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Summer School on Novel Quantum Phases and Non-Equilibrium Phenomena in Cold Atomic Gases

27 August - 7 September, 2007

Thermalization and its mechanism for generic isolated quantum systems

Marcos Rigol
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ICTP, Trieste, Italy
August 30, 2007

On the blackboard

If in an isolated quantum system

$$|\psi_I\rangle \neq |\Psi_\alpha\rangle \quad \text{where} \quad \widehat{H}|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle,$$

then the evolution of an observable A is dictated by

$$A(t) \equiv \langle\psi(t)|\widehat{A}|\psi(t)\rangle \quad \text{where} \quad |\psi(t)\rangle = e^{-i\widehat{H}t}|\psi_I\rangle.$$

Will a generic A in a generic system thermalize?

$$A(t) \longrightarrow_{t\to\infty} \approx A(E_0) = A(T).$$

But one can always write

$$A(t) = \sum_{\alpha',\alpha} C^\star_{\alpha'} C_\alpha e^{i(E_{\alpha'}-E_\alpha)t} A_{\alpha'\alpha} \quad \text{rewriting} \quad |\psi_I\rangle = \sum_\alpha C_\alpha|\Psi_\alpha\rangle,$$

and taking the infinite time average

$$\overline{\langle\hat{A}\rangle} = \sum_\alpha |C_\alpha|^2 A_{\alpha\alpha},$$

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

Outline

1. Introduction
   - Classical vs Quantum thermalization
   - Experiments and numerical simulations
2. Non-equilibrium dynamics in a two-dimensional system
   - Time evolution vs exact time average
   - Statistical description after relaxation
   - Eigenstate thermalization hypothesis
   - Time fluctuations
3. Integrable systems
   - Generalized Gibbs ensemble
4. Summary

Classical statistical mechanics

Generic isolated systems thermalize

Nonlinear evolution (dynamical chaos) drive a system with many particles to explore ergodically the constant-energy manifold, with precisely the micro-canonical measure

Not all classical systems thermalize

Integrable systems do not thermalize

Integrability

- Hamiltonian $H(p,q)$ with $q=(q_1,\cdots,q_N)$ and $p=(p_1,\cdots,p_N)$
- N *functionally* independent constants of the motion in involution

$$I=(I_1,\cdots,I_N), \quad \{I_\alpha,H\}=0, \quad \{I_\alpha,I_\beta\}=0$$

In between there is the KAM theorem

Under small enough perturbations around an integrable point the system does not thermalize

Quantum mechanics

Time evolution is linear

$$|\psi(t)\rangle = e^{-i\widehat{H}t}|\psi_I\rangle$$

Integrability: Can we just change $\{\cdots\} \rightarrow [\cdots]$?
Then find N functionally independent operators

$$\left[\hat{I}_\alpha, \hat{H}\right] = 0, \qquad \left[\hat{I}_\alpha, \hat{I}_\beta\right] = 0$$

No, because operators that commute with $\hat{H}$ are functionally dependent on it

$$\hat{I}_\alpha = \sum_{k=1}^{D} \lambda_k^\alpha \hat{H}^{k-1}$$

Sets of linearly independent conserved quantities for *any* quantum system

$$\widehat{P}_\alpha = |\Psi_\alpha\rangle\langle\Psi_\alpha|, \quad \text{where } \hat{H}|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle$$
$$\hat{H}^n, \quad \text{with } n = 1, \ldots, D$$

