From unitary dynamics to statistical mechanics in isolated quantum systems

Marcos Rigol

Department of Physics
The Pennsylvania State University

Equilibration Mechanisms in Weakly and Strongly Coupled Quantum Field Theory
Institute for Nuclear Theory
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Outline

1. Introduction
   - Foundations of quantum statistical mechanics
   - Experiments with ultracold gases
   - Unitary evolution and thermalization
2. Generic (nonintegrable) systems
   - Time evolution vs exact time average
   - Statistical description after relaxation
   - Eigenstate thermalization hypothesis
   - Time fluctuations
3. Integrable systems
   - Time evolution
   - Generalized Gibbs ensemble
4. Summary

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Foundations of quantum statistical mechanics

Quantum ergodicity: John von Neumann '29
(Proof of the ergodic theorem and the H-theorem in quantum mechanics)

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Recent works:

Tasaki '98
(From Quantum Dynamics to the Canonical Distribution...)

Goldstein, Lebowitz, Tumulka, and Zanghi '06
(Canonical Typicality)

Popescu, Short, and A. Winter '06
(Entanglement and the foundation of statistical mechanics)

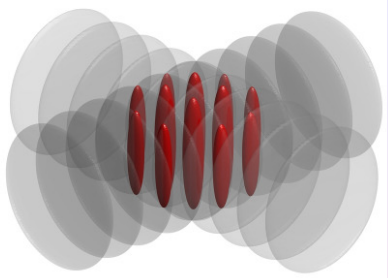
Goldstein, Lebowitz, Mastrodonato, Tumulka, and Zanghi '10
(Normal typicality and von Neumann's quantum ergodic theorem)

MR and Srednicki '12
(Alternatives to Eigenstate Thermalization)

P. Reimann '15
(Generalization of von Neumann's Approach to Thermalization)

Outline

Experiments with ultracold gases in 1D



Effective one-dimensional δ potential

M. Olshanii, PRL **81**, 938 (1998).

$$U_{1D}(x) = g_{1D}\delta(x)$$

where

$$g_{1D} = \frac{2\hbar a_s \omega_\perp}{1 - C a_s \sqrt{\frac{m\omega_\perp}{2\hbar}}}$$

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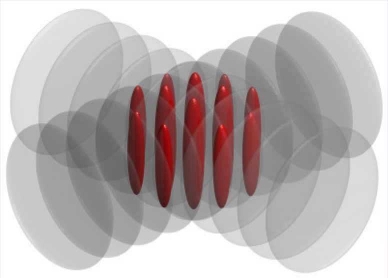

Girardeau '60, Lieb and Liniger '63

T. Kinoshita, T. Wenger, and D. S. Weiss, Science **305**, 1125 (2004).

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$\gamma_{\text{eff}} = \frac{m g_{1D}}{\hbar^2 \rho}$

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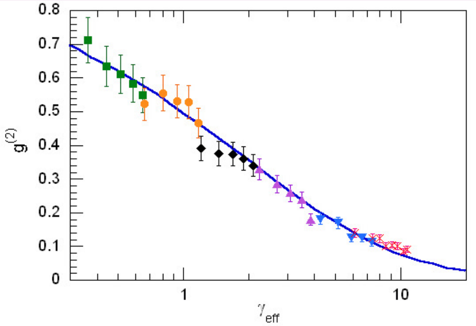
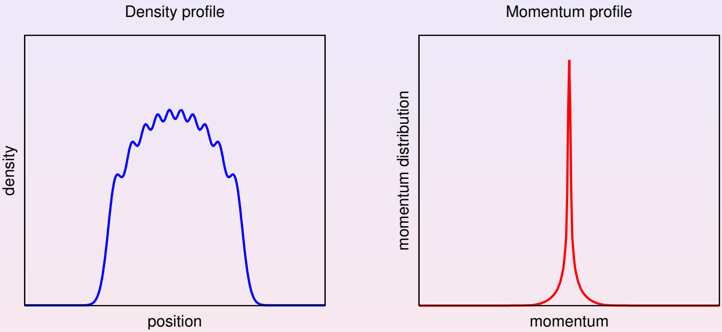


Absence of thermalization in 1D



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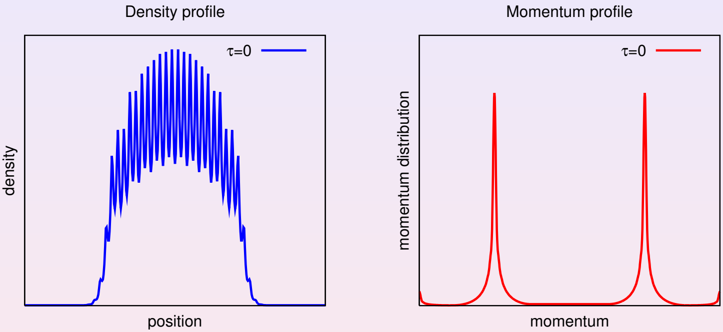

