Entropy and typicality

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Isolated system

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

Open system

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

Diagonal entropy
(Shannon entropy in a specific basis)

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

Similarities with studies of thermalization and entropies by the quantum chaos community: Izrailev, Flambaum, Horoi, Zelevinsky

Zelevinsky et al, Phys. Rep. **276**, 85 (1996)
Flambaum & Izrailev, PRE **56**, 5144 (1997)

PART I

ISOLATED SYSTEM

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

Shannon entropy

$$|\alpha\rangle = \sum_n a_n |n\rangle \Rightarrow S_{hannon} = -\sum_n |a_n|^2 \ln |a_n|^2$$

<u>*Our work about isolated system*</u>

$$H_{in}, \phi_k \xrightarrow{\text{quench}} H_f, \psi_n$$

$$\Psi(0) = \phi_{in} = \sum C_n \psi_n$$

$$S_{hannon}^{\phi(\psi)} = -\sum_n |C_n|^2 \ln |C_n|^2 \xrightarrow{\textbf{chaotic}} S_{th} \propto \ln \eta(E_\psi)$$

$$H_0, \phi_k$$

<u>*Quantum chaos community*</u>

$$H, \psi_n$$

$$\psi_n = \sum A_k^n \phi_k$$

$$S_{th} \propto \ln \eta(E_\phi) \xleftarrow{\textbf{chaotic}} S_{hannon}^{\psi(\phi)} = -\sum_k |A_k|^2 \ln |A_k|^2$$

Chaotic regime: thermodynamic relations

In the chaotic domain:

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

$$S_{\phi} = S_{d} \rightarrow S_{th} \propto \ln \eta(E)$$

- Quantum chaos community.

$$S_{\psi} \rightarrow S_{th} \propto \ln \eta(E)$$

Zelevinsky et al, Phys. Rep. **276**, 85 (1996)
Flambaum & Izrailev, PRE **56**, 5144 (1997)
(occupation number of single particle states: FD, BE distributions)

- 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

Diagonal ensemble and diagonal entropy

Isolated system out of equilibrium
The **von Neumann entropy is conserved** for any process in an isolated system

Initial state: $|\Psi(0)\rangle = \sum_n C_n |\psi_n\rangle$

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

Time evolution of a generic observable:

$$\langle O(\tau)\rangle = \langle \Psi(\tau)|O|\Psi(\tau)\rangle = \sum_{n,m} C_n^* C_m e^{i(E_n - E_m)\tau} O_{nm} \qquad O_{nm} = \langle \psi_n | O | \psi_m \rangle$$

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

$$\overline{\langle O(\tau)\rangle} = O_{diag} = \sum_n |C_n|^2 \, O_{nn}$$

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

$$S_d = \rho_d \ln \rho_d \rightarrow S_{hannon} = -\sum_n |C_n|^2 \ln |C_n|^2$$

Entropy of the diagonal ensemble:

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

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

Diagonal entropy: thermodynamic entropy

The diagonal entropy is a proper definition of thermodynamic entropy for quantum systems out of equilibrium

It satisfies the properties of a thermodynamic entropy:

- it is uniquely related to the energy distribution
- it is additive
- it is conserved for adiabatic processes,

The diagonal entropy is consistent with the second law of thermodynamics:

- it increases when is taken out of equilibrium,

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

Entropy of the diagonal ensemble:

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

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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

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

Smooth part of the diagonal entropy

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

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

$$\begin{cases} S_{smooth} = \int dE W(E) S_{th}(E) \\ S_{fluctuating} = -\int dE W(E) \ln[W(E)\delta E] \end{cases}$$

energy dispersion (δE)

$$W(E) = \sum_n \rho_{nn} \delta(E - E_n)$$ is the energy distribution

- When *W(E)* is narrow on the scale of changes of the equilibrium entropy: $S_{smooth} \approx S_{th} = \ln[\eta(E)\delta E]$ (δE is subextensive)
- If *W(E)* is a smooth function of *E*: $S_{fluctuating}$ is subextensive

