\lambda) = \int_{\lambda_i}^{\lambda} d\lambda' \frac{E_n(\lambda')}{\dot{\lambda}'} \qquad \dot{\lambda} = \delta$$

In the limit $\dot{\lambda} \to 0$ only term with n=m (assuming there are no degenarcies) survives.

Perturbative analysis, keep only term with m=0 in the sum.

$$\alpha_n(t) \approx -\int_{t_i}^{t} dt' \langle n|\partial_{t'}|0\rangle \mathrm{e}^{i(\Theta_n(t')-\Theta_0(t'))}$$

$$\alpha_n(t) \approx -\int_{t_i}^{t} dt' \langle n|\partial_{t'}|0\rangle \mathrm{e}^{i(\Theta_n(t')-\Theta_0(t'))}$$

Infinite integration limits

$$|\alpha_n|^2 \propto \exp[-2\Im(\Theta_n(\lambda^\star) - \Theta_0(\lambda^\star))]$$

where λ^* is the complex root of $E_n(\lambda^\star) - E_0(\lambda^\star) = 0$

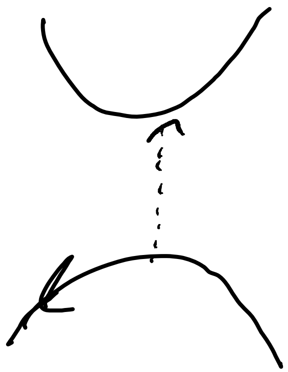
Finite integration limits:

$$\alpha_n(t_f) \approx i\frac{\langle\phi_n|\partial_t|\phi_0\rangle}{E_n(t)-E_0(t)}\mathrm{e}^{i(\Theta_n(t)-\Theta_0(t))}\Bigg|_{t_i}^{t_f} = i\delta\frac{\langle\phi_n|\partial_\lambda|\phi_0\rangle}{E_n(\lambda)-E_0(\lambda)}\mathrm{e}^{i(\Theta_n(\lambda)-\Theta_0(\lambda))}\Bigg|_{\lambda_i}^{\lambda_f}$$

$$|\alpha_n(\lambda_f)|^2 \approx \delta^2\left[\frac{|\langle\phi_n|\partial_{\lambda_i}|\phi_0\rangle|^2}{(E_n(\lambda_i)-E_0(\lambda_i))^2} + \frac{|\langle\phi_n|\partial_{\lambda_f}|\phi_0\rangle|^2}{(E_n(\lambda_f)-E_0(\lambda_f))^2}\right] - 2\delta^2\frac{\langle\phi_n|\partial_{\lambda_i}|\phi_0\rangle}{E_n(\lambda_i)-E_0(\lambda_i)}\frac{\langle\phi_n|\partial_{\lambda_f}|\phi_0\rangle}{E_n(\lambda_f)-E_0(\lambda_f)}\cos\left[\Delta\Theta_{n0}\right]$$

(1

Landau-Zener problem



$$\mathcal{H} = \lambda\sigma_z + g\sigma_x$$

$$E_\pm = \pm\sqrt{\lambda^2 + g^2}.$$

Change coupling λ in the infinite range. Exact solution:

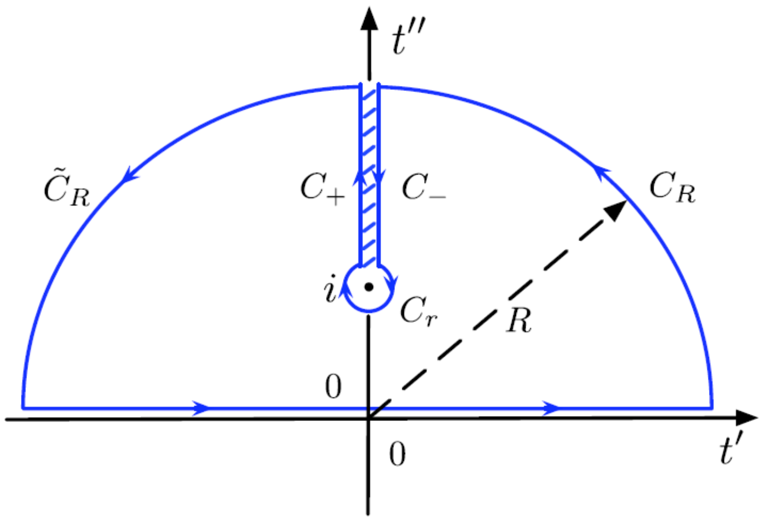
$$|a_+|^2 = \exp\left[-\frac{\pi g^2}{\delta}\right]$$