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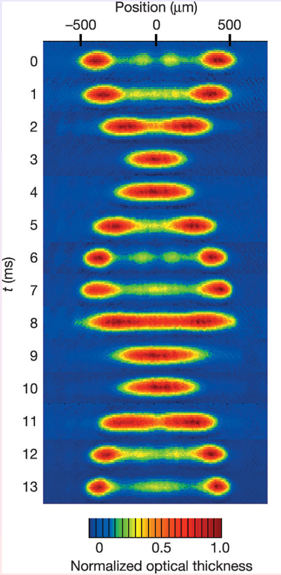
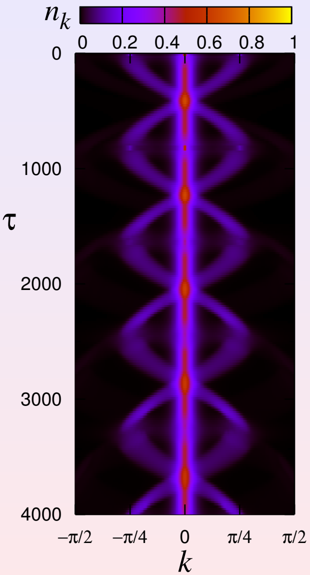
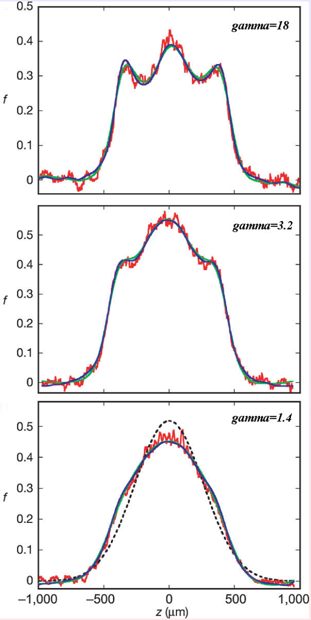
Experiment





Theory

Absence of thermalization in 1D



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$$\gamma = \frac{m g_{1D}}{\hbar^2 \rho}$$

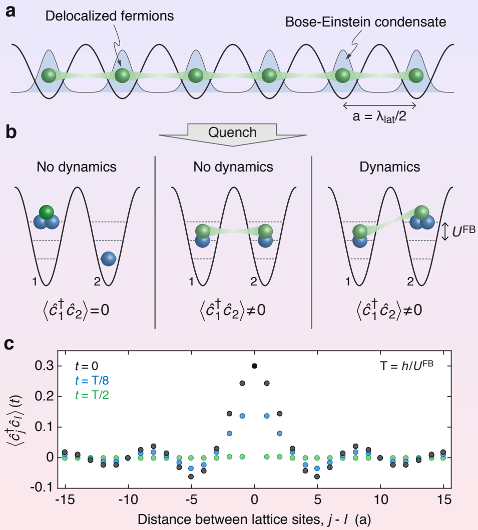
g_{1D}: Interaction strength
ρ: One-dimensional density

If $\gamma \gg 1$ the system is in the strongly correlated Tonks-Girardeau regime

If $\gamma \ll 1$ the system is in the weakly interacting regime

Gring *et al.*, Science **337**, 1318 (2012).

Coherence after quenches in Bose-Fermi mixtures



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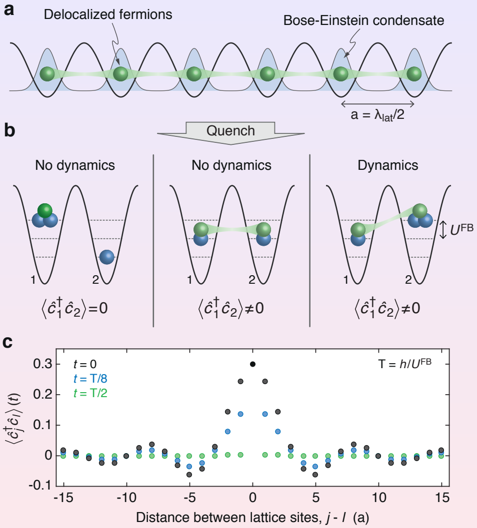

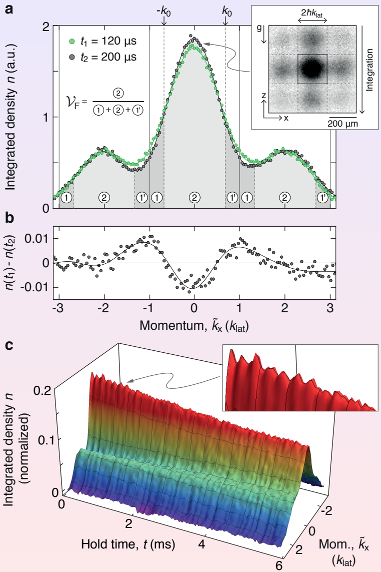

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Outline

Exact results from quantum mechanics

If the initial state is not an eigenstate of $\widehat{H}$

$$|\psi_0\rangle \neq |\alpha\rangle \quad \text{where} \quad \widehat{H}|\alpha\rangle = E_\alpha|\alpha\rangle \quad \text{and} \quad E_0 = \langle\psi_0|\widehat{H}|\psi_0\rangle,$$

then a generic observable O will evolve in time following

$$O(\tau) \equiv \langle\psi(\tau)|\widehat{O}|\psi(\tau)\rangle \quad \text{where} \quad |\psi(\tau)\rangle = e^{-i\widehat{H}\tau}|\psi_0\rangle.$$

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One can rewrite

$$O(\tau) = \sum_{\alpha',\alpha} C^\star_{\alpha'} C_\alpha e^{i(E_{\alpha'}-E_\alpha)\tau} O_{\alpha'\alpha} \quad \text{where} \quad |\psi_0\rangle = \sum_\alpha C_\alpha|\alpha\rangle,$$

Taking the infinite time average (diagonal ensemble $\hat{\rho}_{\text{DE}} \equiv \sum_\alpha |C_\alpha|^2|\alpha\rangle\langle\alpha|$)

$$\overline{O(\tau)} = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau d\tau'\langle\Psi(\tau')|\hat{O}|\Psi(\tau')\rangle = \sum_\alpha |C_\alpha|^2 O_{\alpha\alpha} \equiv \langle\hat{O}\rangle_{\text{diag}},$$

which depends on the initial conditions through $C_\alpha = \langle\alpha|\psi_0\rangle$.