} **chaotic systems**

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

System Model

Hardcore bosons in 1D:

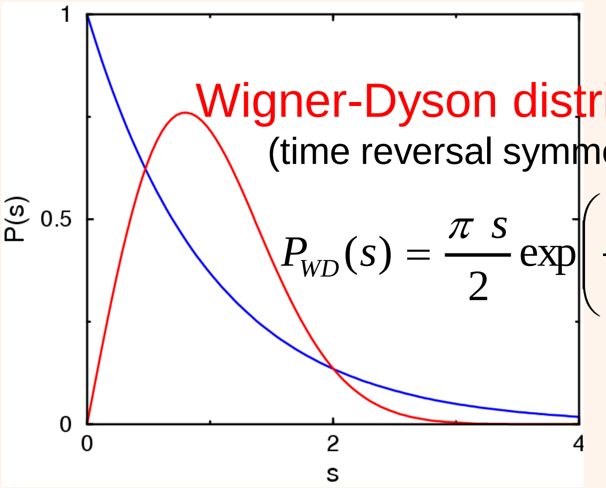
$$\hbar = 1$$

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

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

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

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



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

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

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

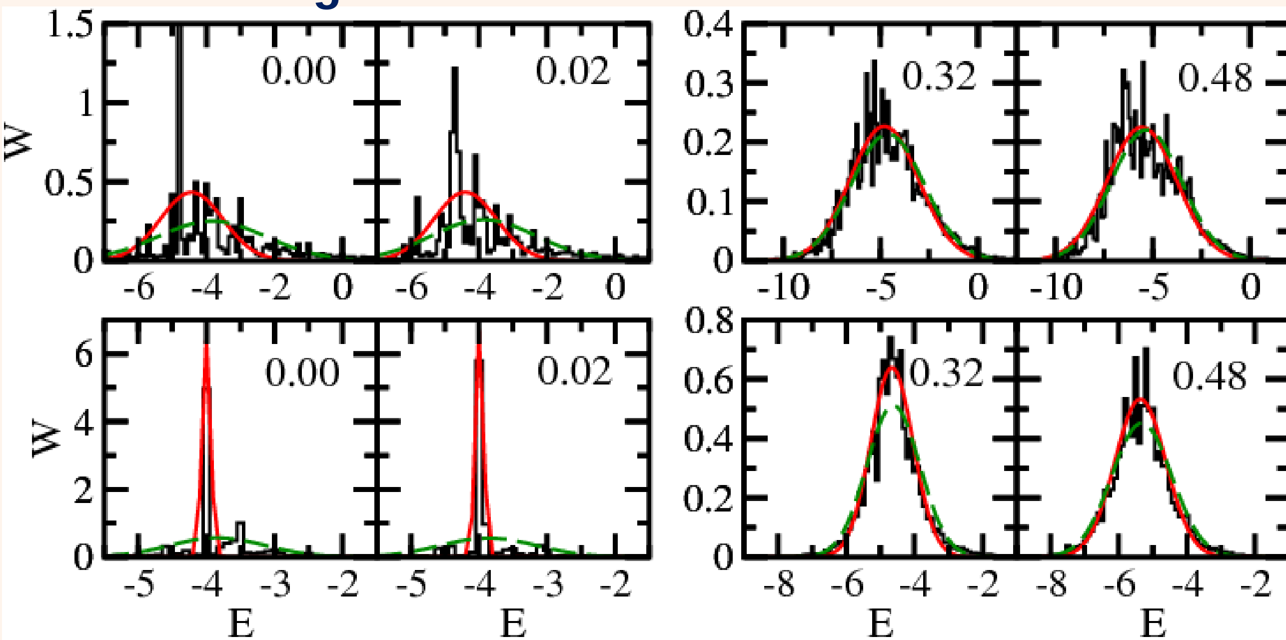
$$H_{f} = \sum_{i=1} \left[\begin{array}{l} -t_{f} \left(b_i^+ b_{i+1} + h.c. \right) + V_{f} \left(n_i^b - \frac{1}{2} \right) \left(n_{i+1}^b - \frac{1}{2} \right) \\ - t' \left(b_i^+ b_{i+2} + h.c. \right) + V' \left(n_i^b - \frac{1}{2} \right) \left(n_{i+2}^b - \frac{1}{2} \right) \end{array} \right]$$