Perturbative solution. Eigenstates:

$$|-\rangle = \begin{pmatrix} \sin(\theta/2) \\ -\cos(\theta/2) \end{pmatrix}, \quad |+\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix} \qquad \tan\theta = g/\lambda$$

$$\langle +|\partial_t|-\rangle = \dot{\theta}/2 = -\frac{1}{2}\frac{\dot{\lambda}g}{\lambda^2 + g^2}$$

$$\alpha_+(\infty) \approx \frac{1}{2}\int_{-\infty}^{\infty} \frac{\delta g}{g^2+(\delta t)^2} \exp\left[2i\int_0^t d\tau\sqrt{(\delta\tau)^2+g^2}\right]$$

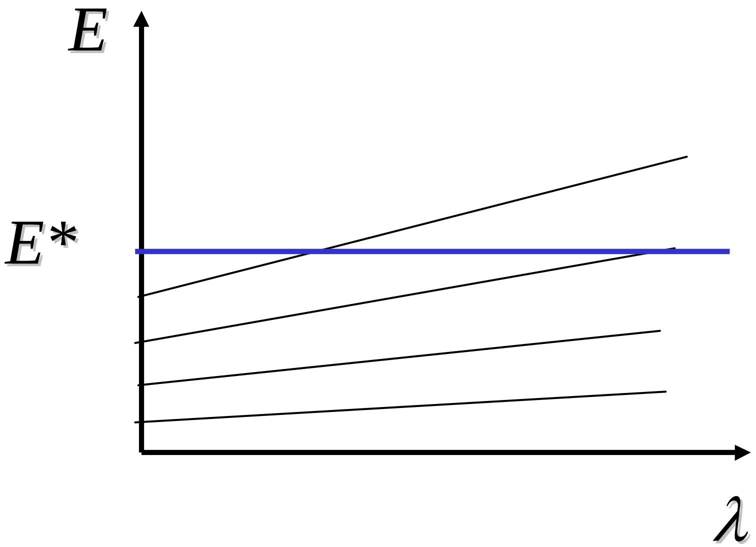


$$|\alpha_+(\infty)|^2 \approx \frac{\pi^2}{9}\exp\left[-\frac{\pi g^2}{\delta}\right]$$

Spurious factor $\pi^2/9$

Gapless systems with quasi-particle excitations

Ramping in generic gapless regime (low energy contribution)



$$\frac{dE^*}{dt} \sim (E^*)^2 \Rightarrow \frac{dE^*}{d\lambda}\dot{\lambda} \sim (E^*)^2$$