B. Sutherland, *Beautiful Models*

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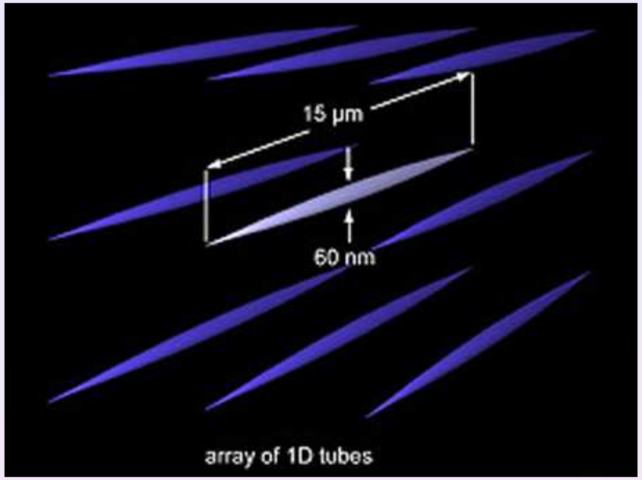
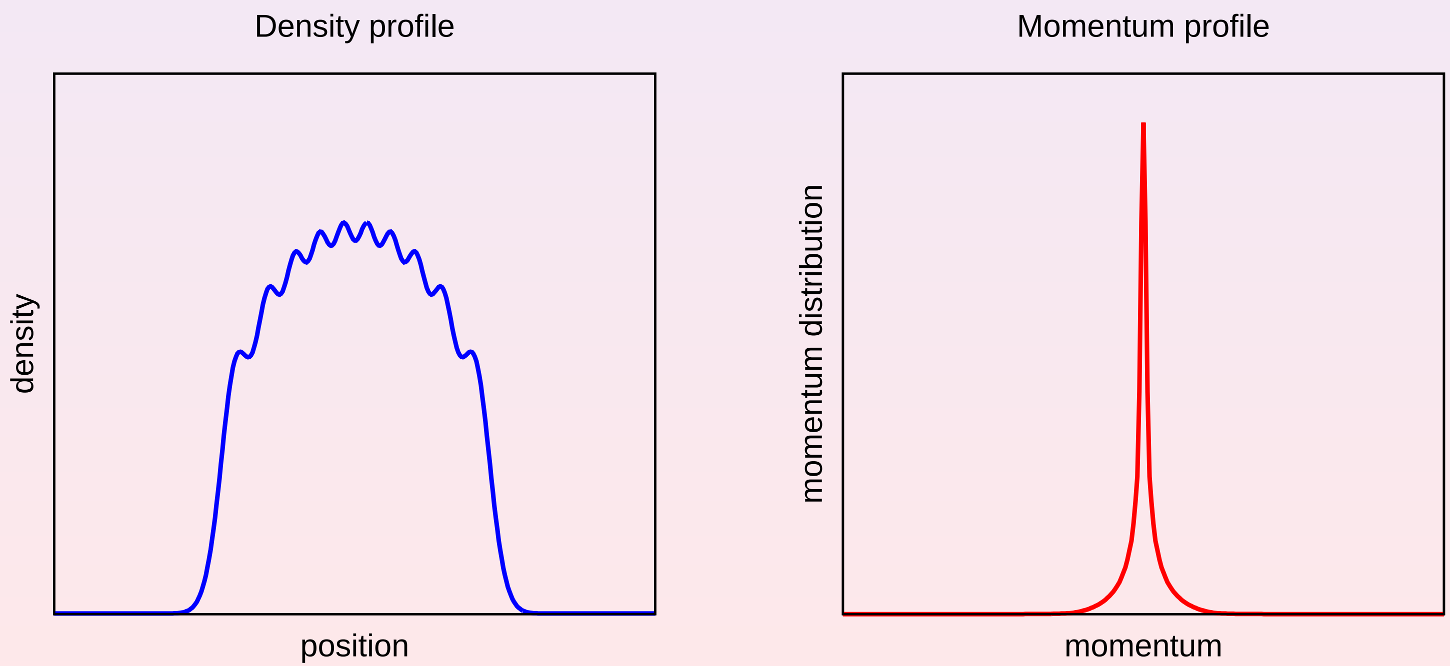
Absence of thermalization in 1D