Distribution Function of Energy: Gaussian

$$W(E) = \sum_n \rho_{nn} \delta(E - E_n)$$

$$S_{smooth} = \int dE W(E) S_{micro}(E)$$
$$S_{fluctuating} = -\int dE W(E) \ln[W(E)\delta E]$$

Integrable **Chaotic**



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

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

green dashed line:

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

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

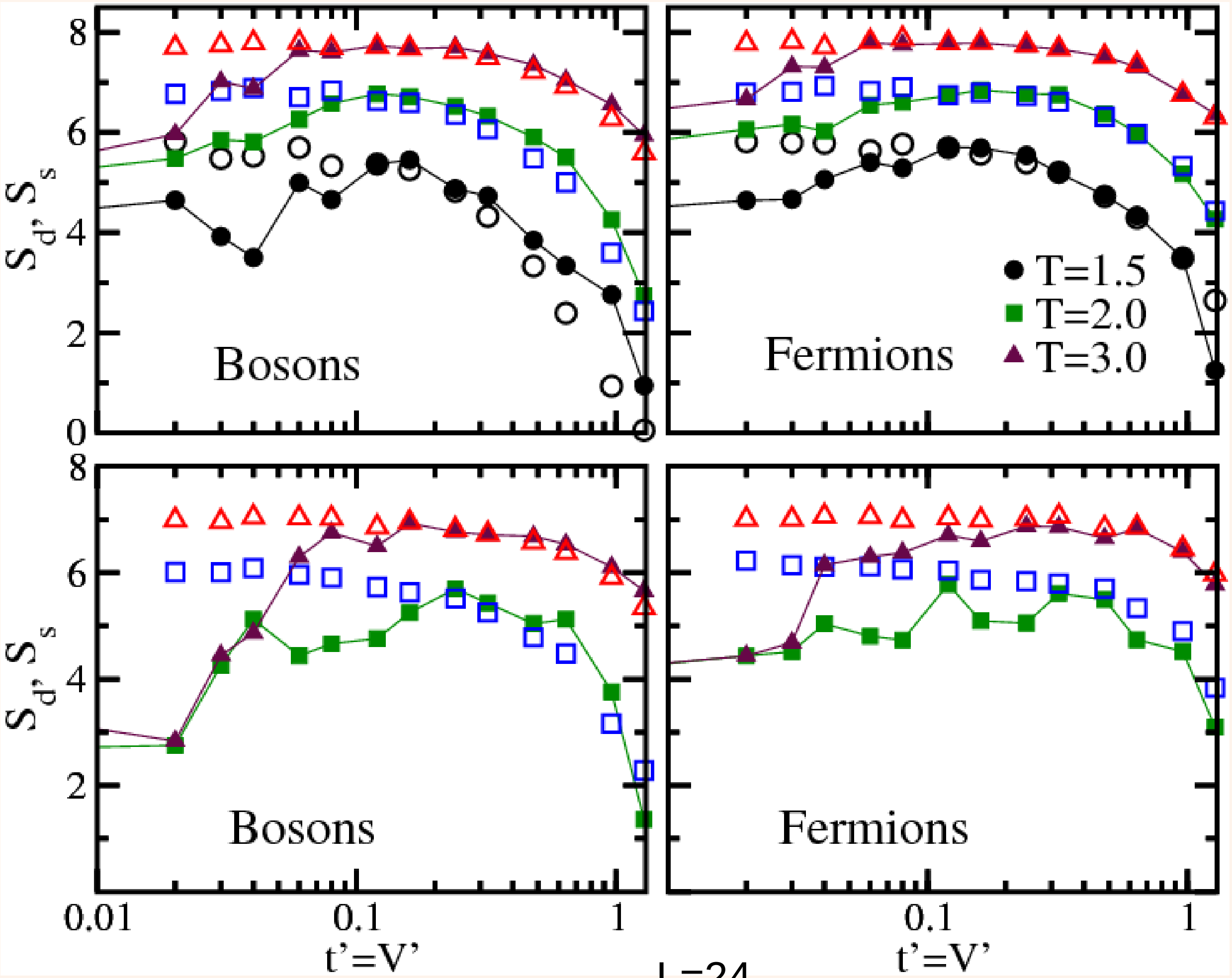
LFS, A. Polkovnikov, M. Rigol
PRL **107**, 040601 (2011)

