Relationship between chaos and thermalization in isolated quantum many-body systems

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Isolated
quantum many-body systems

Thermalization

Quantum chaos

Outline

1D: integrable and chaotic domains

THERMALIZATION

- Thermalization of isolated quantum many-body systems occurs in the chaotic limit (chaotic eigenstates)

RELAXATION PROCESS

- Dynamics and relaxation process of isolated quantum many-body systems after a QUENCH

ENTROPY and TYPICALITY

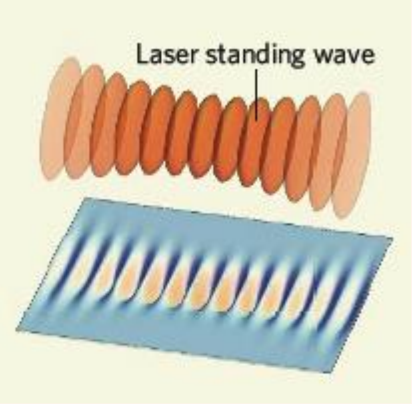
- Entropy to describe quantum many-body systems out of equilibrium

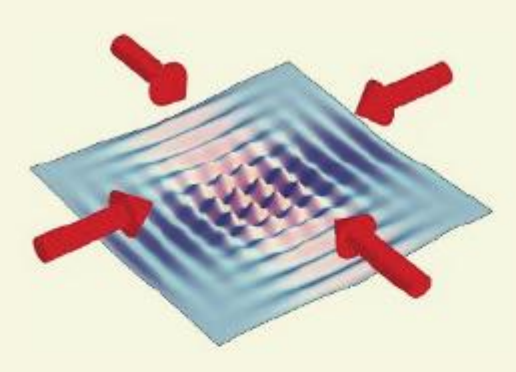
Optical lattices

<u>Optical lattices</u>: crystals formed by interfering laser beams
ultracold atoms play the role of electrons in solid crystal

Real solid materials are complex:
disorder, vibrations of lattice, Coulomb interactions of electrons, etc
cannot be described by the simple theoretical models proposed.

Optical lattices: can realize these simple models, very large (millions of sites)
highly controllable systems – interactions, level of disorder, 1,2,3D
isolated



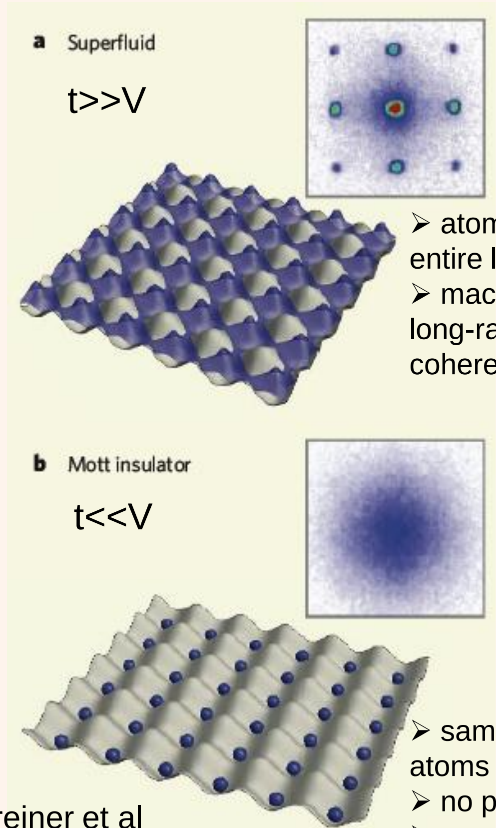


Greiner & Fölling
Nature **453**, 736 (2008)

Experiments in optical lattices

Superfluid -- Mott insulator transition

Bose-Hubbard model with repulsive interaction
t: tunneling strength; V: interaction strength



- atoms spread over entire lattice,
- macro wavefunction long-range phase coherence

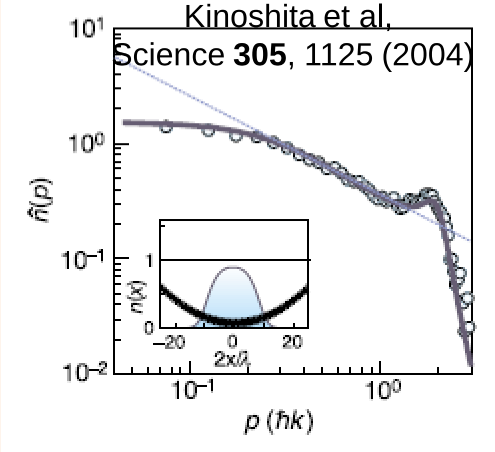
- same number of atoms per site
- no phase coherence
- gap in the spectrum

Greiner et al
Nature **41**, 39 (2002)

Tonks-Girardeau gas

- strong repulsive interaction of bosons in **1D**,
- one boson per site (**hardcore bosons**)
- resemble non-interacting fermions
- same spatial density distribution, different momentum distribution

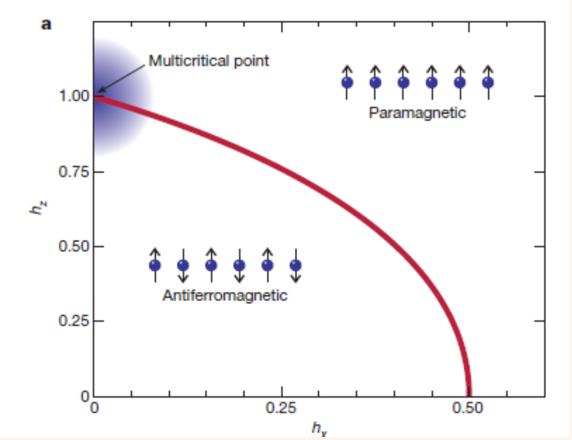
Paredes et al,
Nature **429**, 277 (2004)
Kinoshita et al,
Science **305**, 1125 (2004)



Simulation of spin chains

- spinless bosons simulate a chain of interacting quantum Ising spins as they undergo a phase transition

Simon et al,
Nature **472**, 307 (2011)



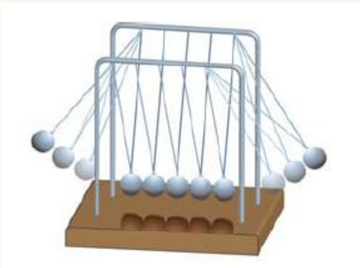
Optical lattices: thermalization in 1D

Quantum Newton's cradle:

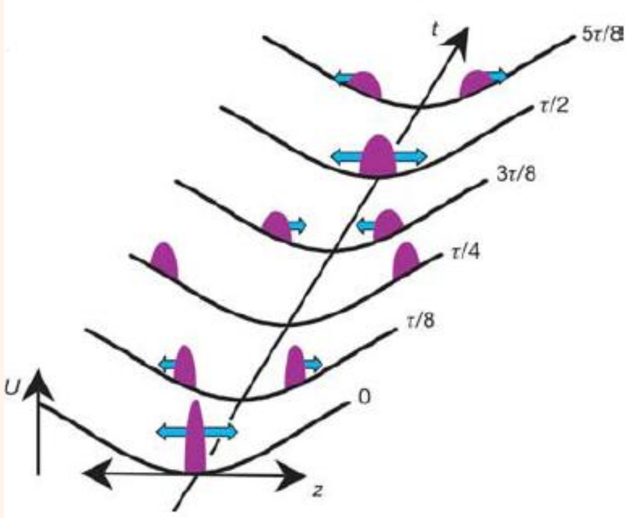
Kinoshita et al
Nature **440**, 900 (2006)

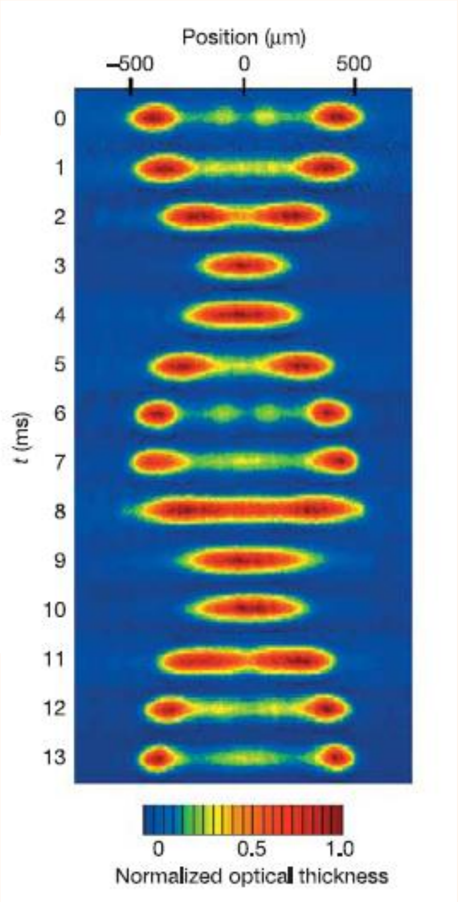
$\gamma = \frac{E_{\text{int}}}{E_{\text{kin}}}$

$\gamma >> 1$
Tonks-Girardeau regime

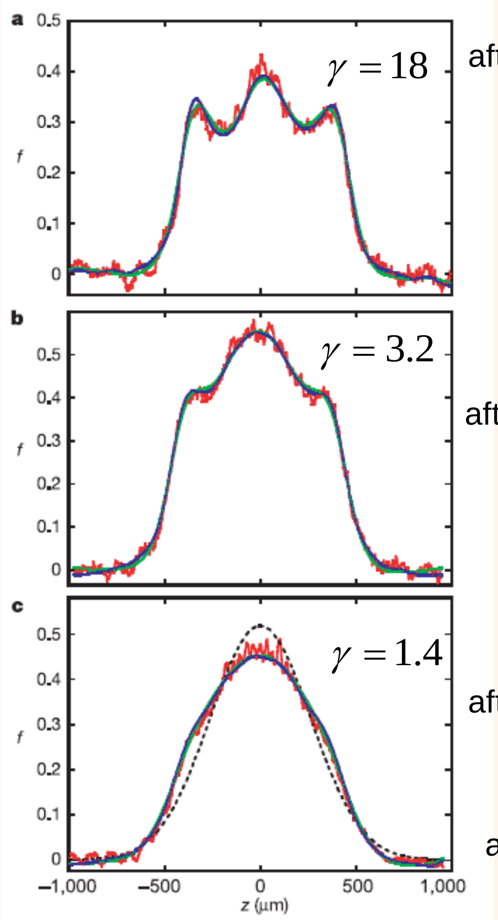


1D Bose gas of ^{87}Rb (BEC)
do not thermalize
after thousands of collisions





Momentum distribution



after 600 collisions

after 2750 collisions

after 6250 collisions

In **3D**:
thermalization
after 3 collisions!