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

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

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





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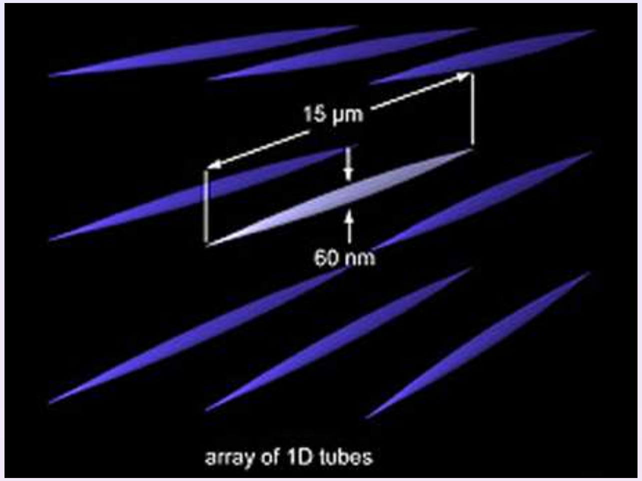
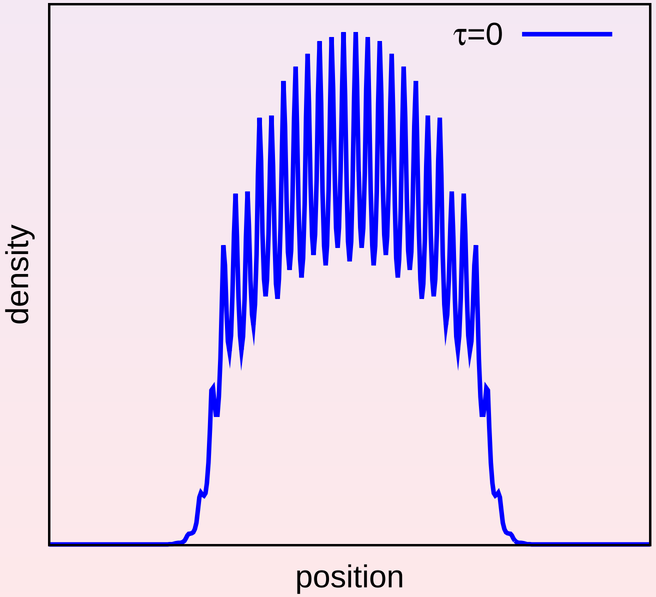
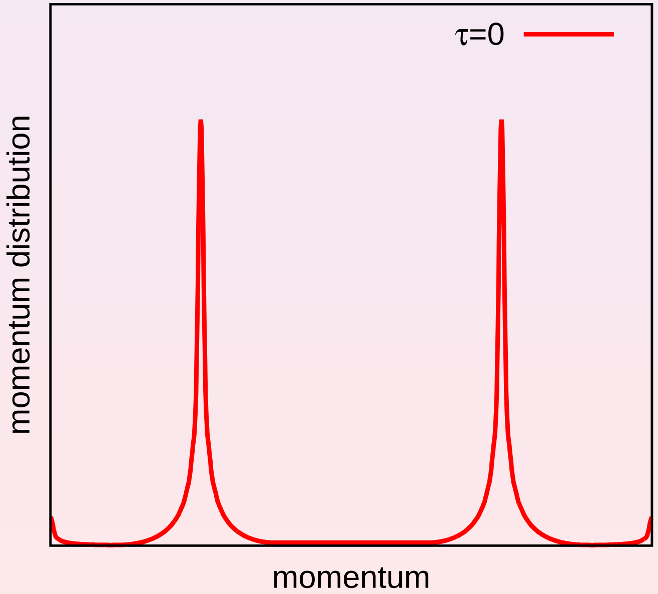