Uniform system: $E(\lambda) = c(\lambda)k^z$

$$E^* \sim \dot{\lambda}\frac{d\ln c}{d\lambda}$$

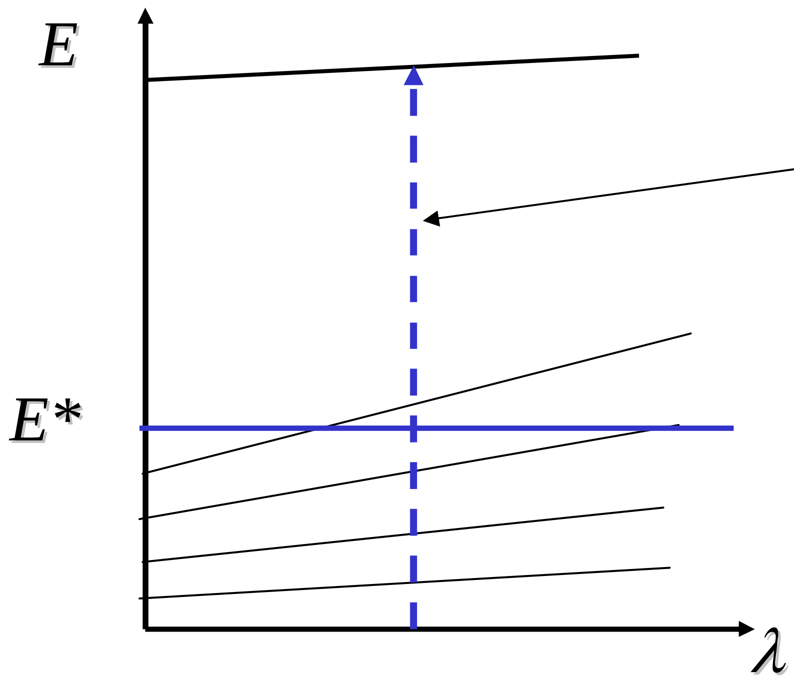
Density of quasi-particles (entropy): $n_{ex} \sim \int_0^{E^*} \rho(E)dE \sim |\dot{\lambda}|^{d/z}$

Absorbed energy density (heating): $Q \sim |\dot{\lambda}|^{(d+z)/z}$

Low energy contribution:

$$n_{ex}, s \propto |\dot{\lambda}|^{d/z}, \quad Q \propto |\dot{\lambda}|^{(d+z)/z}$$

High energy contribution.



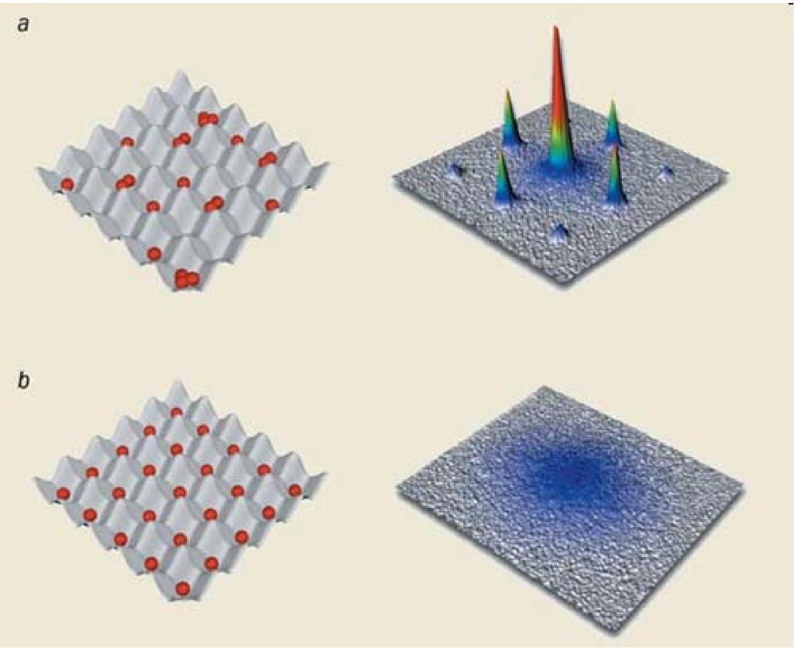
$$p_{ex}(E) \propto \frac{|\dot{\lambda}|^2}{E^6}$$

$$n_{ex} \sim \int p_{ex}(E)\rho(E)dE \propto |\dot{\lambda}|^2$$

Similarly $\quad Q \sim |\dot{\lambda}|^2$

High dimensions: high energies dominate dissipation, low-dimensions – low energies dominate dissipation.

Adiabatic crossing quantum critical points.



Relevant for adiabatic quantum computation, adiabatic preparation of correlated states.

$$\boxed{V = \delta t, \quad \delta \to 0}$$

How does the number of excitations (entropy, energy) scale with δ?