PART I

THERMALIZATION

Quench

$H_{initial}$ —quench→ H_{final}

$eigenstates : \phi_k$ $eigenstates : |\psi_\alpha\rangle$

Initial state **(any)**

$\Psi(0) = \phi_{in}$

$$\underbrace{|\Psi(0)\rangle = |\phi_{in}\rangle = \sum_\alpha C_\alpha |\psi_\alpha\rangle}$$

$$\Downarrow$$

$$|\Psi(\tau)\rangle = \sum_\alpha C_\alpha e^{-iE_\alpha \tau} |\psi_\alpha\rangle$$

Thermalization in an isolated quantum system

Quantum system $H|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$

Quantum system:
linear time evolution
discrete spectrum

Initial state: $|\Psi(0)\rangle = \sum_\alpha C_\alpha |\psi_\alpha\rangle$

Time evolution of a generic observable:

$$\langle O(\tau)\rangle = \langle \Psi(\tau)|O|\Psi(\tau)\rangle = \sum_{\alpha,\beta} C_\alpha^* C_\beta e^{i(E_\alpha - E_\beta)\tau} O_{\alpha\beta}$$

$$O_{\alpha\beta} = \langle\psi_\alpha|O|\psi_\beta\rangle$$

Infinite time average: (generic system with nondegenerate and incommensurate spectrum)

$$\overline{\langle O(\tau)\rangle} = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} = O_{diag}$$

$$\overline{\langle O(\tau)\rangle} = \lim_{\lambda\to\infty} \frac{1}{\lambda}\int_0^\lambda O(\tau)d\tau$$

Will the system thermalize?
Will the predictions from the **diagonal ensemble** coincide with the predictions of the **microcanonical** ensemble?

$$O_{diag} \equiv \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} \overset{=?}{\longleftrightarrow} O_{micro} \equiv \frac{1}{\mathcal{N}_{E_0,\Delta E}} \sum_{\substack{\alpha \\ |E_0 - E_\alpha| < \Delta E}} O_{\alpha\alpha}$$

depends on the initial conditions

depends only on the energy

Eigenstate Thermalization Hypothesis

$$O_{diag} \equiv \sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} \stackrel{=?}{\longleftrightarrow} O_{micro} \equiv \frac{1}{\mathcal{N}_{E_0,\Delta E}} \sum_{\substack{\alpha \\ |E_0 - E_\alpha| < \Delta E}} O_{\alpha\alpha}$$

depends on the initial conditions | depends only on the energy

Equation holds for all initial states that are narrow in energy when…

ETH: the expectation values $O_{\alpha\alpha}$ of few-body observables do not fluctuate for eigenstates close in energy

Deutsch, PRA **43**, 2046 (1991); NJP **12** 075021 (2010)

Srednicki, PRE **50**, 888 (1994); JPA **29** L75 (1996)

Onset of chaos is associated with the onset of **chaotic eigenstates**

delocalized states; large number of uncorrelated components, described statistically; **pseudo-random vectors**

Percival's conjecture (1973): uniformization of the eigenstates

Berry's conjecture (1977): eigenstates are random vectors

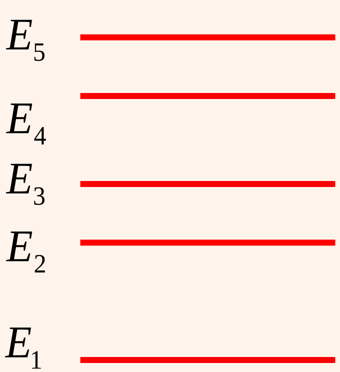
$$\psi^{(j)} = \sum_{i=1}^{N} c_i^{(j)} \phi_i$$

Random matrices

Matrices filled with random numbers and respecting the symmetries of the system.

Wigner in the 1950's used random matrices to study the spectrum of nuclei
(atoms, molecules, quantum dots)

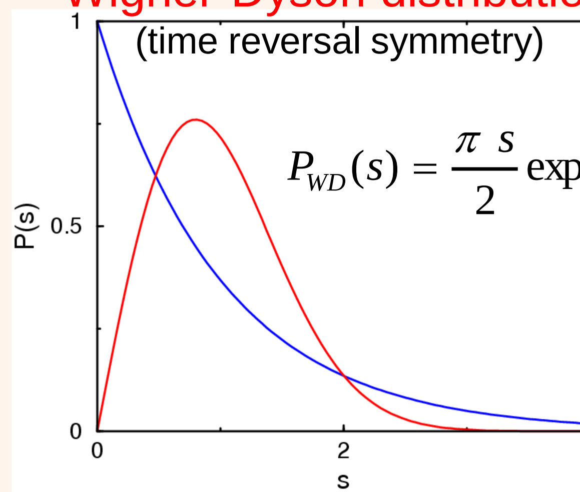
Level spacing distribution



$$s_4 = E_5 - E_4$$
$$s_3 = E_4 - E_3$$
$$s_2 = E_3 - E_2$$
$$s_1 = E_2 - E_1$$

Wigner-Dyson distribution

(time reversal symmetry)



$$P_{WD}(s) = \frac{\pi s}{2} \exp\left(-\frac{\pi s^2}{4} \right)$$

Wigner Dyson distribution – quantum chaos
Quantum chaos = signatures of chaos

Level repulsion
(also in quantum billiards)

(i) Time-reversal invariant systems with rotational symmetry
(or time reversal, integer spin, broken rotational symmetry):
Hamiltonians are real and symmetric
Gaussian Orthogonal Ensemble (GOE)

(ii) Systems without invariance under time reversal (atom in an external magnetic field)
Gaussian Unitary Ensemble (GUE)
Hamiltonians are Hermitian**)**

(iii) Time-reversal invariant systems,
half-integer spin, broken rotational symmetry
Gaussian Sympletic Ensemble (GSE)

Systems with few-body interactions

- ➢ Realistic systems are not described by random matrices;
- ➢ they have with few(two)-body interactions; the density of states is Gaussian;
- ➢ only states in the middle of the spectrum may become chaotic;
- ➢ therefore, in the chaotic limit, thermalization can occur only far from edges

Structure of the eigenstates is key to studies of thermalization

❖ Wigner banded matrices

❖TBRE (two-body random ensembles)
(introduction of a "microcanonical" partition function)
Flambaum & Izrailev PRE **56** 5144 (1997); Izrailev cond-mat/9911297

❖ Shell model (eigenstates and basis dependence – no random elements in *H*)
Zelevinsky et al, Phys. Rep. **276** 85 (1996)

System Model

Hardcore bosons in 1D: (<u>clean</u>, periodic)

$$H=\sum_{i=1}^{L}\left[-t\left(b_i^{+}b_{i+1}+h.c.\right)+V\left(n_i^b-\frac{1}{2}\right)\left(n_{i+1}^b-\frac{1}{2}\right)-t'\left(b_i^{+}b_{i+2}+h.c.\right)+V'\left(n_i^b-\frac{1}{2}\right)\left(n_{i+2}^b-\frac{1}{2}\right)\right]$$

$$\boxed{n_i^b=b_i^{+}b_{i+1}}$$

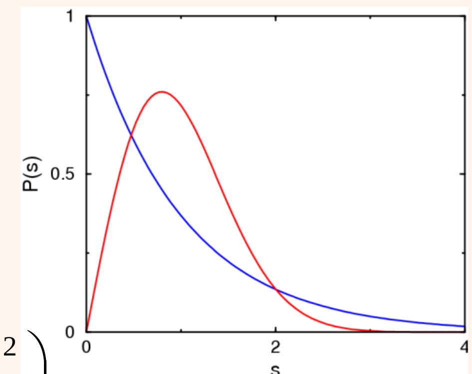
$t',V'=0$ system is integrable

$$P_P(s)=\exp(-s)$$

$t',V'>0$

$t'=0,V'>0$ system may become chaotic

$$P_{WD}(s)=\frac{\pi\, s}{2}\exp\left(-\frac{\pi\, s^2}{4}\right)$$



WD for each subspace

Periodic: conservation of total momentum *k*

(diagonalization for each *k*-sector)

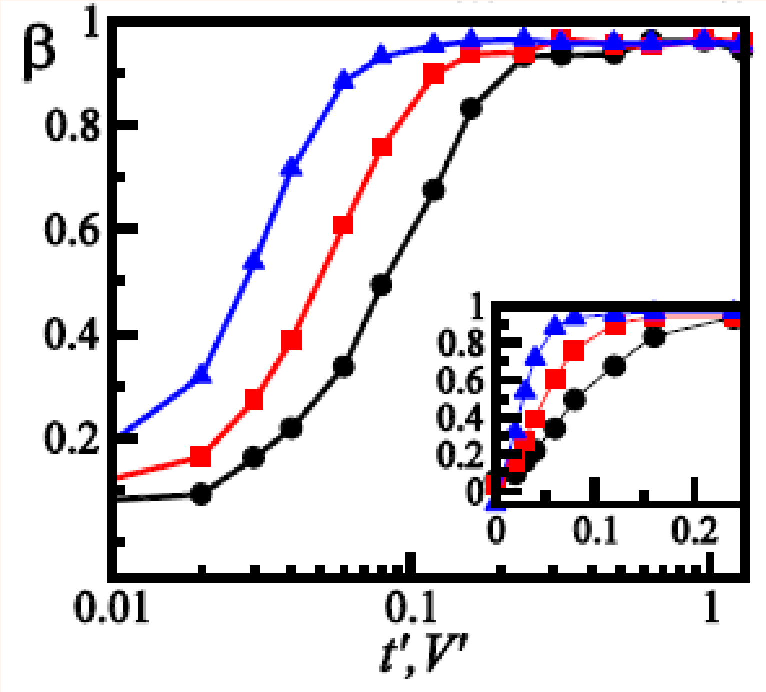
Crossover to chaos

Brody distribution

$$P_B(s) = (\beta+1) b s^{\beta} \exp(-b s^{\beta+1})$$

$$b = \left[\Gamma\left(\frac{\beta+2}{\beta+1}\right)\right]^{\beta+1}$$

$t = V = 1$
$t' = V'$



Chaotic system:

Wigner-Dyson distribution

$\beta = 1$ $$P_{WD}(s) = \frac{\pi s}{2} \exp\left(-\frac{\pi s^2}{4}\right)$$

Integrable system:

Poisson distribution

$\beta = 0$ $$P_P(s) = \exp(-s)$$

1/3 filling
Average over k's

L=24
L=21
L=18

thermodynamic limit?

LFS & M. Rigol
PRE **81** 036206 (2010)

Structure of the eigenstates

Delocalization Measure

Inverse Participation Ratio

$$\psi^{(j)} = \sum_{i=1}^{D} c_i^{(j)} \phi_i \Rightarrow \boxed{IPR^{(j)} \equiv \frac{1}{\sum_{i=1}^{D} |c_i^{(j)}|^4}}$$

IPR – small   localization

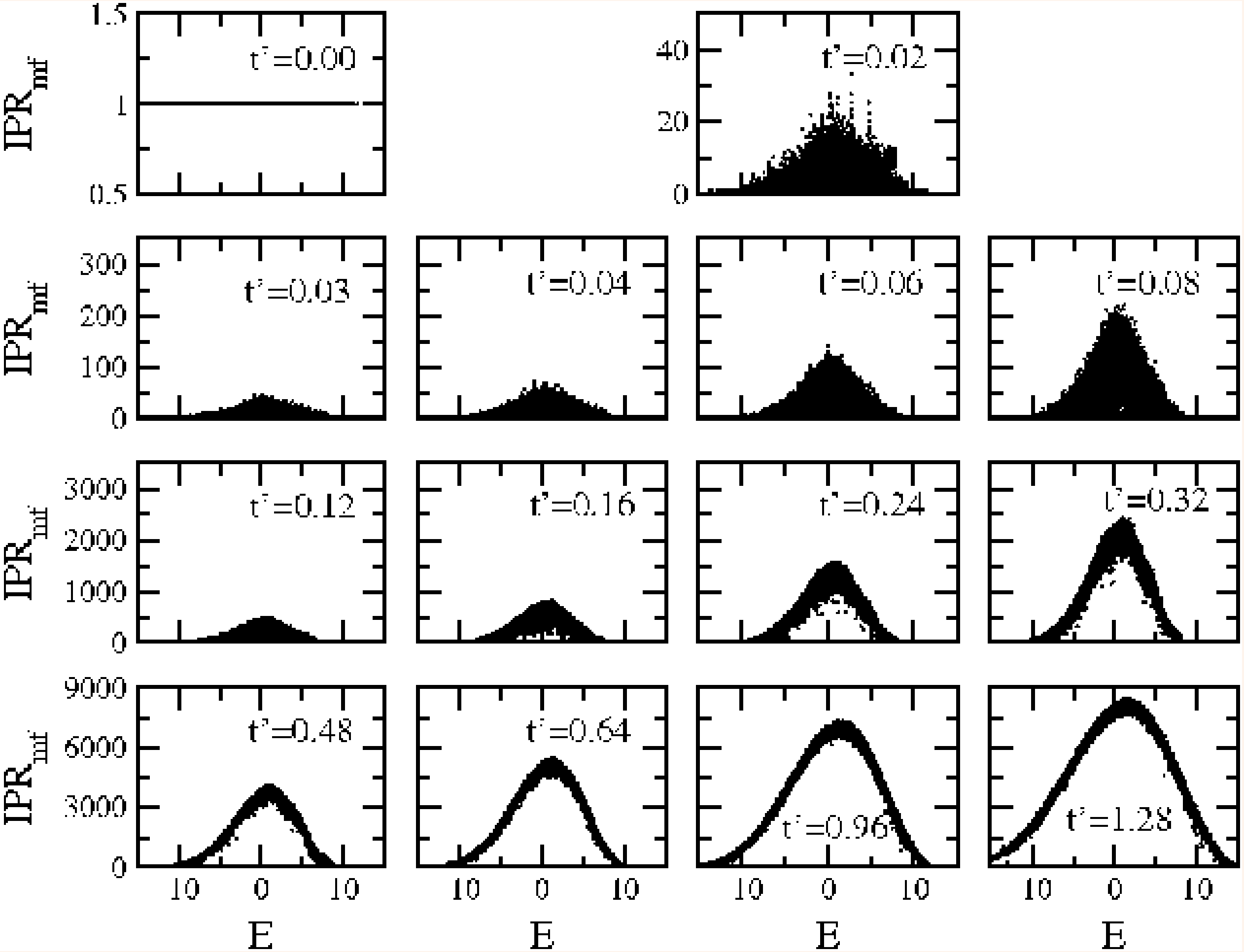
$IPR \sim \dim/3$ maximum delocalization
chaotic states - GOE