Width of the energy density after a sudden quench

Initial state $|\psi_0\rangle = \sum_\alpha C_\alpha |\alpha\rangle$ is an eigenstate of $\widehat{H}_0$. At $\tau = 0$

$$\widehat{H}_0 \to \widehat{H} = \widehat{H}_0 + \widehat{W} \qquad \text{with} \quad \widehat{W} = \sum_j \hat{w}(j) \quad \text{and} \quad \widehat{H}|\alpha\rangle = E_\alpha|\alpha\rangle.$$

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The width of the weighted energy density ΔE is then

$$\Delta E = \sqrt{\sum_\alpha E_\alpha^2|C_\alpha|^2 - (\sum_\alpha E_\alpha|C_\alpha|^2)^2} = \sqrt{\langle\psi_0|\widehat{W}^2|\psi_0\rangle - \langle\psi_0|\widehat{W}|\psi_0\rangle^2},$$

or

$$\Delta E = \sqrt{\sum_{j_1,j_2\in\sigma} [\langle\psi_0|\hat{w}(j_1)\hat{w}(j_2)|\psi_0\rangle - \langle\psi_0|\hat{w}(j_1)|\psi_0\rangle\langle\psi_0|\hat{w}(j_2)|\psi_0\rangle]} \overset{N\to\infty}{\propto} \sqrt{N},$$

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Since $E \propto N$, then the ratio

$$\frac{\Delta E}{E} \overset{N\to\infty}{\propto} \frac{1}{\sqrt{N}},$$

so, as in any thermal ensemble, it vanishes in the thermodynamic limit.

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Outline

Relaxation dynamics of hard-core bosons in 2D

Hard-core boson Hamiltonian

$$\widehat{H} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j, \qquad \hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

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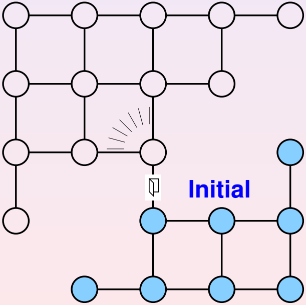
Nonequilibrium dynamics in 2D



Weak n.n. $U = 0.1J$

$N_b = 5$ bosons

$N = 21$ lattice sites

Hilbert space: $D = 20349$

All states are used!

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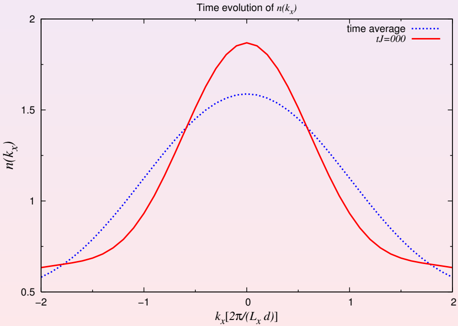

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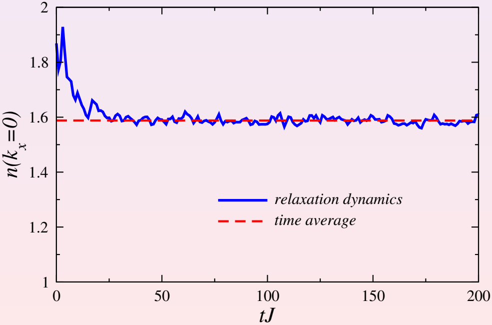

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Statistical description after relaxation

Canonical calculation

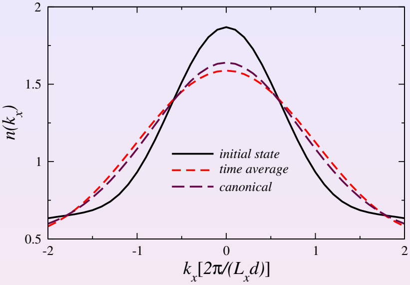
$$O = \mathrm{Tr}\left\{\hat{O}\hat{\rho}\right\}$$

$$\hat{\rho} = Z^{-1}\exp\left(-\hat{H}/k_B T\right)$$

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

$$E_0 = \mathrm{Tr}\left\{\hat{H}\hat{\rho}\right\} \qquad T = 1.9J$$

Momentum distribution



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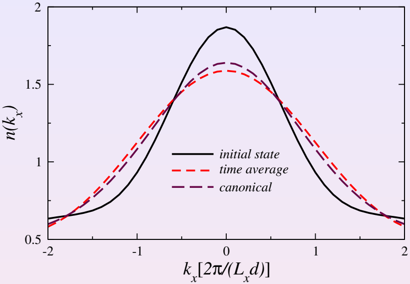
Microcanonical calculation

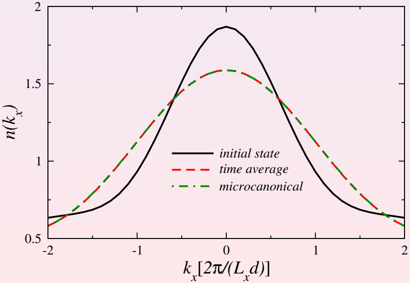
$$O = \frac{1}{N_{states}}\sum_{\alpha}\langle\Psi_\alpha|\hat{O}|\Psi_\alpha\rangle$$

with $E_0 - \Delta E < E_\alpha < E_0 + \Delta E$

N_{states} : # of states in the window

Momentum distribution





Outline

Eigenstate thermalization hypothesis

Paradox?

$$\sum_{\alpha} |C_\alpha|^2 O_{\alpha\alpha} = \langle O \rangle_{\text{microcan.}}(E_0) \equiv \frac{1}{N_{E_0,\Delta E}} \sum_{|E_0 - E_\alpha| < \Delta E} O_{\alpha\alpha}$$