Use scaling arguments in the adiabatic perturbation theory

$$n_{ex} = \sum_k |\alpha_k|^2 , \quad Q = \sum_k \varepsilon_k |\alpha_k|^2 , \ldots$$

$$\alpha_k \simeq \int_{\lambda_i}^{\lambda_f} \langle k | \partial_\lambda | 0 \rangle \, e^{i \theta_{k0}(\lambda)} \, d\lambda$$

$$\Theta_k(\lambda) - \Theta_0(\lambda) = \frac{1}{\delta}\int_{\lambda_i}^{\lambda} d\lambda' (\varepsilon_k(\lambda') - \varepsilon_0(\lambda')) \qquad \varepsilon_k(\lambda) - \varepsilon_0(\lambda) = \lambda^{z\nu} F(k^z/\lambda^{z\nu})$$

$$\langle k|\partial_\lambda|0\rangle = \frac{\langle k|V|0\rangle}{\varepsilon_k(\lambda) - \varepsilon_0(\lambda)} = \frac{1}{\lambda} G(k^z/\lambda^{z\nu}) \qquad \lambda = \xi \delta^{\frac{1}{z\nu+1}}, \quad k = \eta \delta^{\frac{\nu}{z\nu+1}}$$

$$n_{\text{ex}} \sim 2\int \frac{d^d k |\alpha_k|^2}{(2\pi)^d} = 2|\delta|^{\frac{d\nu}{z\nu+1}} \int \frac{d^d\eta}{(2\pi)^d} |\alpha(\eta)|^2,$$

$$\alpha(\eta) = \int_{\xi_i}^{\xi_f} d\xi \frac{1}{\xi} G\left(\frac{\eta^z}{\xi^{z\nu}}\right) \exp\left[i \int_{\xi_i}^{\xi} d\xi_1 \xi_1^{z\nu} F(\eta^z/\xi_1^{z\nu})\right]$$

$$n_{ex} \propto |\delta|^{\frac{d\nu}{z\nu+1}}, \quad \frac{d\nu}{z\nu+1} < 2$$

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

$$n_{ex} \propto \delta^2, \quad \frac{d\nu}{z\nu+1} \geq 2$$

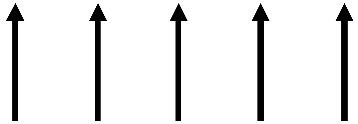
Nontrivial power corresponds to nonlinear response!

$d_c = 2(z + 1/\nu)$ is analogous to the upper critical dimension.

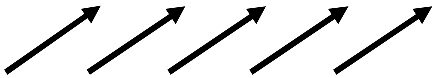
Transverse field Ising model.

$$\boxed{\mathcal{H}_I = -\sum_j g\sigma_j^x + \sigma_j^z \sigma_{j+1}^z}$$

$$g \to 0 \quad \Rightarrow \quad \left\langle \sigma_i^z \sigma_j^z \right\rangle \to 1$$



$$g \to \infty \quad \Rightarrow \quad \left\langle \sigma_i^x \right\rangle \to 1$$



There is a phase transition at g=1.

This problem can be exactly solved using Jordan-Wigner transformation:

$$\sigma_i^x = 2c_i^\dagger c_i - 1, \quad \sigma_i^z = \prod_{j \le i-1} (c_j^\dagger c_j - 1)\ (c_j + c_j^\dagger)$$

$$\mathcal{H}_I = -\sum_j c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}^\dagger + c_{j+1} c_j - 2g c_j^\dagger c_j$$

Spectrum:

Critical exponents: $z=\nu=1 \Rightarrow d\nu/(z\nu+1)=1/2.$

Linear response (Fermi Golden Rule):

$$\boxed{n_{\mathrm{ex}} \approx \int \frac{d^d k}{(2\pi)^d} \left| \int_{-\infty}^{\infty} d\lambda \langle k | \frac{d}{d\lambda} | 0 \rangle e^{i/\delta \int^{\lambda} (\omega_k(\lambda') - \omega_0(\lambda')) d\lambda'} \right|^2}$$