Shannon entropy (information) $S = -\sum_{i=1}^{D} |c_i^{(j)}|^2 \ln |c_i^{(j)}|^2$

<u>Mean-field basis</u>: eigenstates of integrable system (*t'*=*V'*=0)
separates regular from chaotic behavior

Izrailev, Phys. Rep.**196** 299 (1990)
Zelevinsky et al, Phys. Rep. **276** 85 (1996)

Bosons: eigenstates



Fluctuations increase close to integrable point

ETH breaks down

Chaotic region: IPR is a smooth function of E

Middle of spectrum

$$IPR_{mf} \rightarrow IPR_{GOE}$$

LFS & M. Rigol
PRE **81** 036206 (2010)

$t = V = 1$
$t' = V'$

L=24, 8 particles, *k*=2
dim=30624

Bosons in 1D: gapped system

Hardcore bosons in 1D: (<u>clean</u>, periodic)

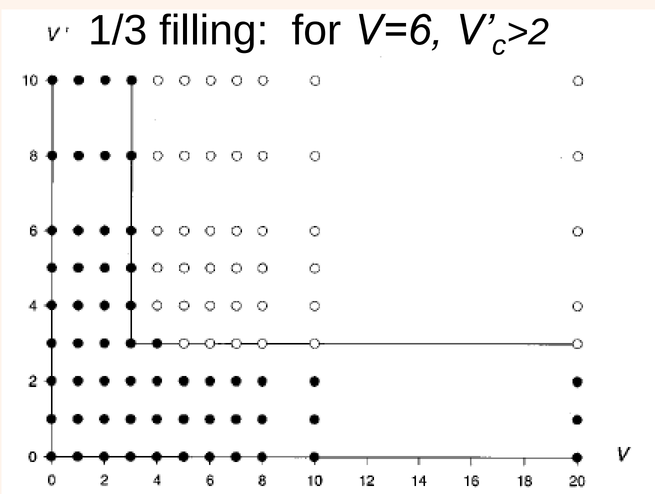
$$H = \sum_{i=1}^{L}\left[-t\left(b_i^+ b_{i+1} + h.c.\right) + V\left(n_i^b - \frac{1}{2}\right)\left(n_{i+1}^b - \frac{1}{2}\right) + V'\left(n_i^b - \frac{1}{2}\right)\left(n_{i+2}^b - \frac{1}{2}\right)\right]$$

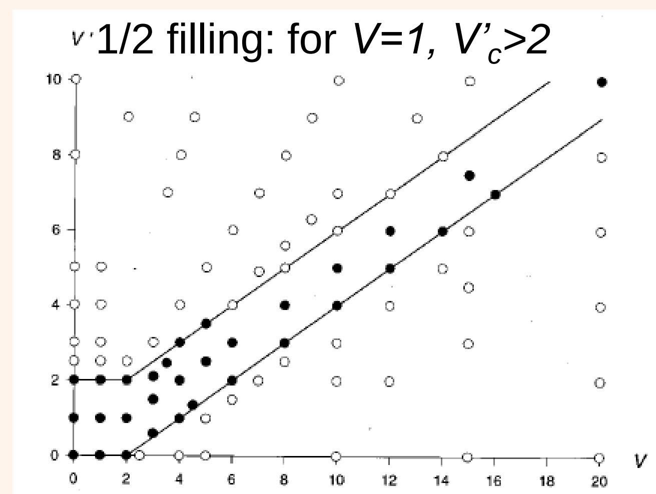
- integrable – chaos transition
- chaos – localization in *k*-space
- gapless superfluid – gapped insulator

- thermalization in gapped system?
- rare events?

Birolli et al,
Mussardo et al

$t = 1$





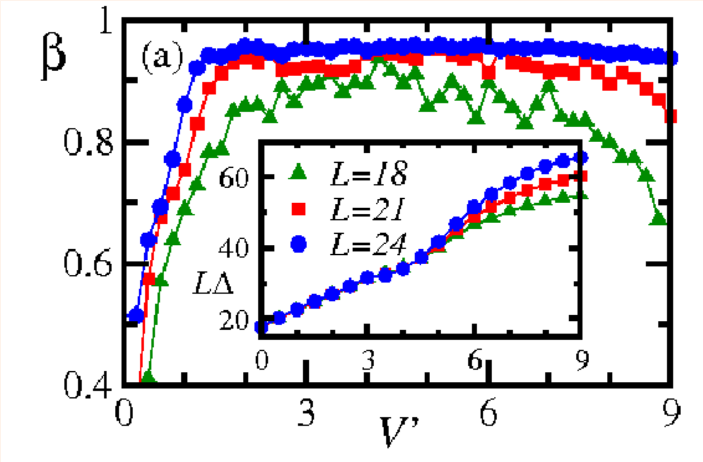
Zhuravlev et al
PRB **86** 12939 (1997)

Gapped phase and chaos

1/3 filling

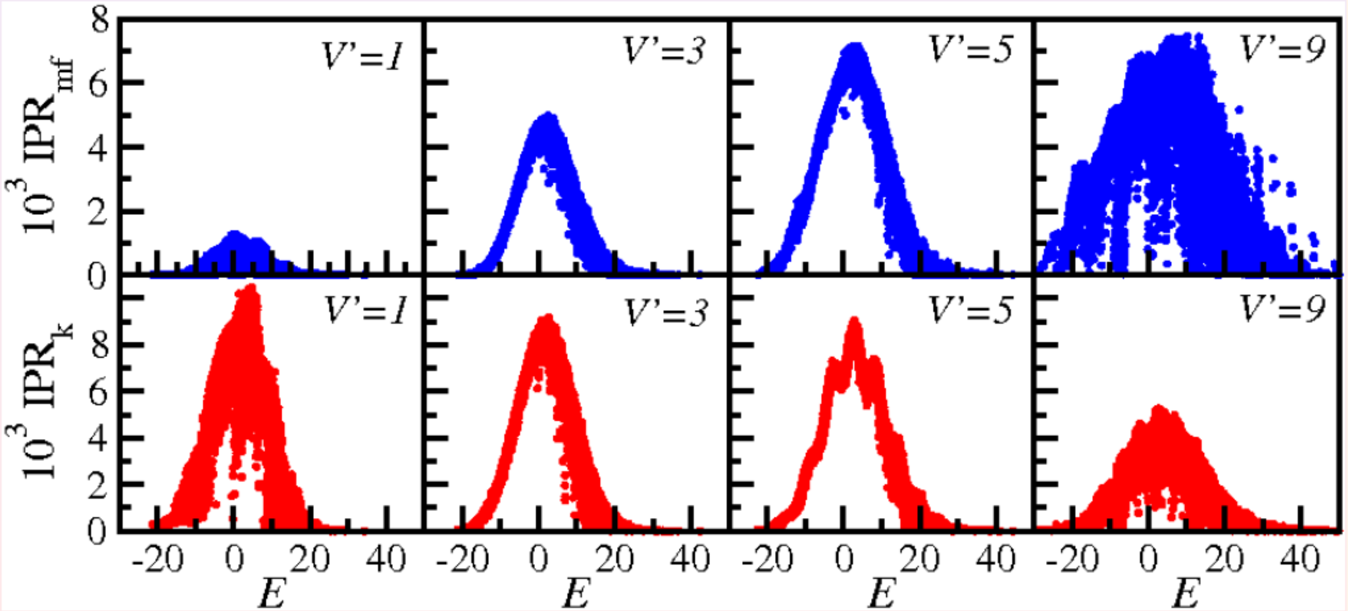
$t = 1, V = 6$

$V'_c = 3$



$L = 24,$

$N = 8$

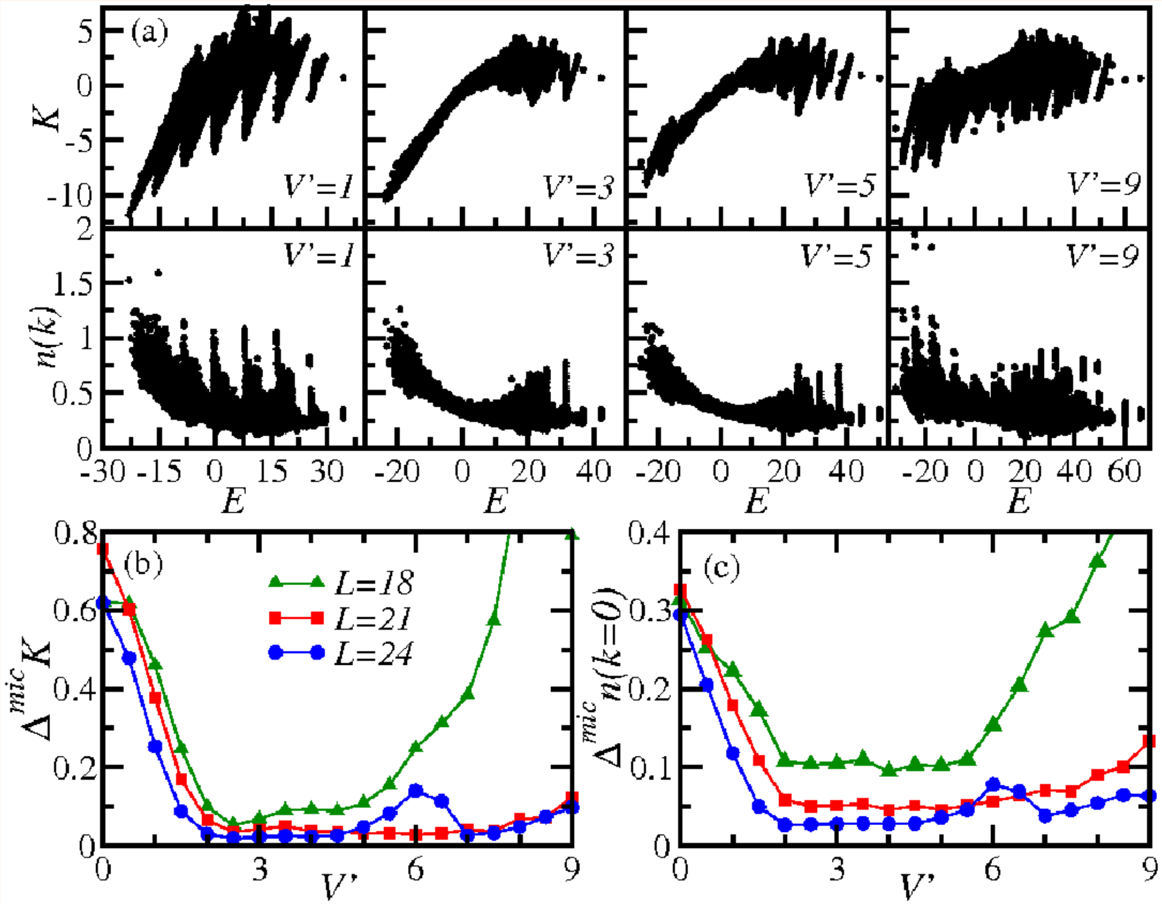


Mean-field basis: eigenstates of the integrable Hamiltonian

Momentum-basis

M. Rigol & LFS
PRA **82** 011604R (2010)

Gapped system: observables



$L = 24,$

$N = 8$

Kinetic energy:

$$K = \sum_i -t\left(b_i^+ b_{i+1} + h.c.\right)$$

Momentum distribution function:

$$n(k) = \frac{1}{L}\sum_{i,j} e^{-k(i-j)} b_i^+ b_j$$

Effective temperature: $T = 3, \Delta E = 0.1$

$$E_\alpha = \frac{1}{Z}\mathrm{Tr}\left\{\hat{H} e^{-\hat{H}/T_\alpha}\right\}$$

$$Z = \mathrm{Tr}\left(e^{-\hat{H}/k_B T}\right) \qquad k_B = 1$$

Average deviation of the EEVs with respect to the microcanonical result:

$$\Delta^{mic} n(k=0) = \frac{\sum_\alpha |n_{\alpha\alpha}(k=0) - n_{mic}(k=0)|}{\sum_\alpha n_{\alpha\alpha}(k=0)}$$