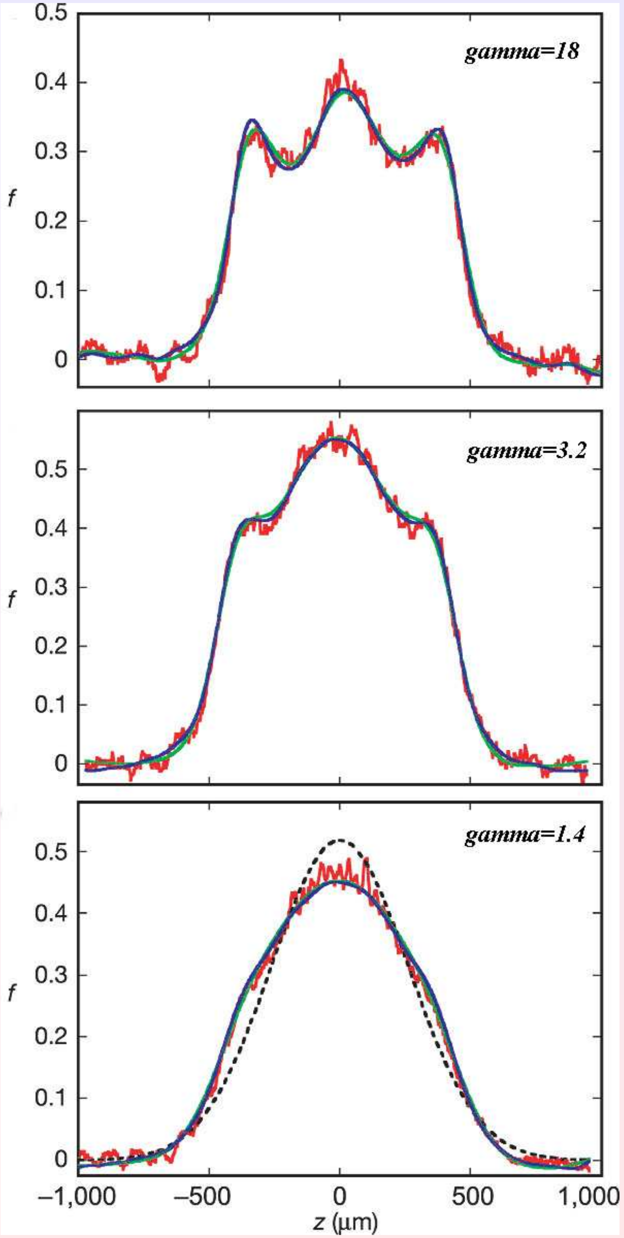
Density profile



Momentum profile



Absence of thermalization in 1D



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

E_{int}: Interaction energy

E_{kin}: Kinetic energy

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

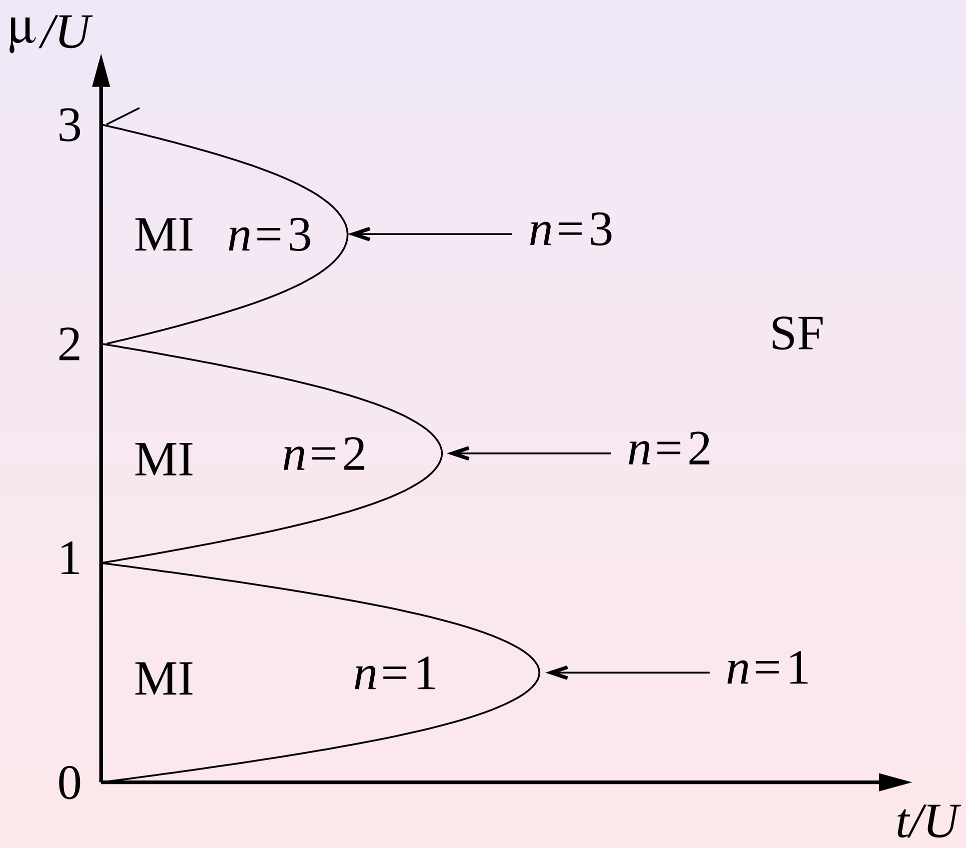
If $\gamma \gg 1$ the system is in the strongly correlated Tonks-Girardeau regime