L=24
8 particles

Bosons, T=4

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

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**

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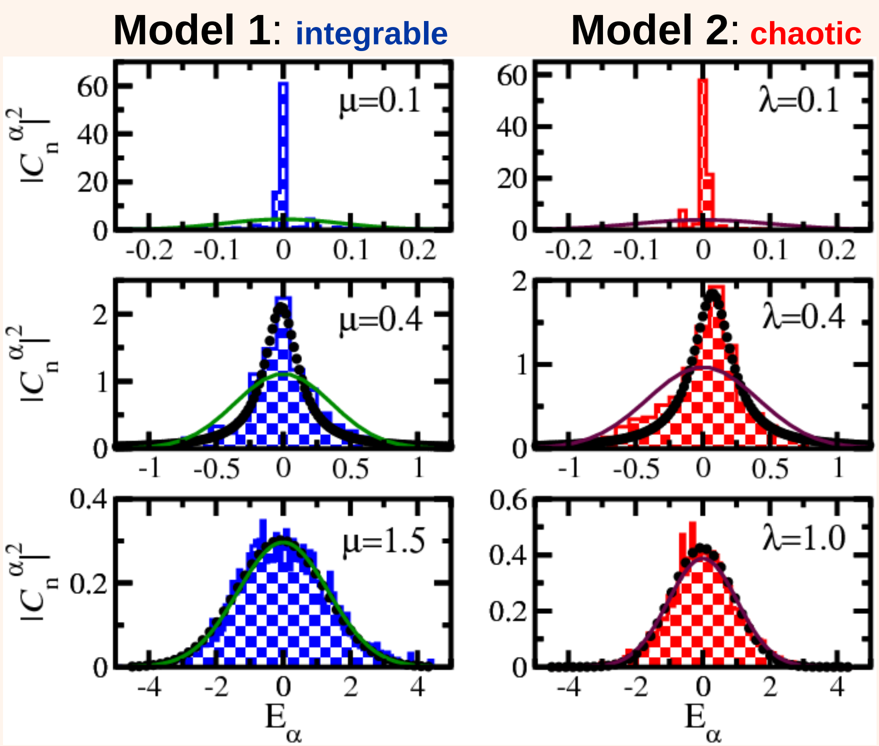
L=24
8 particles

Strength Function and Energy Shell



$$\overbrace{|\phi_n\rangle}^{H_0} = \sum_{\alpha=1}^{D} C_n^\alpha \overbrace{|\psi_\alpha\rangle}^{H=H_0+\lambda V}$$

$$\boxed{P_n(E) = \sum_\alpha |C_n^\alpha|^2 \; \delta(E - E_n)}$$

spread of energy, lifetime of ϕ_n

Chaotic domain:

$$P_n(E) = \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp\left(\frac{-(E-\varepsilon_n)^2}{2\sigma_n^2} \right)$$