M. Rigol & LFS
PRA **82** 011604R (2010)

Quench

Fixed: *t=1,V=6*
Quench: $V'_{in} \rightarrow V'$

Initial state
Effective temperature: *T=3*

$$E_\alpha = \frac{1}{Z}\mathrm{Tr}\left\{\hat{H} e^{-\hat{H}/T_\alpha}\right\}$$

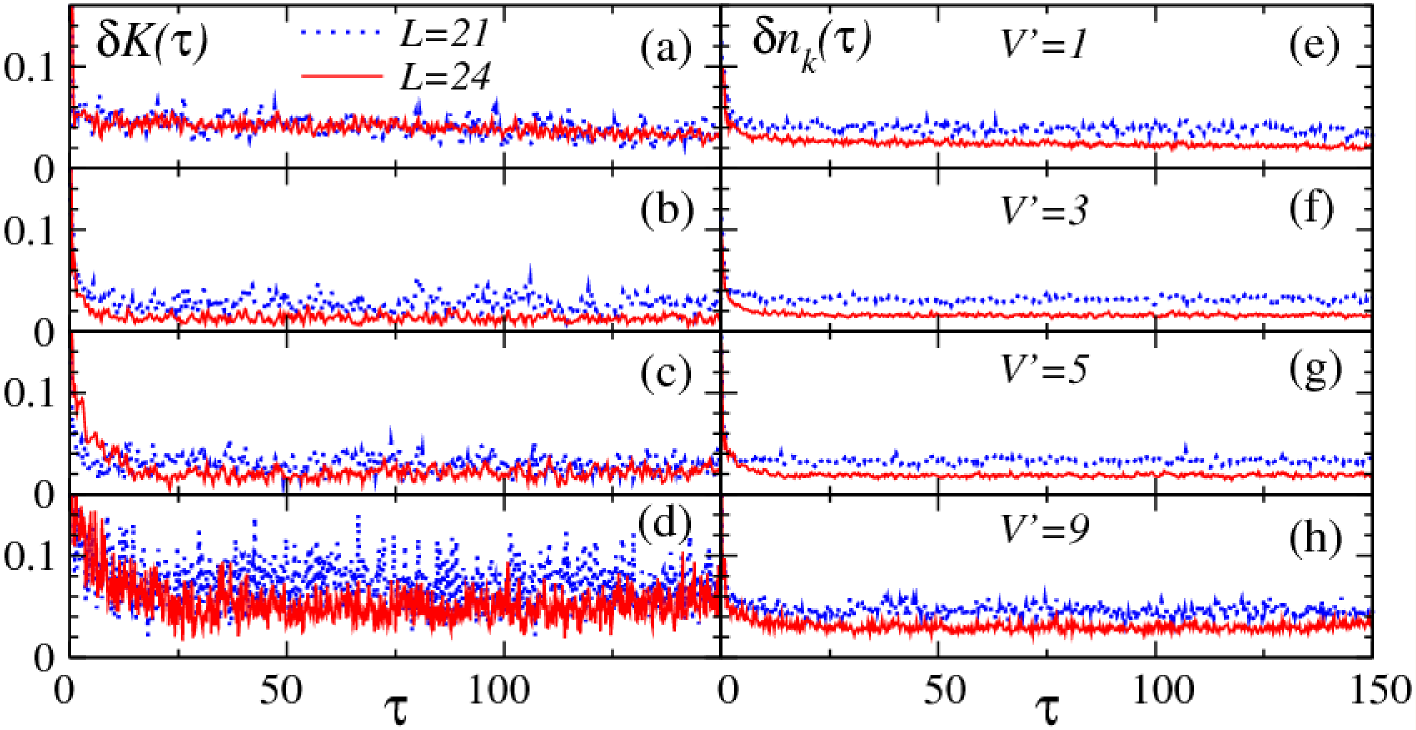
$$Z = \mathrm{Tr}\left(e^{-\hat{H}/k_B T}\right)$$

$$H_{in} = \sum_{i=1}\left[-t\left(b_i^+ b_{i+1} + h.c.\right) + V\left(n_i^b - \frac{1}{2}\right)\left(n_{i+1}^b - \frac{1}{2}\right) + V_{in}'\left(n_i^b - \frac{1}{2}\right)\left(n_{i+2}^b - \frac{1}{2}\right)\right]$$

$$H_f = \sum_{i=1}\left[-t\left(b_i^+ b_{i+1} + h.c.\right) + V\left(n_i^b - \frac{1}{2}\right)\left(n_{i+1}^b - \frac{1}{2}\right) + V'\left(n_i^b - \frac{1}{2}\right)\left(n_{i+2}^b - \frac{1}{2}\right)\right]$$

Long-time dynamics

$\delta K(\tau) = |K(\tau) - K_{\rm diag}|/|K_{\rm diag}|$ $\delta n_k(\tau) = [\sum_k |n(k,\tau) - n_{\rm diag}(k)|]/[\sum_k n_{\rm diag}(k)]$

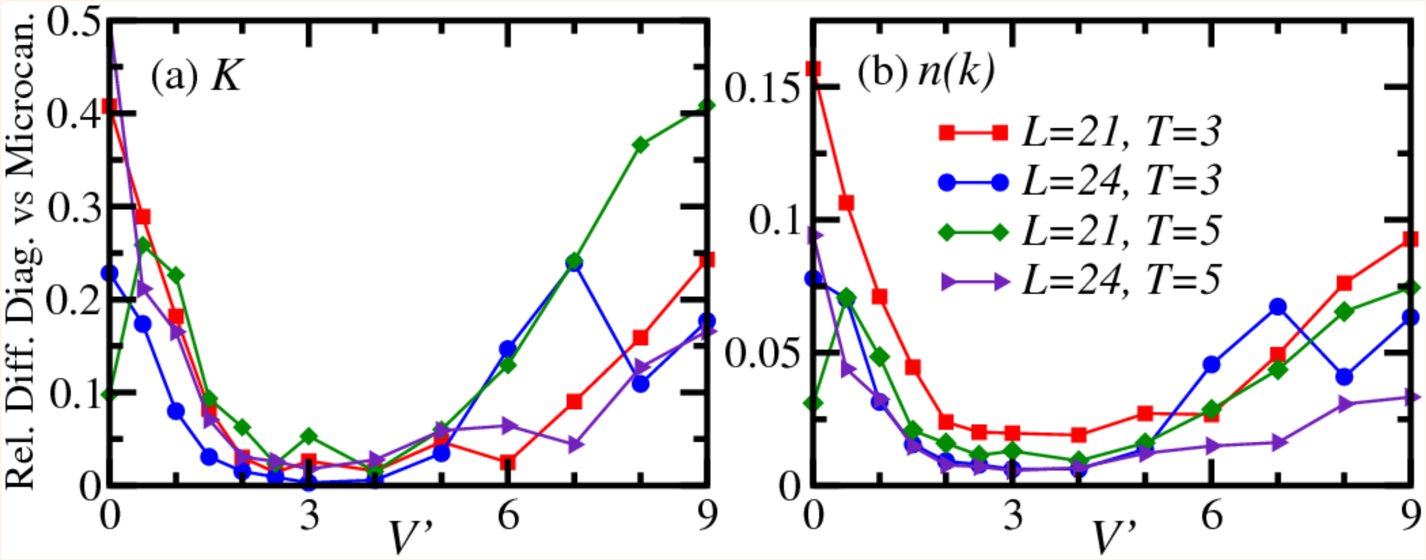


$$\overline{\langle O(\tau)\rangle} = O_{diag} = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha}$$

Average over the evolution of nine initial states selected from the eigenstates of the Hamiltonian with V'_{ini} = 0,1, … 9 (except the V' of the dynamics).

Effective temperature: *T=3* $E_\alpha = \frac{1}{Z}\mathrm{Tr}\left\{\hat{H}e^{-\hat{H}/T_\alpha}\right\}$ $Z = \mathrm{Tr}\,(e^{-\hat{H}/k_B T})$ $k_B = 1$

Time average = microcanonical



M. Rigol & LFS
PRA **82** 011604R (2010)

- Thermalization does occur in the **gapped** phase, it follows the validity of ETH
- ETH is valid in the chaotic limit, away from the edges,
  even if the ground state is an insulator
- As the system size increases, ETH becomes valid deeper into the insulating side

M. Rigol & LFS
PRA **82** 011604R (2010)

Open questions

- What happens to integrable systems?
  They relax to an equilibrium characterized by a Generalized Gibbs Ensemble

Instead of just the energy, the Gibbs exponent contains a linear combination of conserved quantities (for free hardcore bosons, integrals of motion = fermionic (quasi-)momentum distribution operators)

M. Rigol et al
PRL **98** 050405 (2007);
Cazallila, Chung, Iucci
Calabrese, Caux, Essler

- How fast does the system decay to equilibrium?

  Dependence on the initial state, observable

  System size, regime, pre-thermalization

  Gap, symmetries, disorder

Andrei, Eisler, Y. Lin,
Pollmann,
Sen, Stephan

- Transport behavior (diffusive or ballistic)
  spin diffusion

Mazur, McCoy, Zotos
Steinigeweg, Herbrych, and Prelovsek

PART II

RELAXATION

1D spin-1/2 systems

Model 1: **integrable**

$$H_1 = H_0 + \mu V_1$$

$$H_0 = \sum_{n=1}^{L-1} J(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y)$$

Unperturbed part: mean-field basis

$$V_1 = \sum_{n=1}^{L-1} J S_n^z S_{n+1}^z$$

Perturbation

Model 2: **chaotic**

$$H_2 = H_1 + \lambda V_2$$

$$H_1 = J\sum_{n=1}^{L-1}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) + J\Delta \sum_{n=1}^{L-1} S_n^z S_{n+1}^z$$

Unperturbed part: mean-field basis

$$H_2 = \sum_{n=1}^{L-1} J(S_n^x S_{n+2}^x + S_n^y S_{n+2}^y + \mu S_n^z S_{n+2}^z)$$

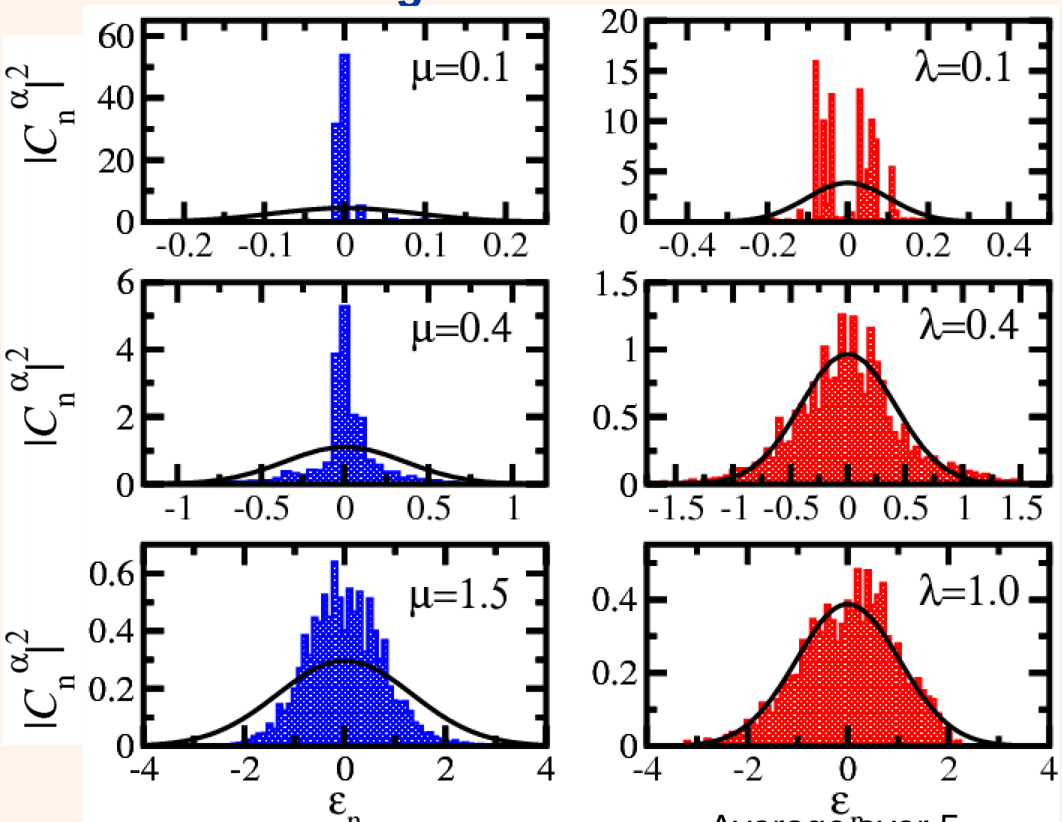
Perturbation

Open boundaries

Energy Shell and Eigenstates

Energy shell is the density of states obtained from a matrix filled only with the **off**-diagonal elements of the perturbation (maximal strength function, local density of states)