Left hand side: Depends on the initial conditions through $C_\alpha = \langle \Psi_\alpha | \psi_I \rangle$
Right hand side: Depends only on the initial energy

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i) For physically relevant initial conditions, $|C_\alpha|^2$ practically do not fluctuate (remember that ΔE is subextensive).

ii) Large (and uncorrelated) fluctuations occur in both $O_{\alpha\alpha}$ and $|C_\alpha|^2$. A physically relevant initial state performs an unbiased sampling of $O_{\alpha\alpha}$.
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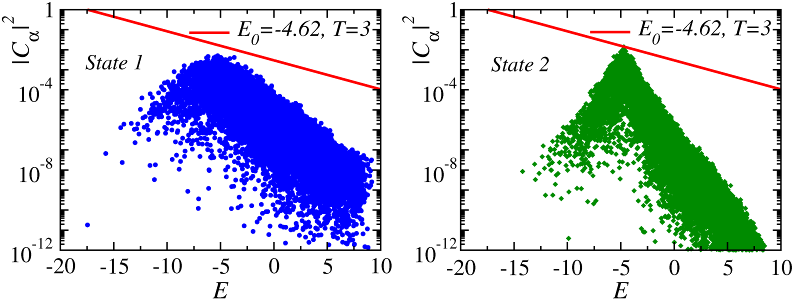

MR, PRA **82**, 037601 (2010).

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Eigenstate thermalization hypothesis (diagonal part)
[J. M. Deutsch, PRA **43** 2046 (1991); M. Srednicki, PRE **50**, 888 (1994);
MR, V. Dunjko, and M. Olshanii, Nature **452**, 854 (2008).]

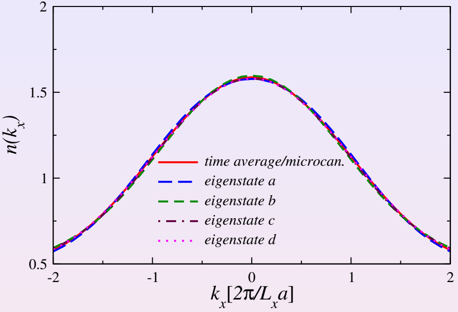
iii) The expectation value $\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle$ of a few-body observable $\widehat{O}$ in an eigenstate of the Hamiltonian $|\Psi_\alpha\rangle$, with energy E_α, of a large interacting many-body system equals the thermal average of $\widehat{O}$ at the mean energy E_α:

$$\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle_{\text{microcan.}}(E_\alpha)$$

Eigenstate thermalization

Momentum distribution

Eigenstates $a - d$ are the ones with energies closest to E_0



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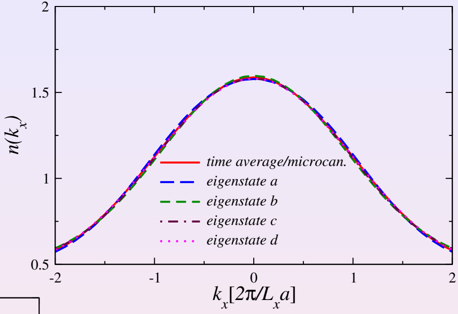

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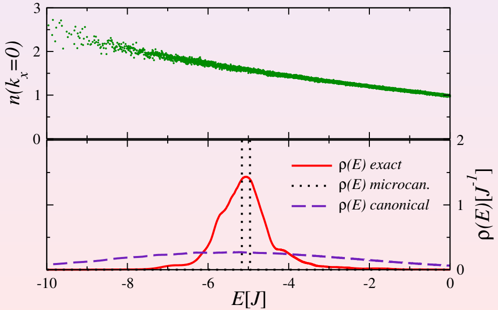


$n(k_x = 0)$ vs energy

$\rho(E) = \text{P(E)} \times \text{dens. stat.}$

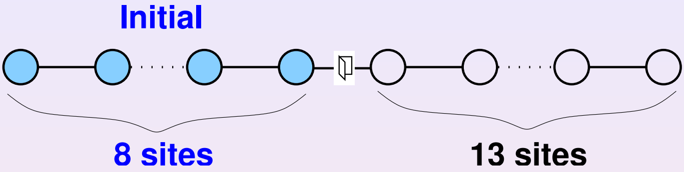
$P(E)_{\text{exact}} \rightarrow |C_\alpha|^2$

$P(E)_{\text{mic}} \rightarrow \text{constant}$

$P(E)_{\text{can}} \rightarrow \exp\left(-E/k_B T\right)$

One-dimensional integrable case

Similar experiment in one dimension



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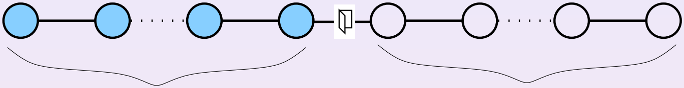
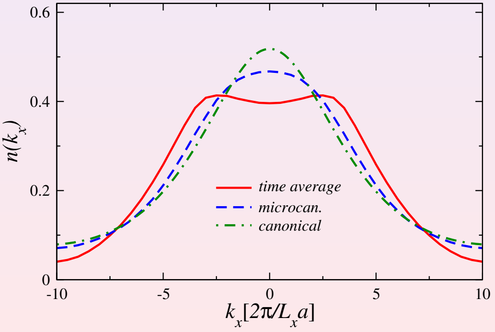
Initial



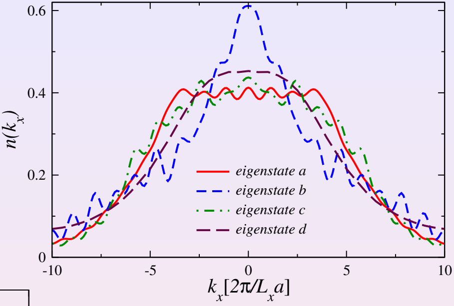
8 sites **13 sites**

Time average vs Stat. Mech.