Dynamics of the 1D Bose-Hubbard model

Bose-Hubbard Hamiltonian

$$H = -J\sum_i (b_i^\dagger b_{i+1} + h.c.) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1)$$

C. Kollath, A. Läuchli, and E. Altman, PRL **98**, 180601 (2007).



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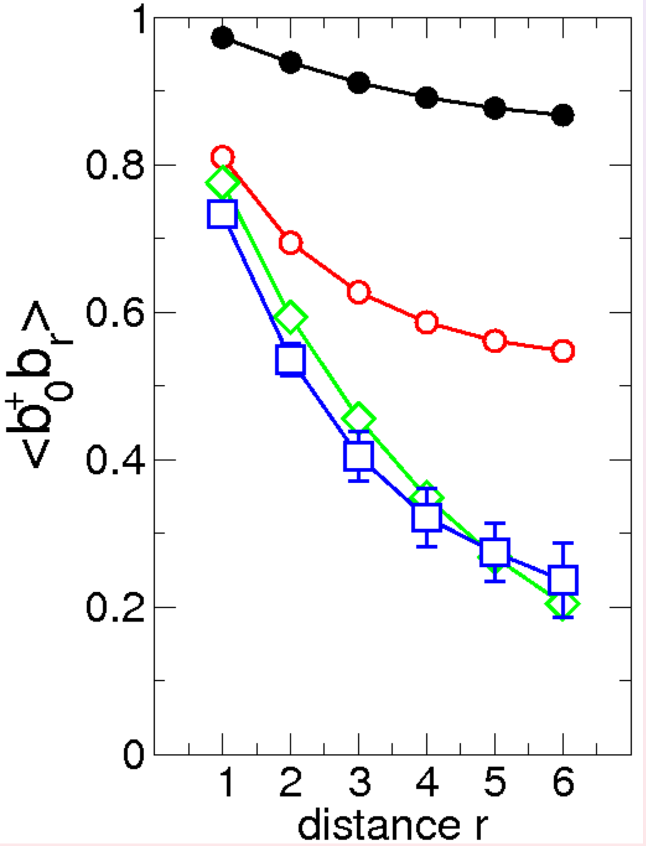
C. Kollath, A. Läuchli, and E. Altman, PRL **98**, 180601 (2007).