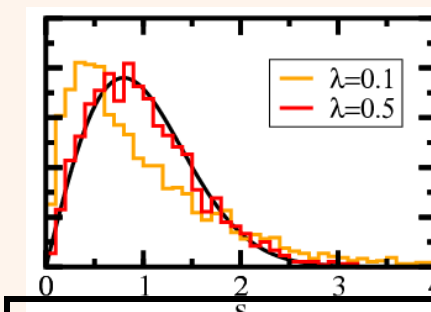
Model 1: **integrable** **Model 2**: **chaotic**



Energy shell:
Gaussian with variance

$$\sigma^2 = \sum_{n \neq m} |H_{nm}|^2$$

$$\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{-(E-\varepsilon)^2}{2\sigma^2} \right)$$



LFS, Borgonovi, Izrailev
PRL **108**, 094102 (2012)
PRE **85**, 036209 (2012)

L=15
5 spins up

Average over 5 eigenstates in the middle of the spectrum

Shannon entropy

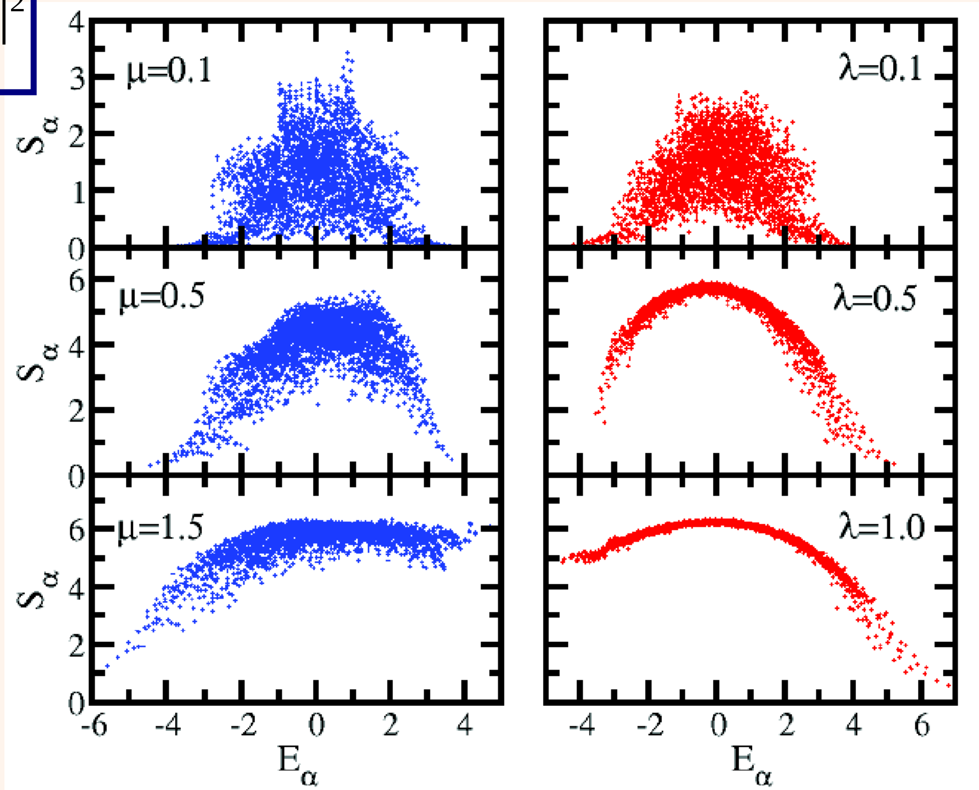
$$S_\alpha = -\sum_{n=1}^{D} |C_n^\alpha|^2 \ln |C_n^\alpha|^2$$

$$|\alpha\rangle = \sum_{n=1}^{D} C_n^\alpha |n\rangle$$

Average over 5 eigenstates in the middle of the spectrum

L=15
5 spins up

Model 1: integrable **Model 2**: chaotic



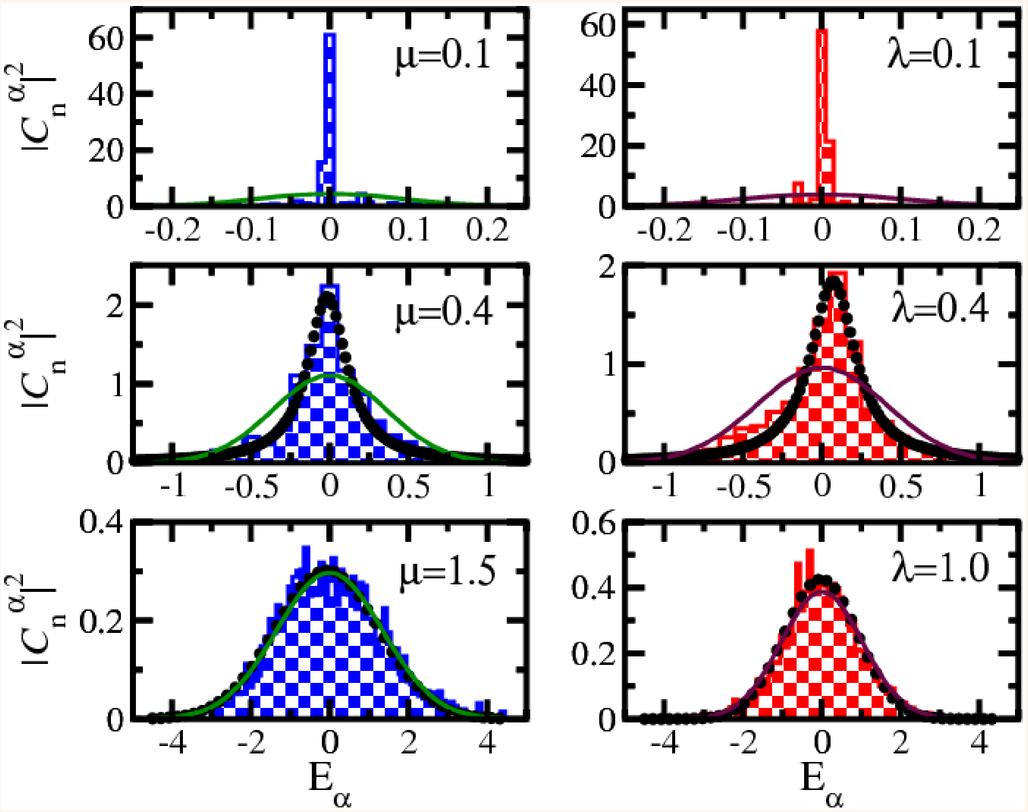
$$IPR_\alpha \equiv \frac{1}{\sum_{n=1}^{D} |C_n^\alpha|^4}$$

LFS, Borgonovi, Izrailev
PRL **108**, 094102 (2012)
PRE **85**, 036209 (2012)

Energy Shell and Strength Functions

Energy shell is the density of states obtained from a matrix filled only with the **off**-diagonal elements of the perturbation (maximal strength function, local density of states)

Model 1: **integrable** **Model 2**: **chaotic**



Energy shell:
Gaussian with variance

$$\sigma^2 = \sum_{n \neq m} |H_{nm}|^2$$

Average over 5 basis states in the middle of the spectrum

L=15
5 spins up

LFS, Borgonovi, Izrailev
PRL **108**, 094102 (2012)
PRE **85**, 036209 (2012)

Relaxation

$$S_\alpha = -\sum_{n=1}^{D} |C_n^\alpha|^2 \ln |C_n^\alpha|^2$$

Initial state: unperturbed state from the middle of the spectrum

- Circles: numerical data
- Solid line: semi-analytical result

$$S_{n_0}(t) = -W_{n_0}(t)\ln W_{n_0}(t) - [1-W_{n_0}(t)]\ln\left(\frac{1-W_{n_0}(t)}{N_{pc}}\right)$$

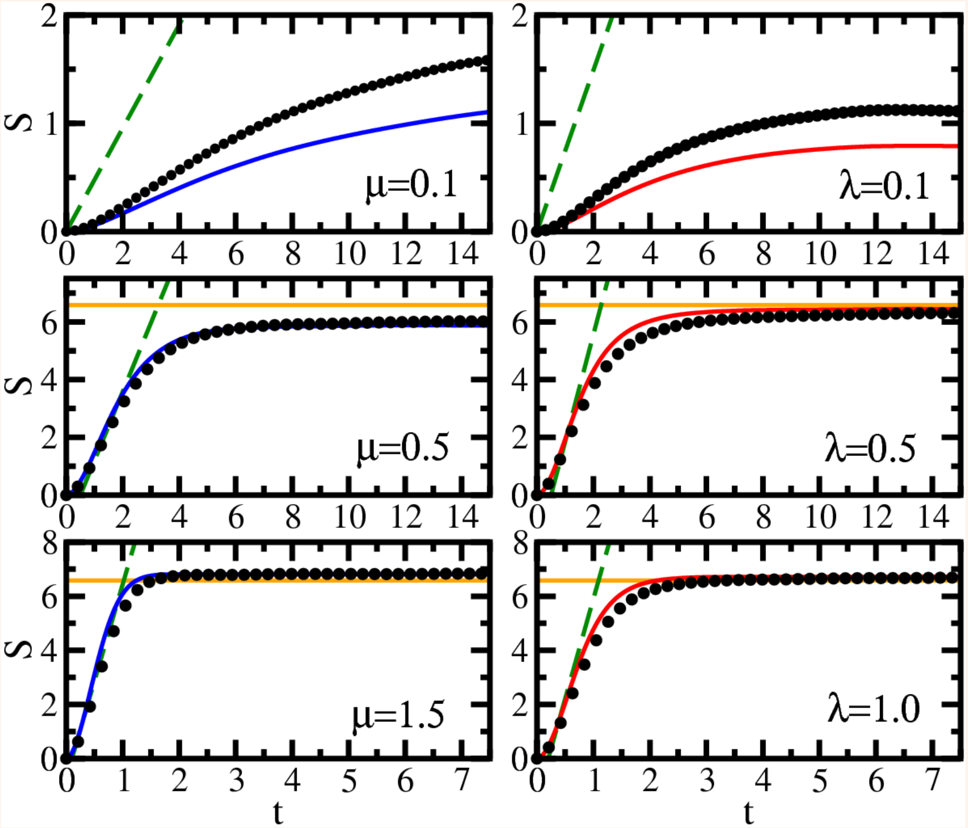
- Dashed line:

$$S_{n_0}(t) \approx \sigma_{n_0} t \ln M_{n_0}$$

$$\sigma^2 = \sum_{n\neq m} |H_{nm}|^2$$

Connectivity

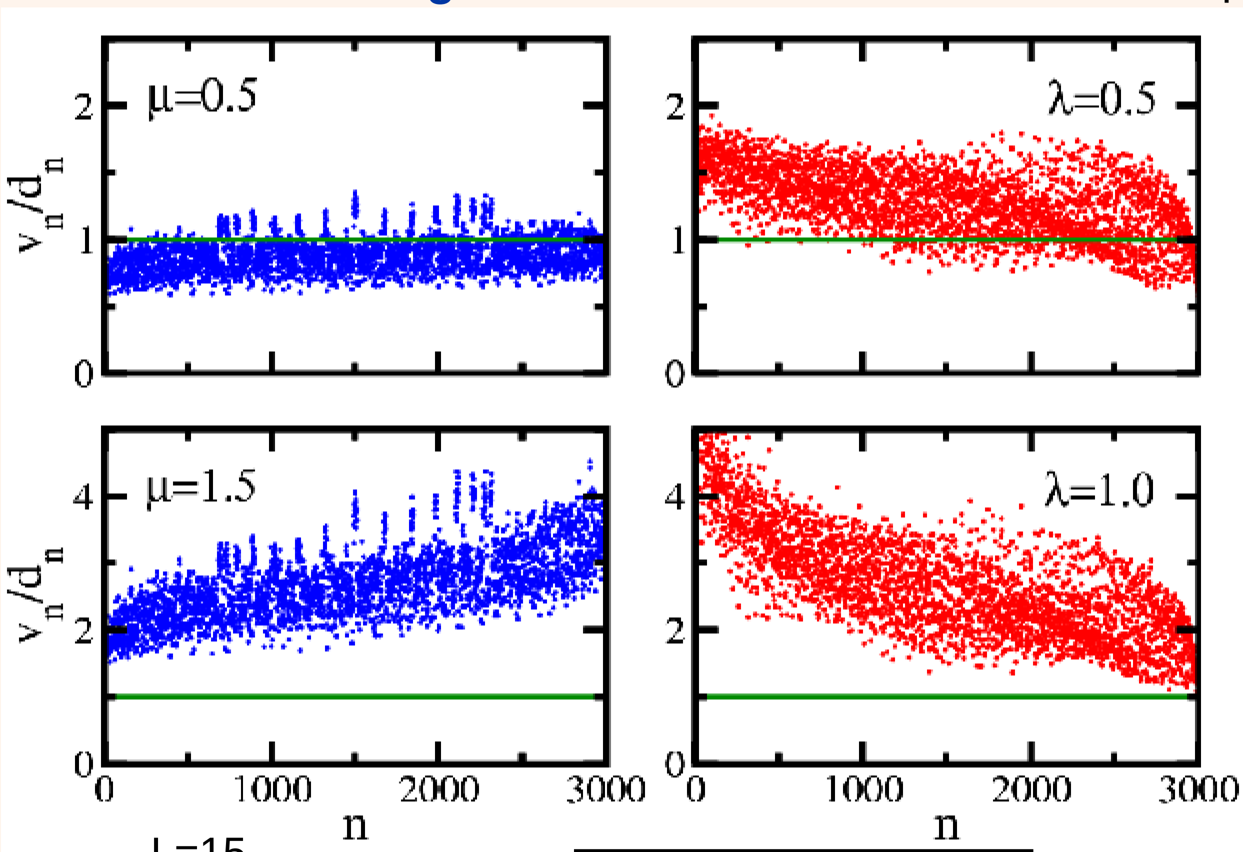
Model 1: integrable **Model 2**: chaotic

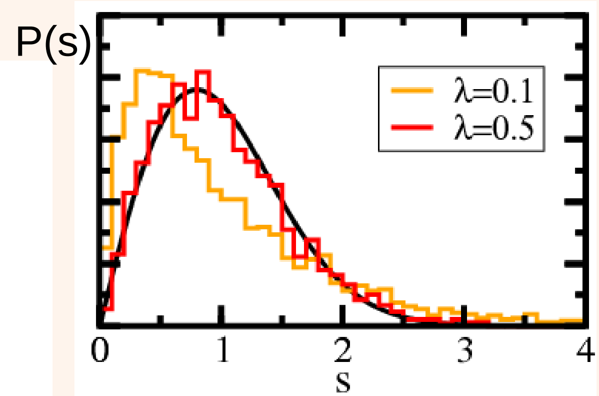


L=15
5 spins up

Coupling strength vs mean level spacing

Model 1: **integrable** **Model 2**: **chaotic**





Average coupling strength

$$v_n = \sum_{m \neq n} | H_{nm} | / M_n$$

mean level spacing
between directly coupled states
for each line n

$$d_n = (\varepsilon_n^{\max} - \varepsilon_n^{\min}) / M_n$$

L=15
5 spins up

LFS, Borgonovi, Izrailev
PRL **108**, 094102 (2012)
PRE **85**, 036209 (2012)

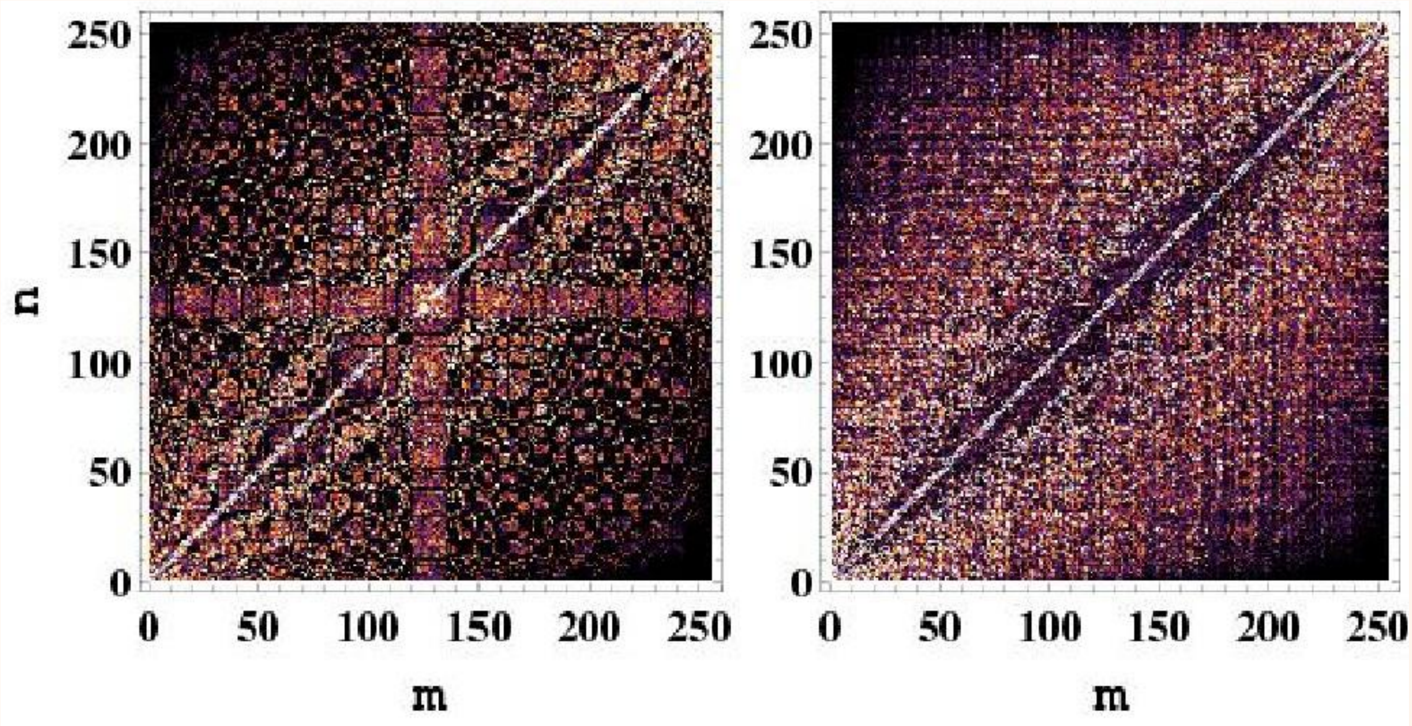
Structure of the Hamiltonian

Model 1:
More zeros (sparse)
More correlations

L=12
4 spins up
even states

Model 1: **integrable** $\mu = 0.5$

Model 2: **chaotic** $\lambda = 0.5$

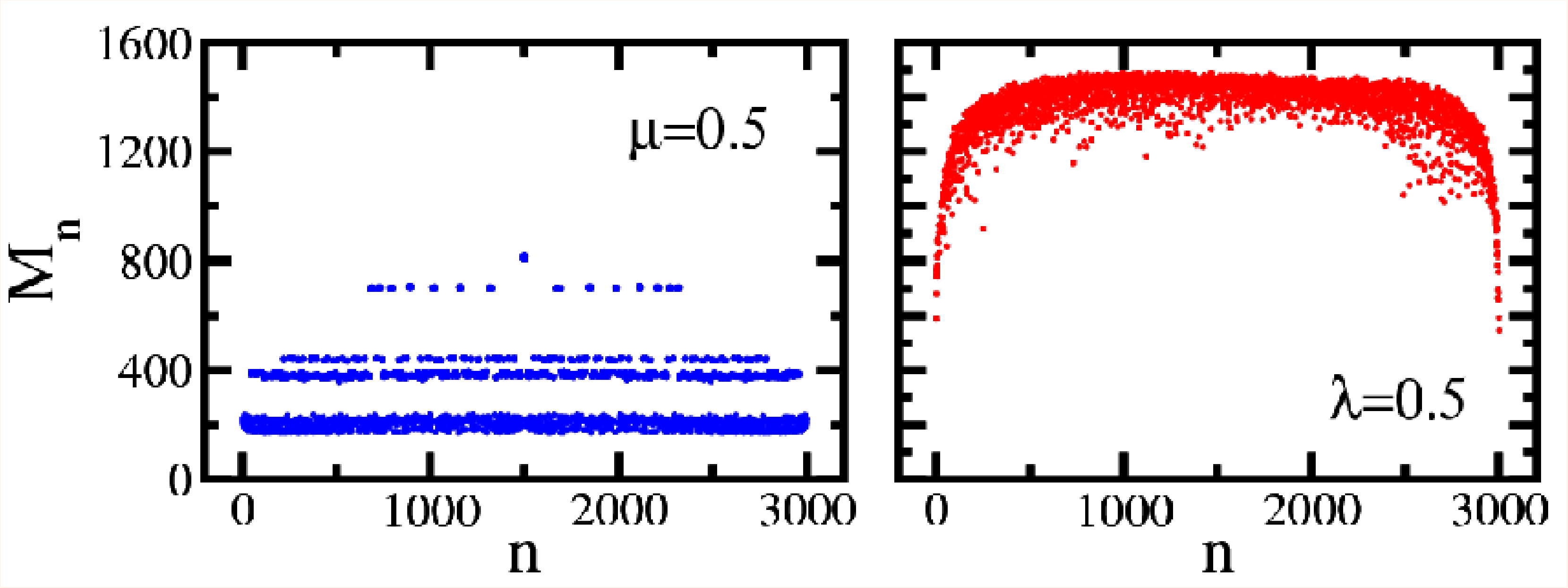


Density plot
Light colors= larger values

Lea F. Santos, Yeshiva University

Connectivity

Model 1: **integrable** **Model 2**: **chaotic**



Model 1:
More sparse
Structure

L=15
5 spins up

Summary of the results for the relaxation process

• Integrable systems, contrary to chaotic systems:

eigenstates are **not** completely delocalized in the **energy shell** (larger fluctuations of delocalization measures, contradicts ETH)

but they are also very delocalized

• Strength functions (initial states) for both regimes are Gaussian and lead to very similar relaxation processes.

• Much information is obtained even **before diagonalization**, by studying the Hamiltonian matrix.

LFS, Borgonovi, Izrailev
PRL **108**, 094102 (2012)
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PART III

ENTROPY

Diagonal entropy

- We need an entropy that can describe the new equilibrium the system will reach

$$|\Psi(0)\rangle = \sum_n C_n |\psi_n\rangle \Rightarrow \rho_{nn} = |C_n|^2$$

$$O_{diag} = \sum_n |C_n|^2 O_{nn} = \sum_n \rho_{nn} O_{nn}$$

$$S_d = -Tr(\rho_{diag} \ln \rho_{diag})$$

A. Polkovnikov
Ann. Phys.**326**, 486 (2011)

$|C_n|^2$ are the diagonal elements of $\rho(\tau) = |\Psi(\tau)\rangle\langle\Psi(\tau)|$ in the energy representation

Entropy of the diagonal ensemble:

$$S_d = -\sum_n |C_n|^2 \ln |C_n|^2 = -\sum_n \rho_{nn} \ln \rho_{nn}$$

In the chaotic domain:

- Diagonal entropy is a thermodynamic entropy, it is determined by the energy of the system only;

LFS, A. Polkovnikov, M. Rigol
PRL **107**, 040601 (2011)

- Entropy from a microscopic theory leads to thermodynamic relations.

$$dE = TdS - Fdx$$

x external parameter

F:generalized force describing the adiabatic response of the system

Smooth part of the diagonal entropy

$$\rho_{nn} = |C_n|^2$$

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

$$S_d = S_{smooth} + S_{fluctuating}$$

$$\begin{cases} S_{smooth} = \sum_n \rho_{nn} \overbrace{\ln[\eta(E_n)\delta E]}^{S_{th}} \\ S_{fluctuating} = -\sum_n \rho_{nn} \ln[\rho_{nn}\eta(E_n)\delta E] \end{cases}$$

$\eta(E) = \sum_n \delta(E - E_n)$ is the density of states

$\delta E^2 = \sum_n \rho_{nn}(E_n - E_{ini})^2$ is the energy variance

- When the distribution of $\rho_{nn} = |C_n|^2$ in energy becomes smooth,
  S_{fluct} becomes negligible and
  S_{smooth} coincides with the thermodynamic entropy S_{th}

chaotic systems

$$S_d \approx S_{smooth} \approx S_{th}$$

System Model

Hardcore bosons in 1D:

$\hbar = 1$

$$H = \sum_{i=1} \left[-t\left(b_i^+ b_{i+1} + h.c.\right) + V\left(n_i^b - \frac{1}{2}\right)\left(n_{i+1}^b - \frac{1}{2}\right) - t'\left(b_i^+ b_{i+2} + h.c.\right) + V'\left(n_i^b - \frac{1}{2}\right)\left(n_{i+2}^b - \frac{1}{2}\right) \right]$$

$$n_i^b = b_i^+ b_{i+1}$$

$t', V' = 0$ system is integrable

$t', V' > 0$ system may become chaotic

Periodic: conservation of total momentum *k*

(diagonalization for each *k*-sector)

Quench

Fixed: t', V'
Quench: $t_{ini}, V_{ini} \rightarrow t = V = 1$

$t', V' = 0$ system is integrable

$t', V' > 0$ system may be chaotic

$$H_{in} = \sum_{i=1} \left[\begin{array}{l} -t_{in} \left(b_i^+ b_{i+1} + h.c. \right) + V_{in} \left(n_i^b - \frac{1}{2} \right) \left(n_{i+1}^b - \frac{1}{2} \right) \\ -t' \left(b_i^+ b_{i+2} + h.c. \right) + V' \left(n_i^b - \frac{1}{2} \right) \left(n_{i+2}^b - \frac{1}{2} \right) \end{array} \right]$$

$$H_f = \sum_{i=1} \left[\begin{array}{l} -t_f \left(b_i^+ b_{i+1} + h.c. \right) + V_f \left(n_i^b - \frac{1}{2} \right) \left(n_{i+1}^b - \frac{1}{2} \right) \\ -t' \left(b_i^+ b_{i+2} + h.c. \right) + V' \left(n_i^b - \frac{1}{2} \right) \left(n_{i+2}^b - \frac{1}{2} \right) \end{array} \right]$$

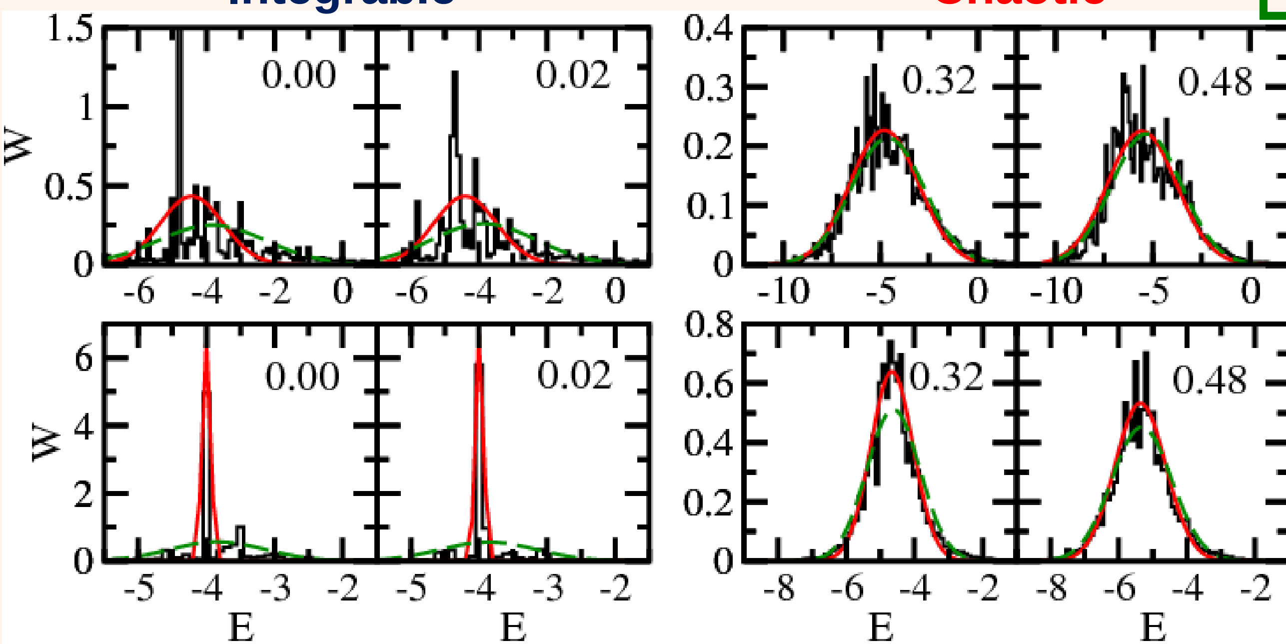
Distribution Function of Energy: Gaussian

$$\rho_{nn} = |C_n|^2 \qquad W(E) = \sum_n \rho_{nn}\delta(E - E_n)$$

green dashed line:

$$\exp\left(\frac{-(E - E_{ini})^2}{2\delta E^2}\right) / \sqrt{2\pi}\delta E$$

Integrable **Chaotic**



$$\delta E^2 = \sum_n \rho_{nn}(E_n - E_{ini})^2$$

energy variance

$$t_{ini} = 0.5, V_{ini} = 2.0$$

$$t_{ini} = 2.0, V_{ini} = 0.5$$

L=24
8 particles

$$E = Z^{-1}\sum_n E_n e^{-E_n/T}$$

Bosons, T=4

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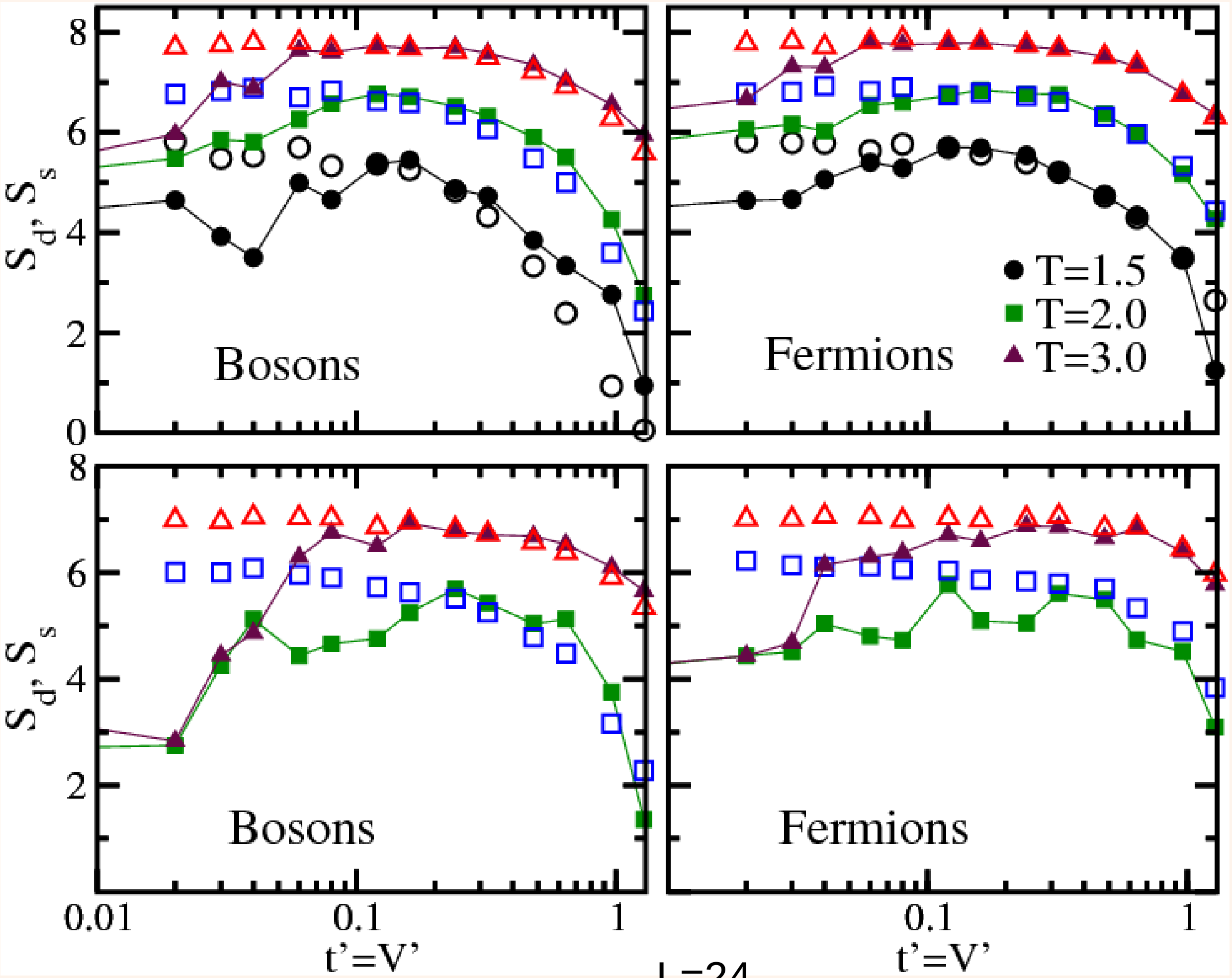
PRL **107**, 040601 (2011)

Diagonal Entropy and Chaos



$t_{ini} = 0.5, V_{ini} = 2.0$

Filled: $S_{diagonal}$
Empty: S_{smooth}

$E = Z^{-1} \sum_n E_n e^{-E_n/T}$

$t_{ini} = 2.0, V_{ini} = 0.5$

Results improve with temperature and **system size**

L=24
8 particles

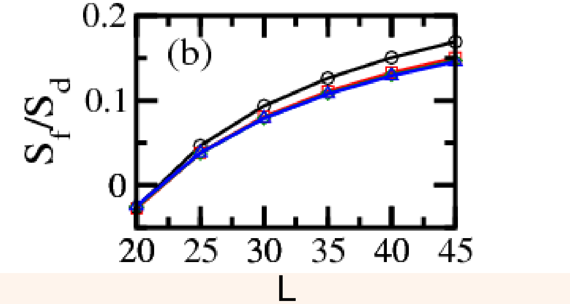
LFS, A. Polkovnikov, M. Rigol
PRL **107**, 040601 (2011)

Integrable regime

1D HCB model with NN hopping ,
an external potential, and OPEN BOUNDARIES

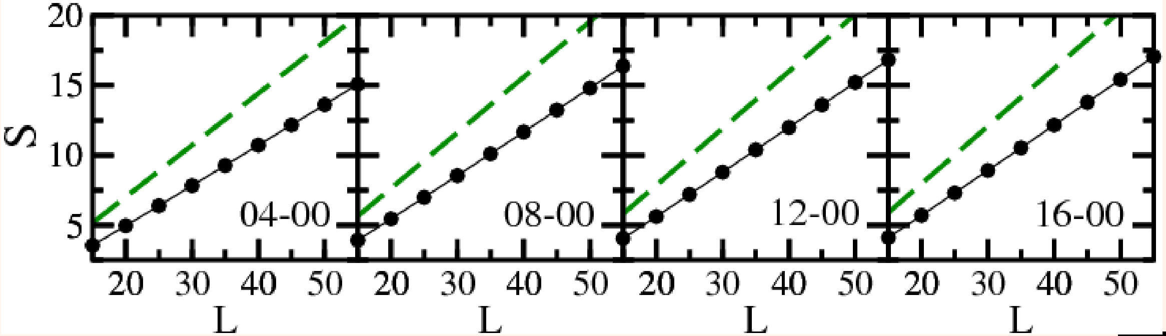
$$H_S = -t\sum_{j=1}^{L-1}(b_j^\dagger b_{j+1} + \text{H.c.}) + A\sum_{j=1}^{L}\cos\left(\frac{2\pi j}{P}\right)b_j^\dagger b_j$$

- S_d is not equivalent to the thermodynamic entropy,
  S_{fluct}/S_d does not decrease with system size (L)



Quench: A from 4, 8, 12, 16 to 0
Period P=5
t=1
1/5 filling

- S_d does not coincide with S_{GGE}.



Green: S_{GGE}
Black: S_d

LFS, A. Polkovnikov, M. Rigol
PRL **107**, 040601 (2011)

PART III.b

TRACE OUT
PART OF THE SYSTEM

Typicality

Tasaki, PRL **80**, 1373 (1998);
Popescu et al, Nature Phys. **2,** 754 (2006);
Goldstein et al, PRL **96,** 050403 (2006).