Energy shell:
Gaussian with variance $\sigma_n^2 = \sum_{m \neq n} |H_{nm}|^2$

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

Average over 5 EFs in the middle of the spectrum; L=15; 5 spins up

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

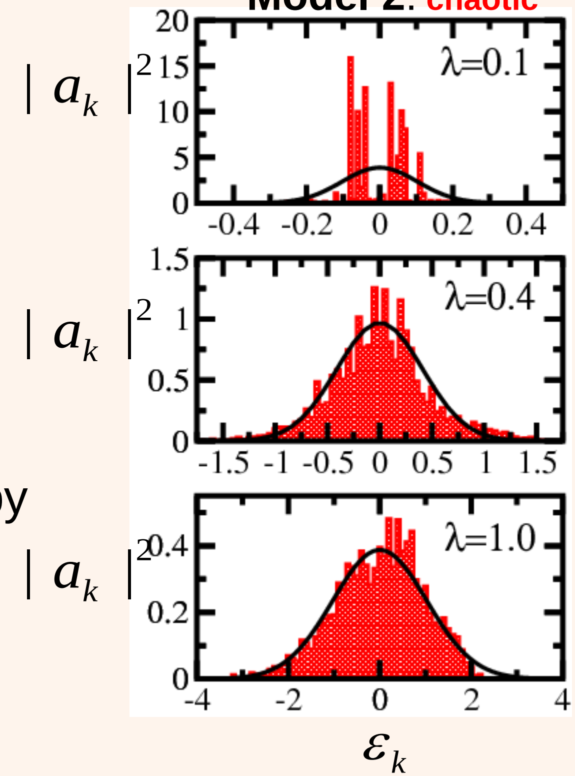
Chaos and Random Matrix Theory

- 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

- Chaotic states = states that fill the energy shell

Shannon entropy coincides with thermodynamic entropy if the state considered fills the energy shell

Model 2: chaotic



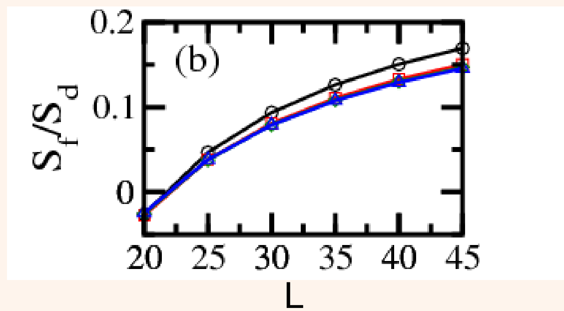
LFS, Borgonovi, Izrailev
PRL **108**, 094102 (2012)
PRE **85**, 036209 (2012)

Integrable regime

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

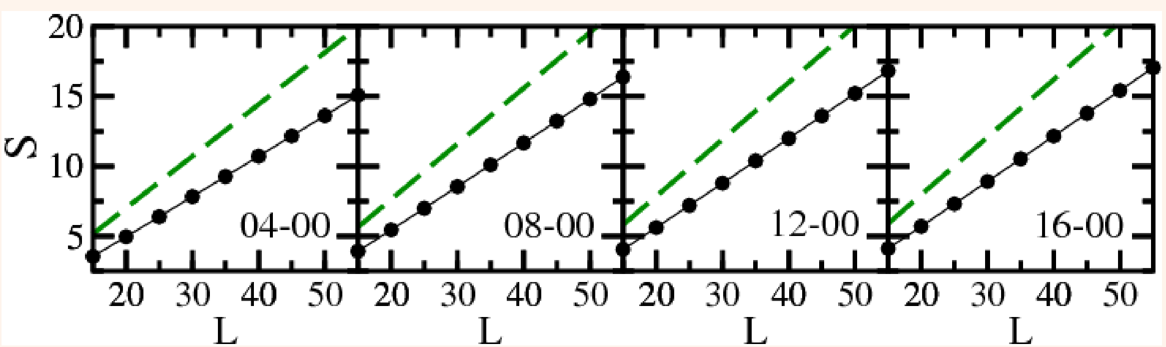
$$H_S = -t\sum_{j=1}^{L-1}(b_j^\dagger b_{j+1} + \text{H.c.}) + A\sum_{j=1}^{L}\cos\left(\frac{2\pi j}{P}\right) b_j^\dagger b_j$$

- 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)

TRACE OUT
PART OF THE SYSTEM

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

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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Entropies: what to expect?