No thermalization!

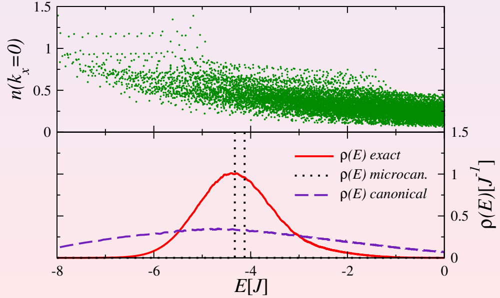


Breakdown of eigenstate thermalization



Momentum distribution

Eigenstates $a - d$ are the ones with energies closest to E_0



$n(k_x = 0)$ vs energy

$\rho(E) = \text{P(E)} \times \text{dens. stat.}$

$P(E)_{\text{exact}} \to |C_\alpha|^2$

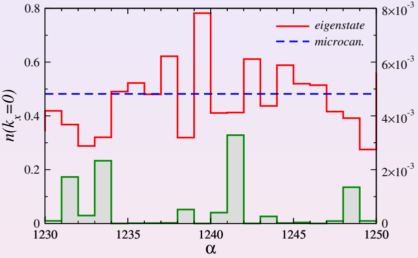
$P(E)_{\text{mic}} \to \text{constant}$

$P(E)_{\text{can}} \to \exp\left(-E/k_B T\right)$

Integrable vs Nonintegrable cases

Correlations between $n(k)$ and C_α

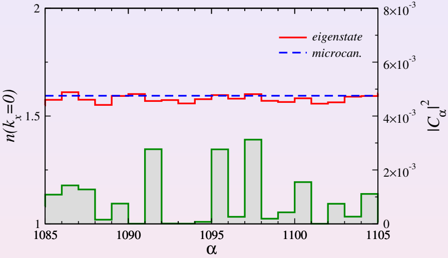
1D (integrable) case



⇓

Conservation laws play a role in integrable models.

2D (nonintegrable) case



⇓

Correlations are not relevant, and they are not present!

Transition between integrability and nonintegrability:

MR, PRL **103**, 100403 (2009); PRA **80**, 053607 (2009).

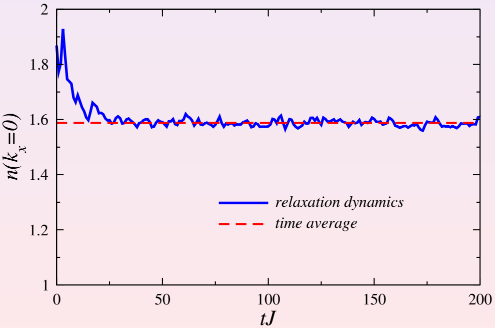
Outline

Relaxation dynamics of hard-core bosons in 2D

Hard-core boson Hamiltonian

$$\widehat{H} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{H.c.} \right) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j, \qquad \hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

Nonequilibrium dynamics in 2D



Weak n.n. $U = 0.1J$

$N_b = 5$ bosons

$N = 21$ lattice sites

Hilbert space: $D = 20349$

All states are used!

Time fluctuations

Are they small because of dephasing?

$$\langle\hat{O}(t)\rangle - \overline{\langle\hat{O}(t)\rangle} = \sum_{\substack{\alpha',\alpha \\ \alpha'\neq\alpha}} C^{\star}_{\alpha'} C_{\alpha} e^{i(E_{\alpha'}-E_{\alpha})t} O_{\alpha'\alpha} \sim \sum_{\substack{\alpha',\alpha \\ \alpha'\neq\alpha}} \frac{e^{i(E_{\alpha'}-E_{\alpha})t}}{N_{\text{states}}} O_{\alpha'\alpha}$$

$$\sim \frac{\sqrt{N^2_{\text{states}}}}{N_{\text{states}}} O^{\text{typical}}_{\alpha'\alpha} \sim O^{\text{typical}}_{\alpha'\alpha}$$

Time fluctuations

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$$\sim \frac{\sqrt{N^2_{\text{states}}}}{N_{\text{states}}} O^{\text{typical}}_{\alpha'\alpha} \sim O^{\text{typical}}_{\alpha'\alpha}$$

Time average of $\langle \hat{O} \rangle$

$$\overline{\langle \hat{O} \rangle} = \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha}$$

$$\sim \sum_{\alpha} \frac{1}{N_{\text{states}}} O_{\alpha\alpha} \sim O^{\text{typical}}_{\alpha\alpha}$$

Time fluctuations

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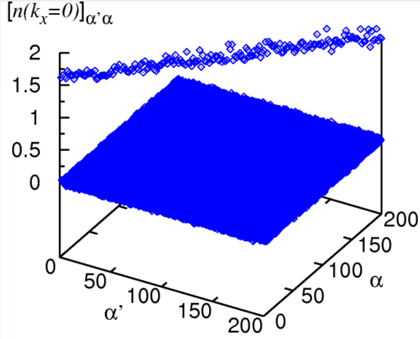

Eigenstate thermalization hypothesis

Eigenstate thermalization hypothesis

M. Srednicki, J. Phys. A **32**, 1163 (1999).

$$O_{\alpha\beta} = O(E)\delta_{\alpha\beta} + e^{-S(E)/2} f_O(E,\omega) R_{\alpha\beta}$$

where $E \equiv (E_\alpha + E_\beta)/2$, $\omega \equiv E_\alpha - E_\beta$, $S(E)$ is the thermodynamic entropy at energy E, and $R_{\alpha\beta}$ is a random number with zero mean and unit variance.