$$n_{ex} \approx 0.21\sqrt{\delta}$$

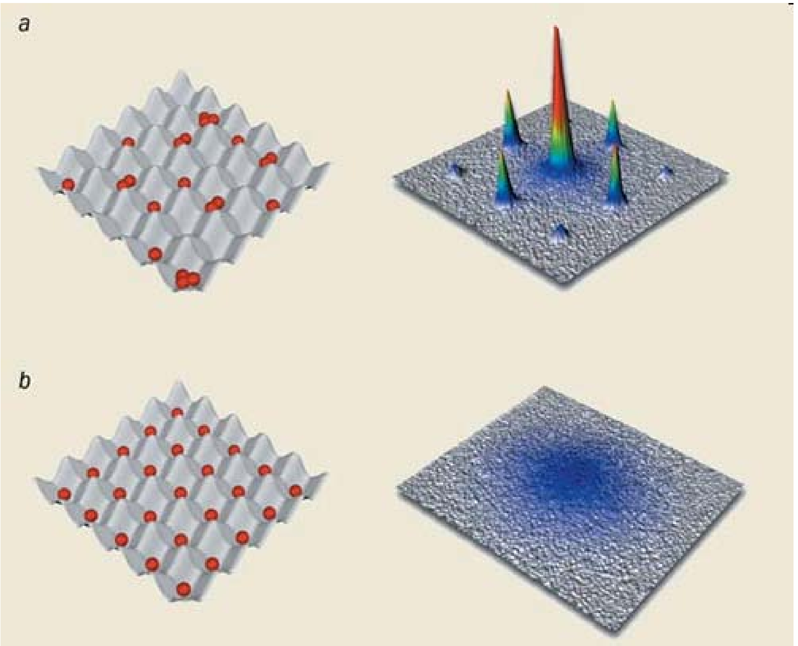
A. P., 2003

Correct result (J. Dziarmaga 2005): $n_{ex} \approx 0.11\sqrt{\delta}$

Interpretation as the Kibble-Zurek mechanism:
W. H. Zurek, U. Dorner, Peter Zoller, 2005

Optimal adiabatic passage through a QCP.

(R. Barankov and A. Polkovnikov, Phys. Rev. Lett. 101, 076801 (2008))



Given the total time T, what is the optimal way to cross the phase transition?

Need to slow down near the phase transition:

$$\boxed{\lambda=(\delta t)^r, \quad \delta \sim 1/T}$$

$$r_{\text{opt}} \approx -\frac{1}{z\nu} \ln\left[\frac{\delta}{C} \ln(C/\delta)\right]$$

optimal power

$$n_{\text{opt}} \sim \left[\frac{\delta}{C} \ln(C/\delta)\right]^{d/z}$$

number of defects at optimal rate.

Three regimes of response to the slow linear 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

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

C. Non-adiabatic – low dimensions, bosonic excitations

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

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

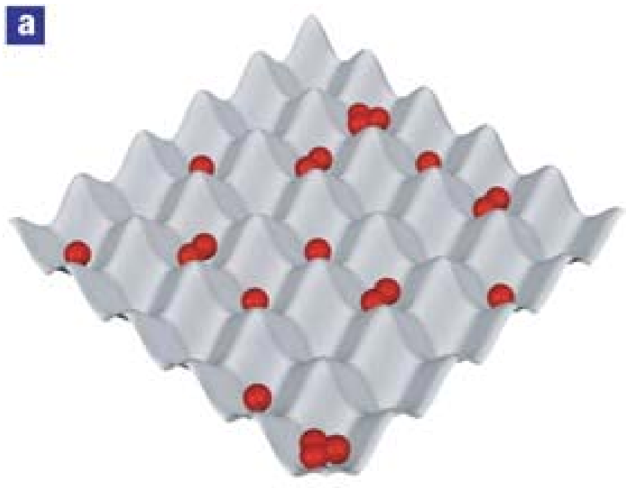
The adiabatic theorem in thermodynamics does follow from the adiabatic theorem in quantum mechanics.