$U_i = J$

$U_f = 4J$

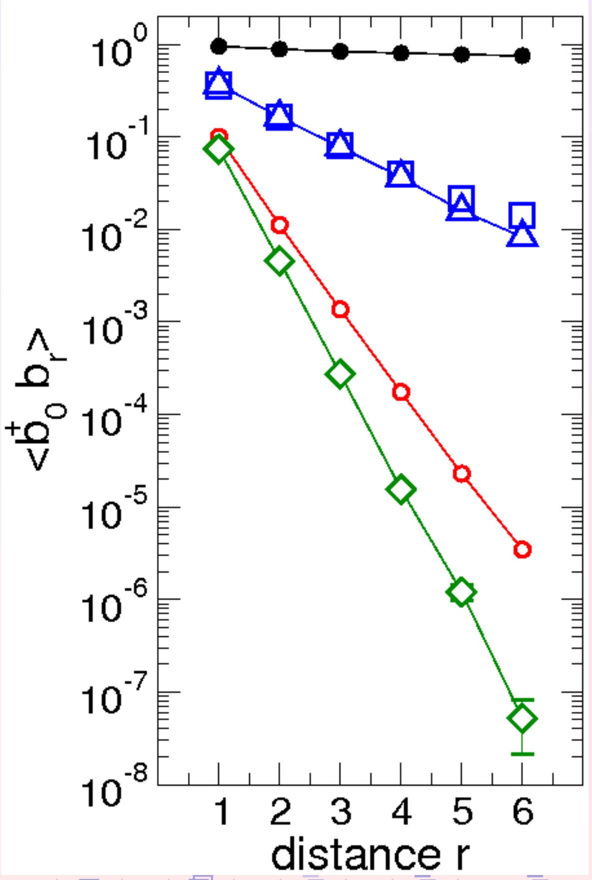
$T = 0.8J$



$U_i = 2J$

$U_f = 40J$

$T = 21.5J$

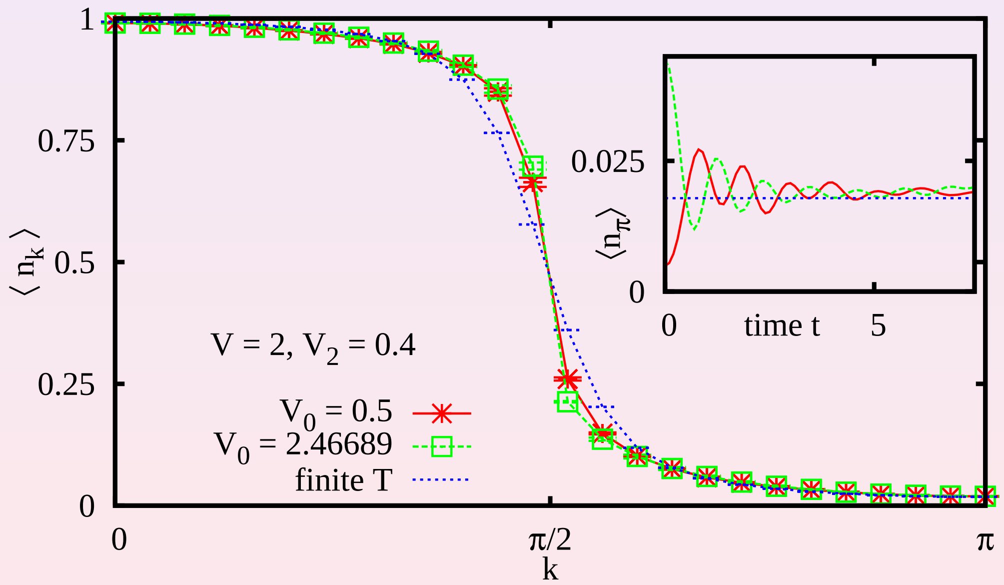


Dynamics of strongly correlated fermions in 1D

Spinless fermions Hamiltonian

$$H = -t\sum_j \left(c^\dagger_{j+1}c_j + h.c.\right) + V\sum_j n_j n_{j+1} + V_2 \sum_j n_j n_{j+2}$$

S. R. Manmana, S. Wessel, R. M. Noack, and A. Muramatsu, PRL **98**, 210405 (2007).



Outline

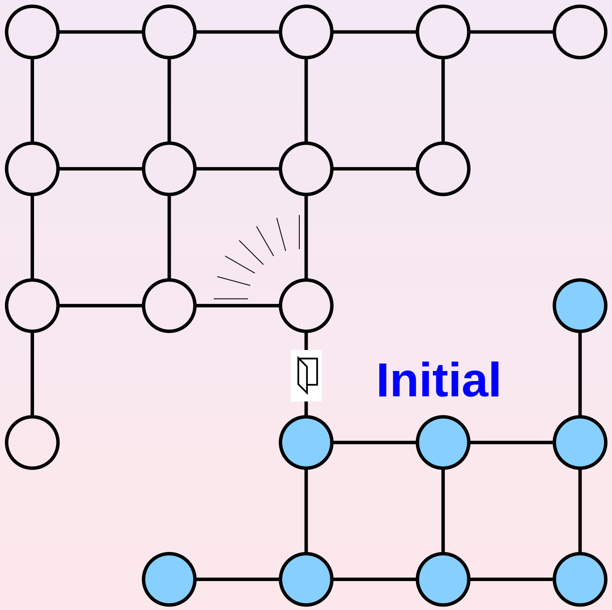
Relaxation dynamics of hard-core boson in 2D

Hard-core boson Hamiltonian

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

MR, V. Dunjko, and M. Olshanii, arXiv:0708.1324 (2007).