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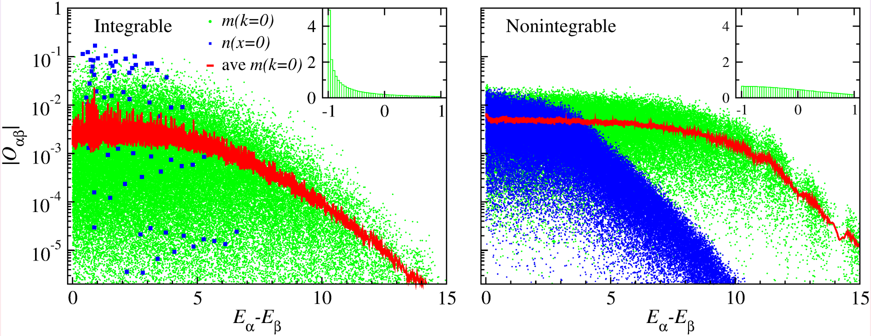
Off-diagonal matrix elements [histogram of $(|O_{\alpha\beta}| - |O_{\alpha\beta}|_{\text{ave}})/|O_{\alpha\beta}|_{\text{ave}}$]



E. Khatami, G. Pupillo, M. Srednicki, and MR, PRL **111**, 050403 (2013).

Outline

1. Introduction
   - Foundations of quantum statistical mechanics
   - Experiments with ultracold gases
   - Unitary evolution and thermalization
2. Generic (nonintegrable) systems
   - Time evolution vs exact time average
   - Statistical description after relaxation
   - Eigenstate thermalization hypothesis
   - Time fluctuations
3. Integrable systems
   - Time evolution
   - Generalized Gibbs ensemble
4. Summary

Bose-Fermi mapping

Hard-core boson Hamiltonian in an external potential

$$\hat{H} = -J \sum_i \left(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.} \right) + \sum_i v_i \ \hat{n}_i$$

Constraints on the bosonic operators

$$\hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

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Constraints on the bosonic operators

$$\hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

$$\Downarrow$$

Map to spins and then to fermions (Jordan-Wigner transformation)

$$\sigma_i^+ = \hat{f}_i^\dagger \prod_{\beta=1}^{i-1} e^{-i\pi \hat{f}_\beta^\dagger \hat{f}_\beta}, \quad \sigma_i^- = \prod_{\beta=1}^{i-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} \hat{f}_i$$

$$\Downarrow$$

Non-interacting fermion Hamiltonian

$$\hat{H}_F = -J \sum_i \left(\hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + \sum_i v_i \ \hat{n}_i^f$$

One-particle density matrix

One-particle Green's function

$$G_{ij} = \langle \Psi_{HCB} | \sigma_i^- \sigma_j^+ | \Psi_{HCB} \rangle = \langle \Psi_F | \prod_{\beta=1}^{i-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} \hat{f}_i \hat{f}_j^\dagger \prod_{\gamma=1}^{j-1} e^{-i\pi \hat{f}_\gamma^\dagger \hat{f}_\gamma} | \Psi_F \rangle$$

$$\Downarrow$$

Time evolution

$$|\Psi_F(\tau)\rangle = e^{-i\hat{H}_F \tau/\hbar} |\Psi_F^I\rangle = \prod_{\delta=1}^{N} \sum_{\sigma=1}^{L} P_{\sigma\delta}(\tau) \hat{f}_\sigma^\dagger \, |0\rangle$$

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One-particle Green's function

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$$\Downarrow$$

Exact Green's function

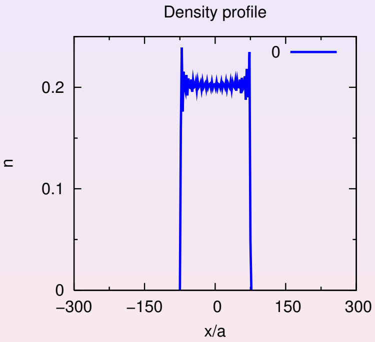
$$G_{ij}(\tau) = \det \left[\left(\mathbf{P}^l(\tau) \right)^\dagger \mathbf{P}^r(\tau) \right]$$

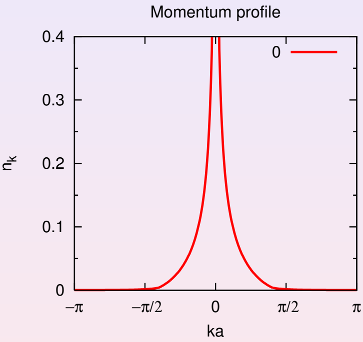
Computation time $\sim L^2 N^3$

3000 lattice sites, 300 particles

MR and A. Muramatsu, PRL **93**, 230404 (2004); PRL **94**, 240403 (2005).

Relaxation dynamics in an integrable system





MR, V. Dunjko, V. Yurovsky, and M. Olshanii, PRL **98**, 050405 (2007).

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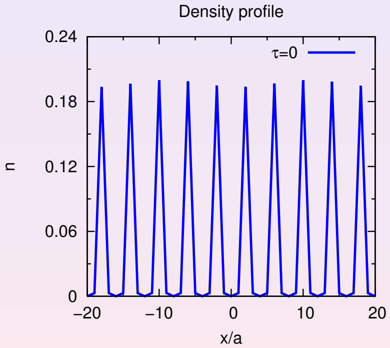

MR, V. Dunjko, V. Yurovsky, and M. Olshanii, PRL **98**, 050405 (2007).