Canonical typicality:
Reduced density matrix of a subsystem of most pure states of many-particle systems is canonical.

$$\rho_\beta = \frac{1}{Z}\exp(-\beta H^{(S)})$$

- How much do we need to trace out in a finite system?
- Which quantities are more or less affected?

What we see…

- Grand-canonical entropy and diagonal entropy are close after the removal of **few sites.**

WEAK TYPICALITY

- The von Neumann entropy should approach the other two after tracing out **many sites.**

STRONG TYPICALITY
additional information

- **Observables**: reduced density matrix, diagonal ensemble, and grand-canonical ensemble give similar results which improve with system size.

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PRE **86** 010102(R) (2012)

Entropies: what to expect?

Composite system $S+\mathcal{E}$ in a pure state $\rho = |\Psi\rangle\langle\Psi|$

- Grand-canonical entropy:

$$S_{GC} = \ln \Xi + \frac{E_S - \mu N_S}{T_{GC}}$$

Grand-partition function
$\Xi = \sum_n e^{(\mu N_n - E_n)/T_{GC}}$
μ: chemical potential

Es,Ns: average energy and number of particles in the remaining system

- Reduced von Neumann entropy

$$S_{vN} \equiv -Tr_S[\rho_S \ln \rho_S] = -Tr_{\varepsilon}[\rho_{\varepsilon} \ln \rho_{\varepsilon}]$$

$$\rho_S = Tr_{\varepsilon}[\rho] \qquad \rho_{\varepsilon} = Tr_S[\rho]$$

Minimum S_{vN}=0 (separable states)

Maximum S_{vN}=ln D (D: dimension of smallest subsystem)

- Diagonal entropy

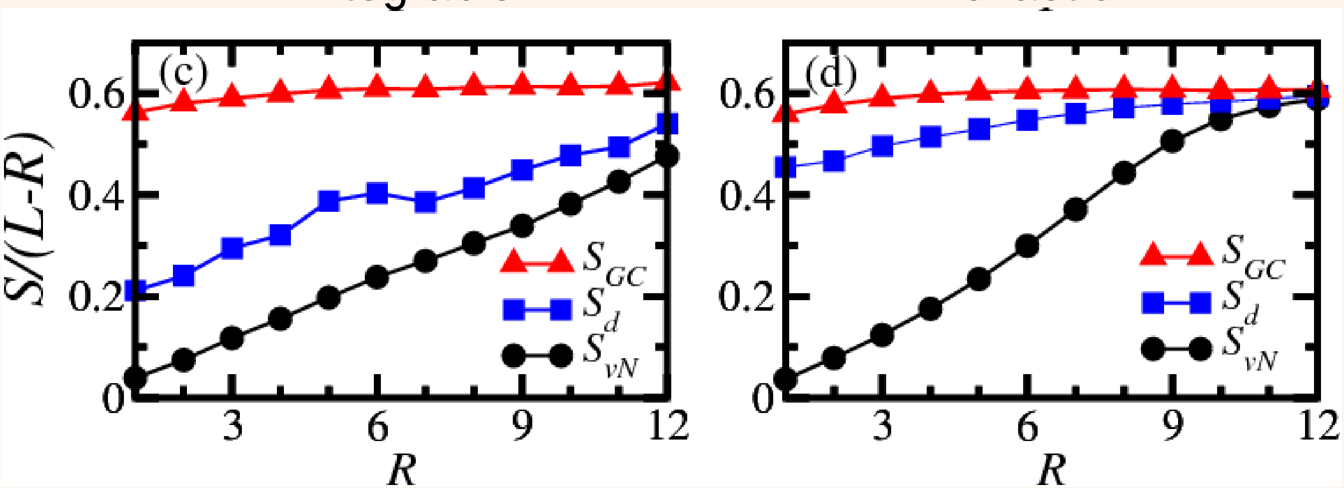
$$S_d = -\sum_n \rho_{nn} \ln \rho_{nn}$$

S_d counts logarithmically the number of energy eigenstates which are occupied.

Entropies vs Number of Sites Traced out

$t', V' = 0.00$ integrable

$t', V' = 0.32$ chaotic



R = number of sites traced out

L=18; 6 particles; T=4

Chaotic region: diagonal part of the density matrix of the reduced system in the energy eigenbasis exhibits a thermal structure

$$S_{\rm vN} \equiv -{\rm Tr}_{\mathcal{S}}\left[\hat{\rho}_{\mathcal{S}} \ln \hat{\rho}_{\mathcal{S}}\right] \equiv -{\rm Tr}_{\mathcal{E}}\left[\hat{\rho}_{\mathcal{E}} \ln \hat{\rho}_{\mathcal{E}}\right]$$

$$S_d \equiv -\sum \rho_{nn} \ln(\rho_{nn}),$$

$$S_{\rm GC} = \ln \Xi + \frac{E_{\mathcal{S}} - \mu N_{\mathcal{S}}}{T_{\rm GC}}$$

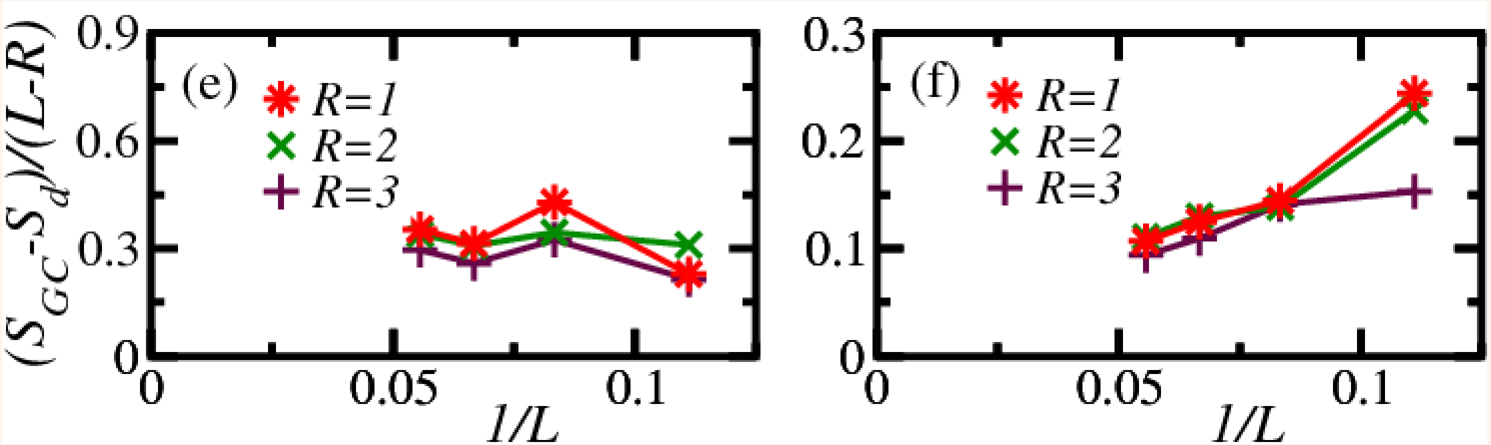
$$\Xi = \sum_n e^{(\mu N_n - E_n)/T_{\rm GC}}$$

$E_{\mathcal{S}} = {\rm Tr}[\hat{H}_{\mathcal{S}} \hat{\rho}_{\mathcal{S}}]$ and $N_{\mathcal{S}} = {\rm Tr}[\hat{N}_{\mathcal{S}} \hat{\rho}_{\mathcal{S}}]$

Entropies vs system size

$t', V' = 0.00$ integrable

$t', V' = 0.32$ chaotic



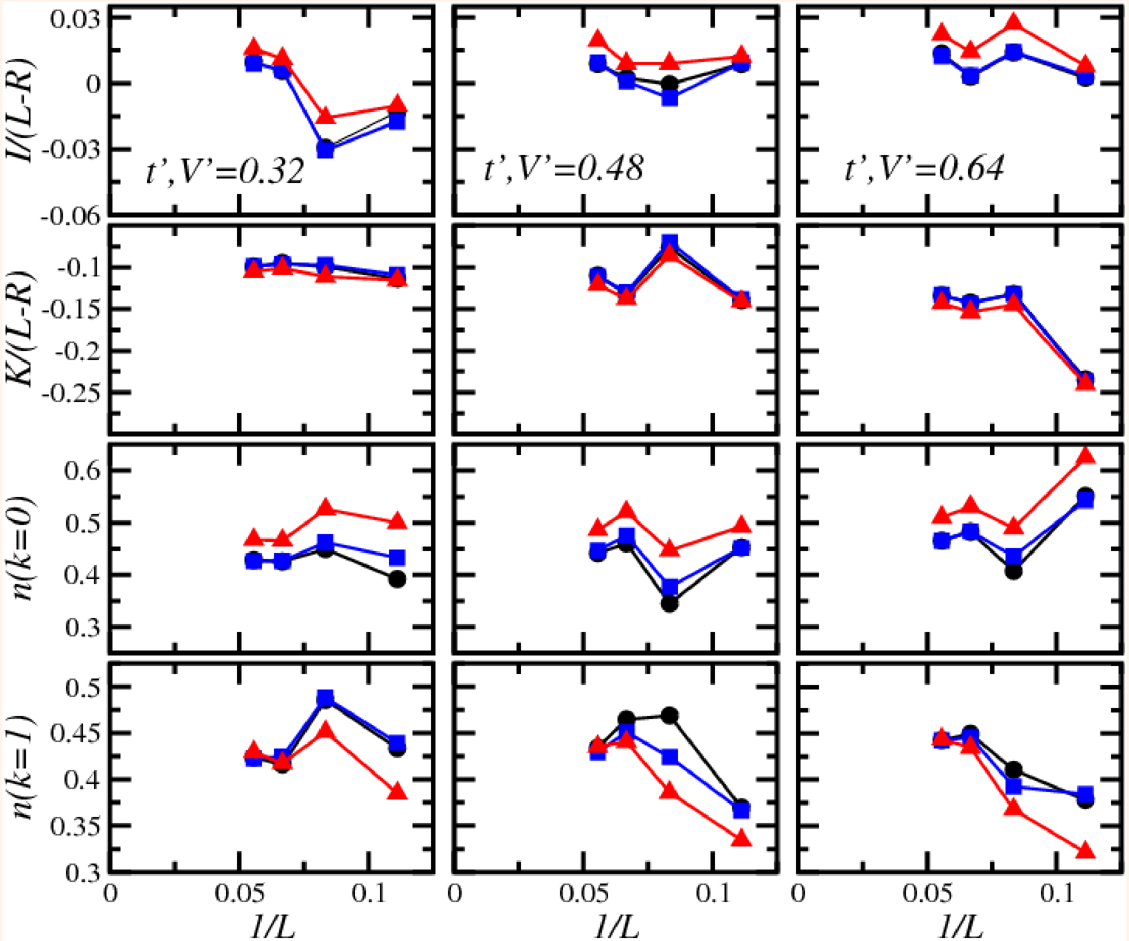
R =number of sites traced out

Chaotic region: the results indicate that in thermodynamic limit S_{GC} and S_d coincide even when just one site is cut

L/3 particles; T=4

LFS, M. Rigol, A. Polkovnikov
PRE **86** 010102(R) (2012)

Observables in the chaotic domain



Tracing out and cutting off and waiting for equilibrium lead to the same results.

Is there any physical observable that could detect this extra information?

Momentum distribution function:

$$n(k) = \frac{1}{L} \sum_{i,j} e^{-k(i-j)} b_i^{+} b_j$$

T=5; R=L/3

Conclusion: typicality

- From a pure state, **traced out** some sites of the lattice:

  Few sites removed: **diagona**l entropy **= canonical** entropy
  (weak typicality)

  Many sites removed: von Neumann = diagonal = canonical entropy
  (strong typicality)

  Observables coincide for the **three cases**, irrespective of how many sites are traced out.
  (reduced density matrix contains irrelevant information)

  Diagonal ensemble describes physical observables.

Conclusion

- Thermalization of isolated quantum many-body systems occurs
  in the chaotic regime away from the edges of the spectrum

- Structure of eigenstates and initial state play an important role (energy shell).

- Information about what to expect is contained in the Hamiltonian before diagonalization.

- Diagonal entropy = thermodynamic entropy in the chaotic regime.
  Entropy from a microscopic theory leads to thermodynamic relations

- There are several open question
  relaxation: how fast, initial state, metastable/pre-thermalization, time scale
  integrable domain, observable, scaling analysis

Thank you!