Composite system $S + \varepsilon$ 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

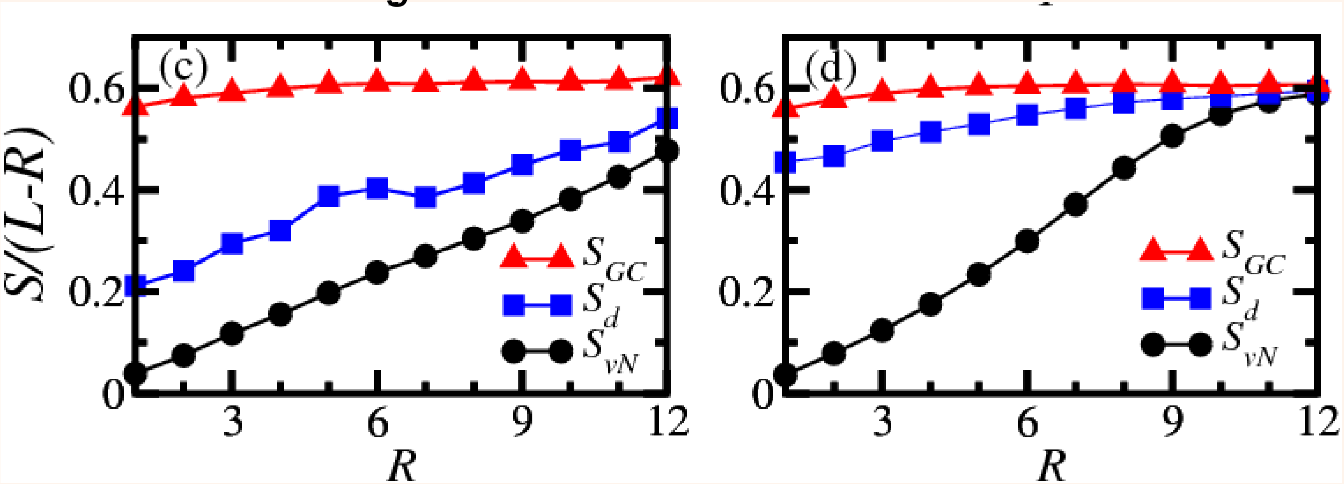
$$S_d = -\sum_n \rho_{nn} \ln \rho_{nn}$$

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

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

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

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

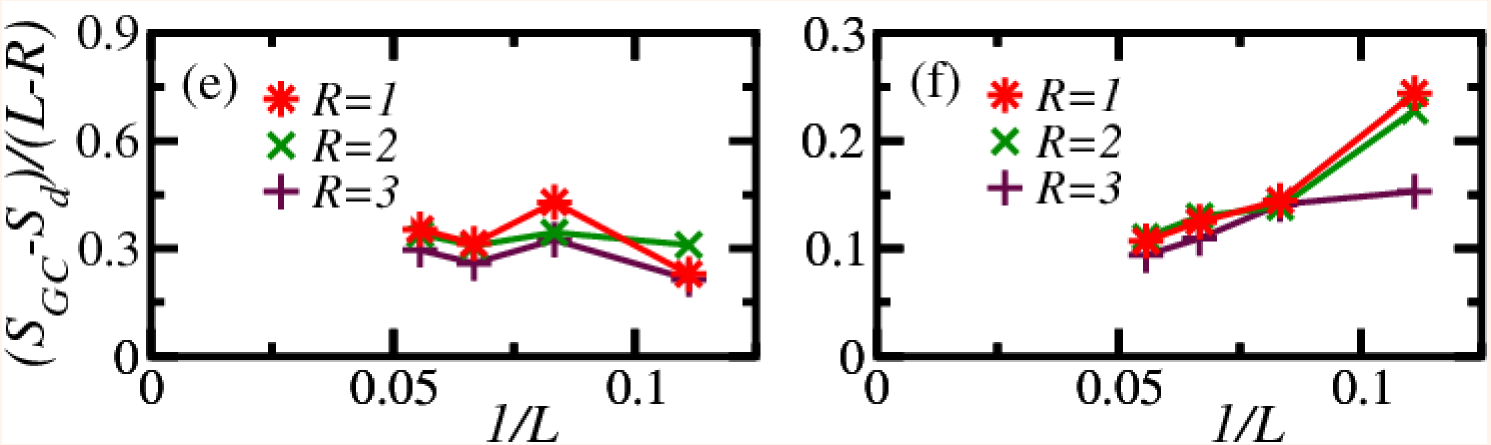
$$\Xi = \sum_n e^{(\mu N_n - E_n)/T_{GC}}$$