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!

Relaxation dynamics of hard-core boson in 2D

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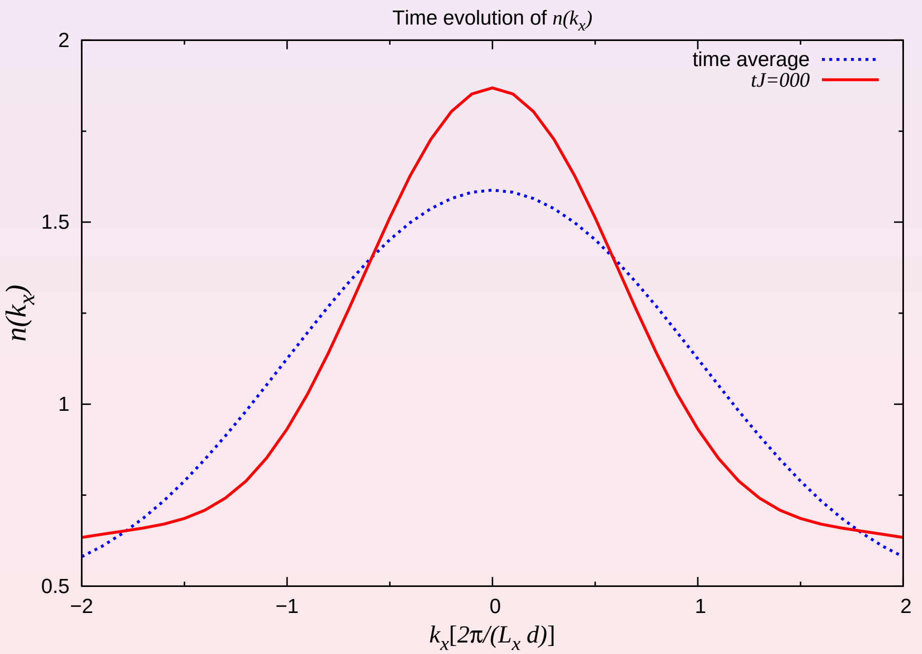

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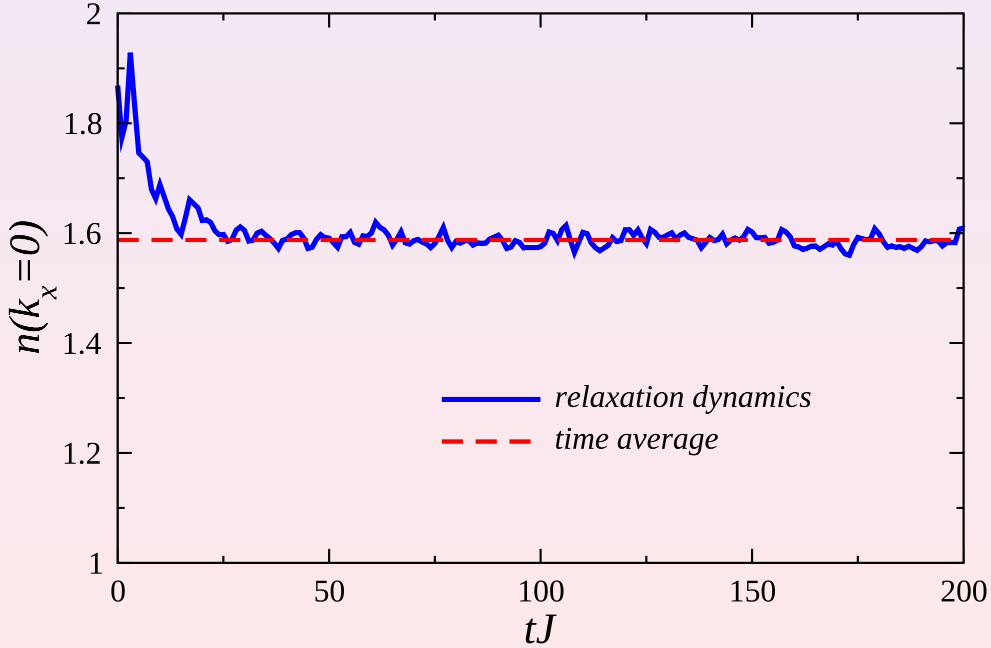