Numerical verification (bosons on a lattice).

$$\boxed{\mathcal{H}_{bh} = -J\sum_{\langle ij\rangle}(a_i^\dagger a_j + a_j^\dagger a_i) + \frac{U(t)}{2}\sum_j a_j^\dagger a_j(a_j^\dagger a_j - 1),}$$

$$U(t) = U_0 \tanh(\delta t)$$

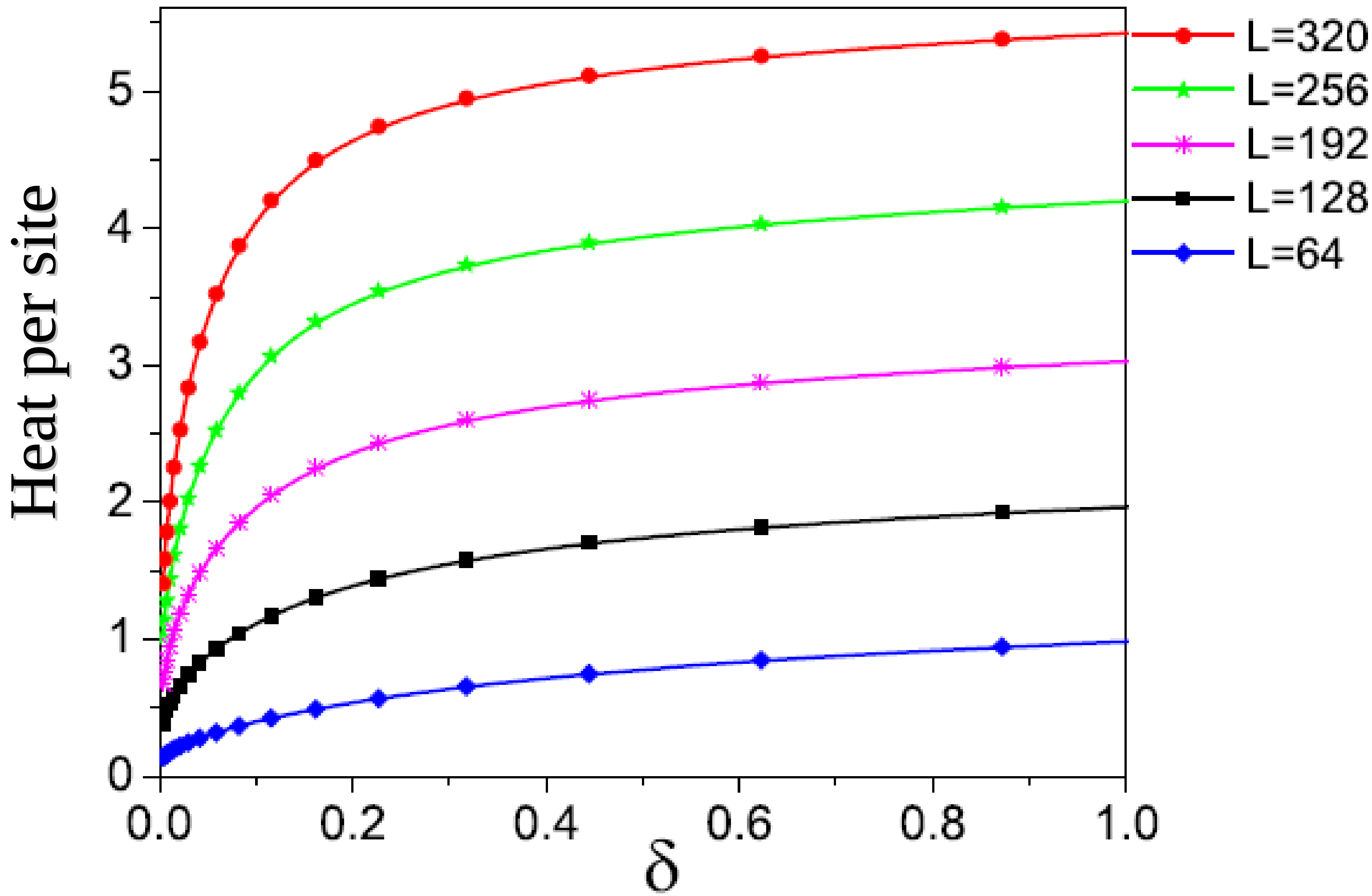
Nonintegrable model in all spatial dimensions, expect thermalization.