Outline

Statistical description after relaxation

Thermal equilibrium

$$\hat{\rho} = Z^{-1} \exp\left[-\left(\hat{H} - \mu \hat{N}_b \right) / k_B T \right]$$

$$Z = \mathrm{Tr}\left\{ \exp\left[-\left(\hat{H} - \mu \hat{N}_b \right) / k_B T \right] \right\}$$

$$E = \mathrm{Tr}\left\{ \hat{H} \hat{\rho} \right\}, \quad N_b = \mathrm{Tr}\left\{ \hat{N}_b \hat{\rho} \right\}$$

MR, PRA **72**, 063607 (2005).

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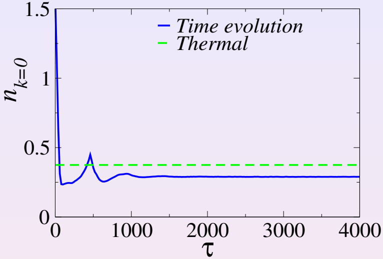
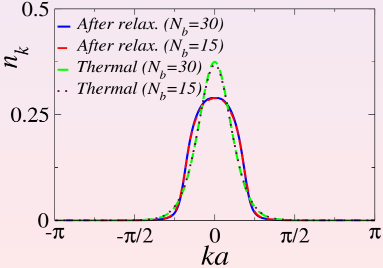
Evolution of $n_{k=0}$



n_k after relaxation



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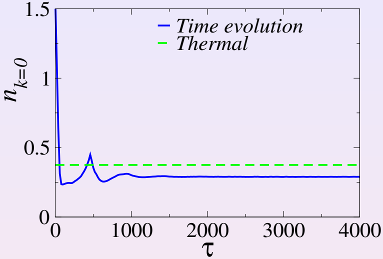

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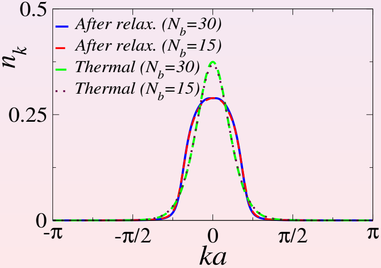

Integrals of motion

(underlying noninteracting fermions)

$$\hat{H}_F \hat{\gamma}_m^{f\dagger}|0\rangle = E_m \hat{\gamma}_m^{f\dagger}|0\rangle$$

$$\left\{\hat{I}_m^f\right\} = \left\{\hat{\gamma}_m^{f\dagger}\hat{\gamma}_m^f\right\}$$

Statistical description after relaxation

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MR, PRA **72**, 063607 (2005).

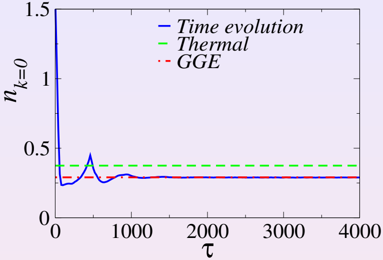
Generalized Gibbs ensemble

$$\hat{\rho}_c = Z_c^{-1} \exp\left[-\sum_m \lambda_m \hat{I}_m\right]$$

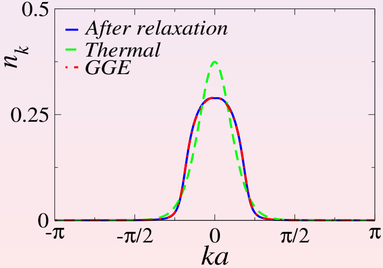
$$Z_c = \mathrm{Tr}\left\{\exp\left[-\sum_m \lambda_m \hat{I}_m\right]\right\}$$

$$\langle \hat{I}_m \rangle_{\tau=0} = \mathrm{Tr}\left\{\hat{I}_m \hat{\rho}_c\right\}$$

Evolution of $n_{k=0}$



n_k after relaxation



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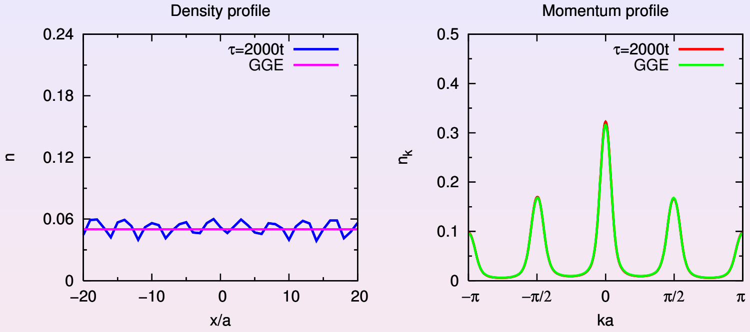

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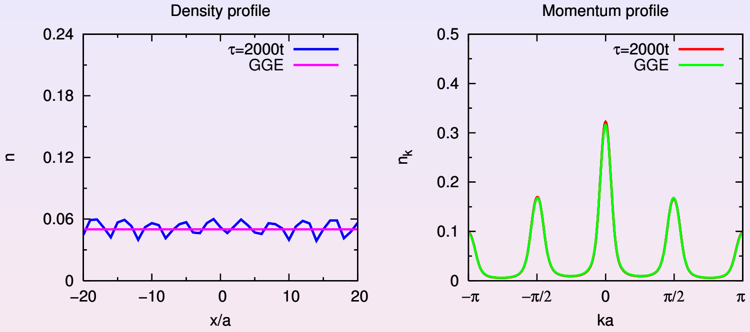

Why does the GGE work?

Generalized eigenstate thermalization:

A. C. Cassidy, C. W. Clark, and MR, Phys. Rev. Lett. **106**, 140405 (2011).

K. He, L. F. Santos, T. M. Wright, and MR, Phys. Rev. A **87**, 063637 (2013).

J.-S. Caux and F. H. L. Essler, Phys. Rev. Lett. 110, 257203 (2013).