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

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

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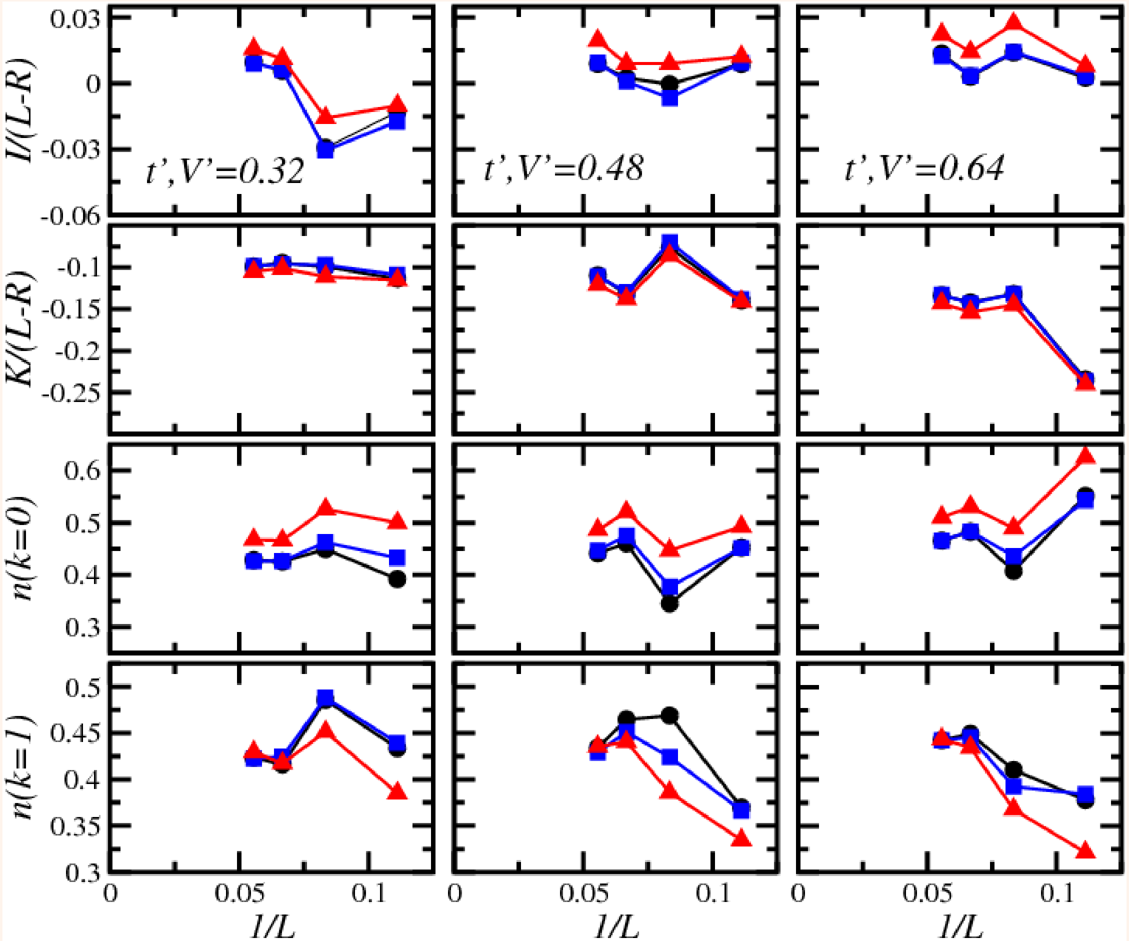
PRE **86** 010102(R) (2012)

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

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

  Few sites removed: **diagonal** 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.