Use the fact that quantum fluctuations are weak in the SF phase and expand dynamics in the effective Planck's constant:

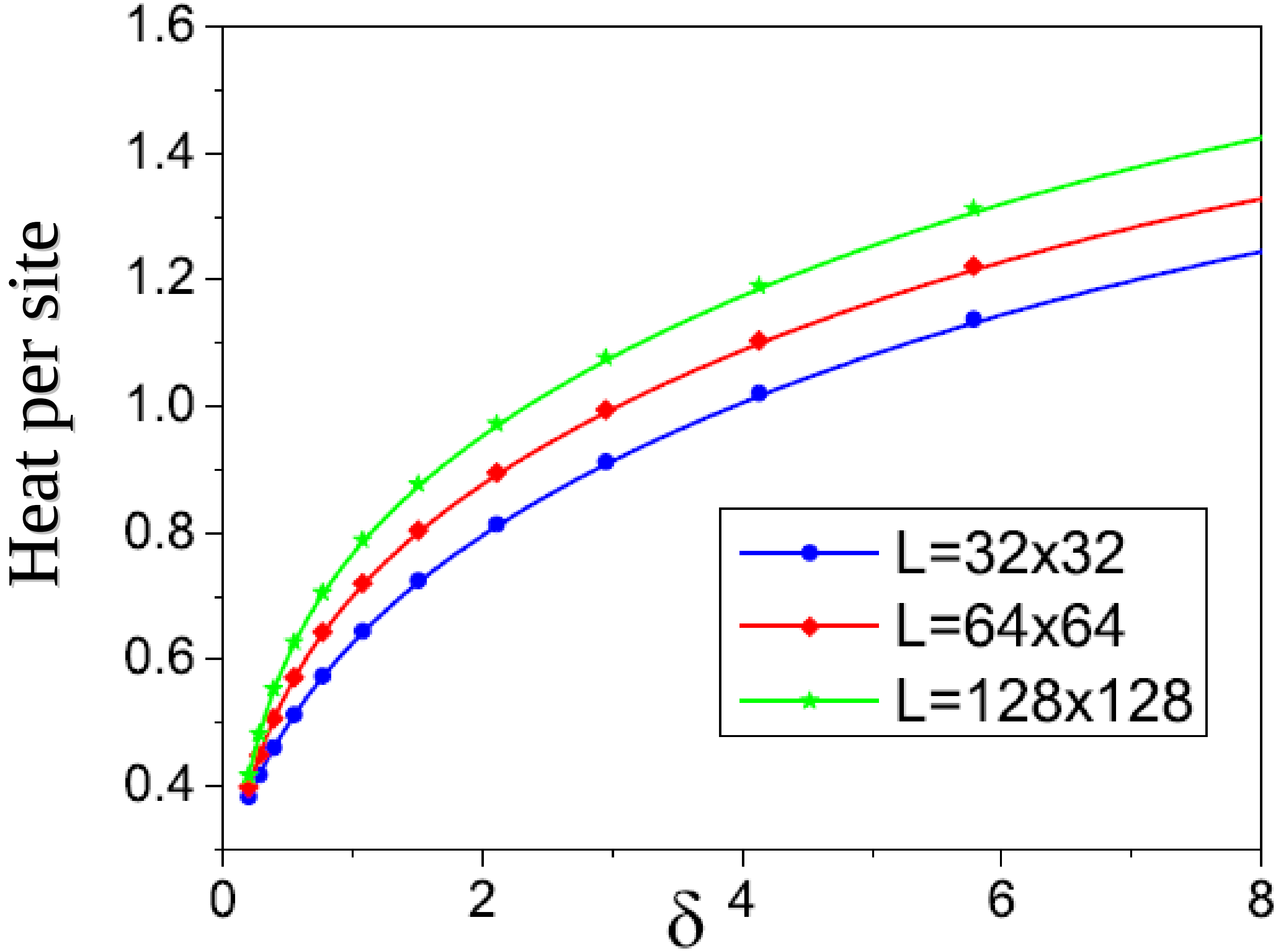
$$\hbar \to \sqrt{U / n_0 J}$$

T=0.02



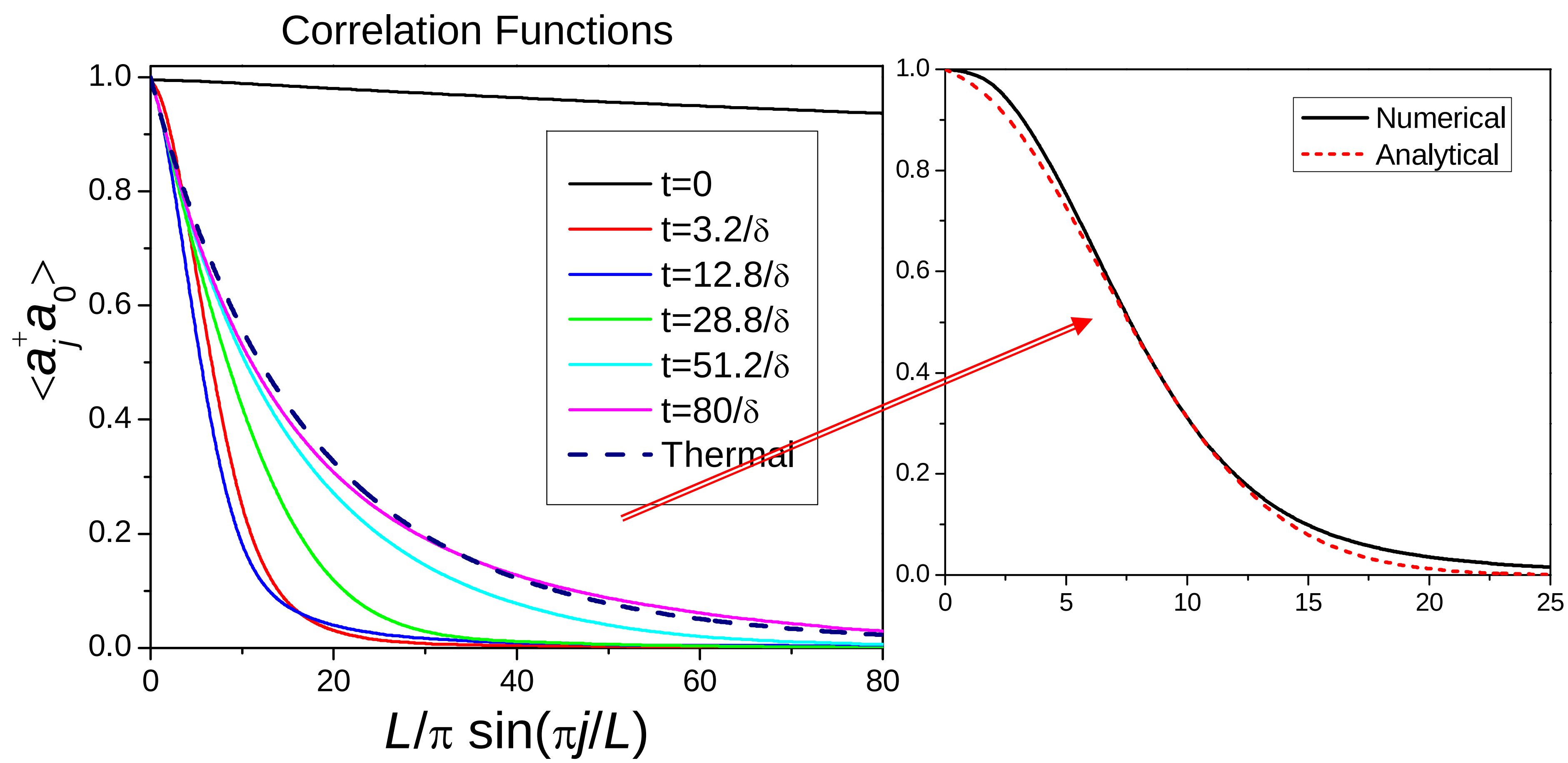
$$\boxed{\Delta E \propto T\, L^{4/3}\, \delta^{1/3}}$$

2D, T=0.2



$$\Delta E \propto T\, L^{1/3}\, \delta^{1/3}$$

Thermalization at long times (1D).



Probing quasi-particle statistics in nonlinear dynamical probes.

(R. Barankov, C. De Grandi, V. Gritsev, A. Polkovnikov, work in progress.)