Summary

- Thermalization occurs in generic isolated systems
  ★ Finite size effects

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  ★ $\langle \Psi_\alpha | \hat{O} | \Psi_\alpha \rangle = \langle O \rangle_{\text{microcan.}}(E_\alpha)$

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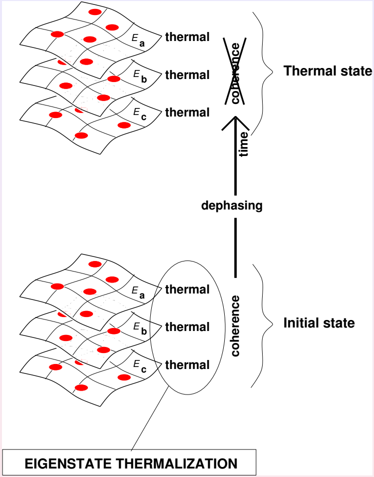

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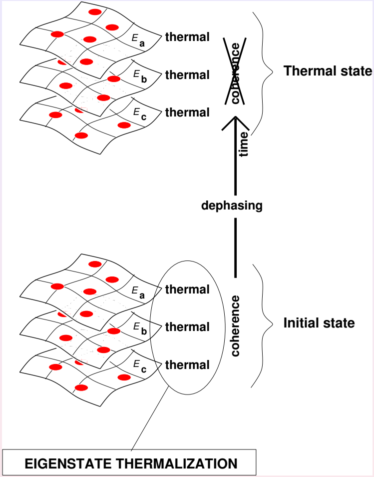
- Thermalization and ETH break down close integrability (finite system)
  - ★ Quantum equivalent of KAM?
- Small time fluctuations $\leftarrow$ smallness of off-diagonal elements
- Time plays only an auxiliary role
- Integrable systems are different (Generalized Gibbs ensemble)



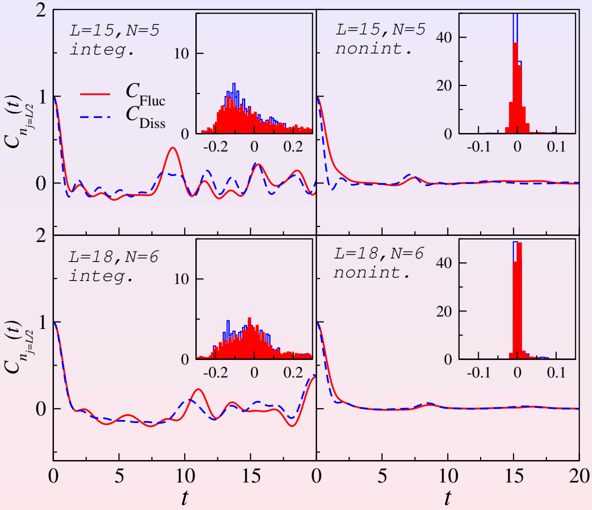
Collaborators

- Vanja Dunjko (U Mass Boston)
- Alejandro Muramatsu (Stuttgart U)
- Maxim Olshanii (U Mass Boston)
- Anatoli Polkovnikov (Boston U)
- Lea F. Santos (Yeshiva U)
- Mark Srednicki (UC Santa Barbara)
- Current group members: Deepak Iyer, Baoming Tang
- Former group members: Kai He (NOAA), Ehsan Khatami (SJSU)

Supported by:

Fluctuation-dissipation theorem (dipolar bosons)

Occupation in the center of the trap ($n_{j=L/2}$)



Hamiltonian

$$\hat{H} = -J \sum_{j=1}^{L-1} \left(\hat{b}_j^\dagger \hat{b}_{j+1} + \text{H.c.} \right)$$
$$+V \sum_{j<l} \frac{\hat{n}_j \hat{n}_l}{|j-l|^3} + g \sum_j x_j^2 \, \hat{n}_j$$

magnetic atoms, polar molecules

Relaxation dynamics

$$O(t) = C(t) O(t=0)$$

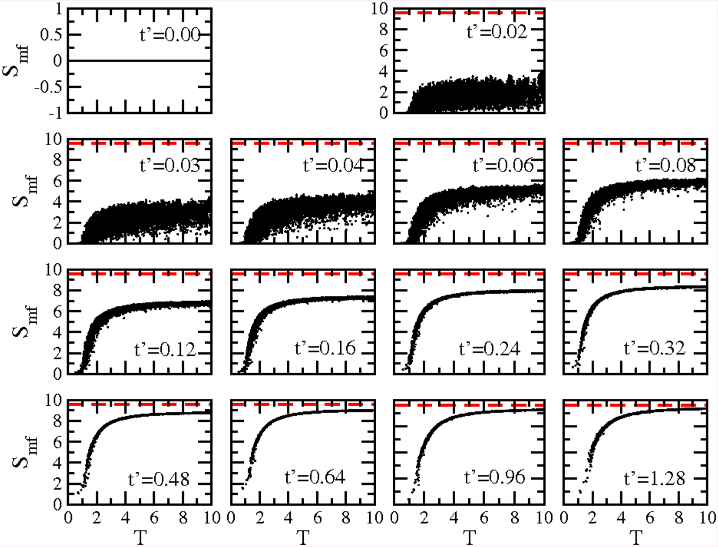
where

$$C(t) = \frac{\overline{O(t+t')O(t')}}{\overline{(O(t'))^2}}$$

Srednicki, JPA **32**, 1163 (1999).

E. Khatami, G. Pupillo, M. Srednicki, and MR, PRL **111**, 050403 (2013).

Information entropy ($S_j = -\sum_{k=1}^{D} |c_j^k|^2 \ln |c_j^k|^2$)



L.F. Santos and MR, PRE **81**, 036206 (2010); PRE **82**, 031130 (2010).