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Outline

Statistical description after relaxation

Canonical calculation

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

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

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

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

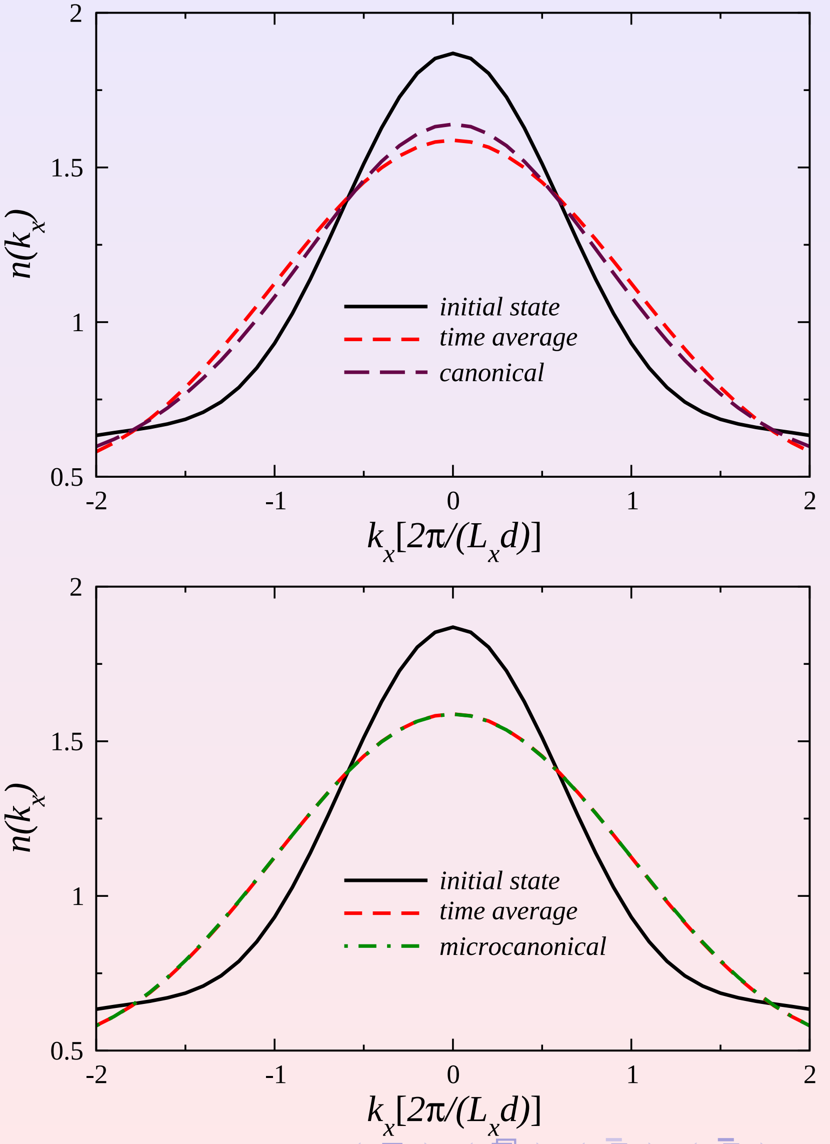
Microcanonical calculation

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

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?

$$\sum_{\alpha} |C_\alpha|^2 A_{\alpha\alpha} = \langle A \rangle_{\text{microcan.}}(E_0)$$

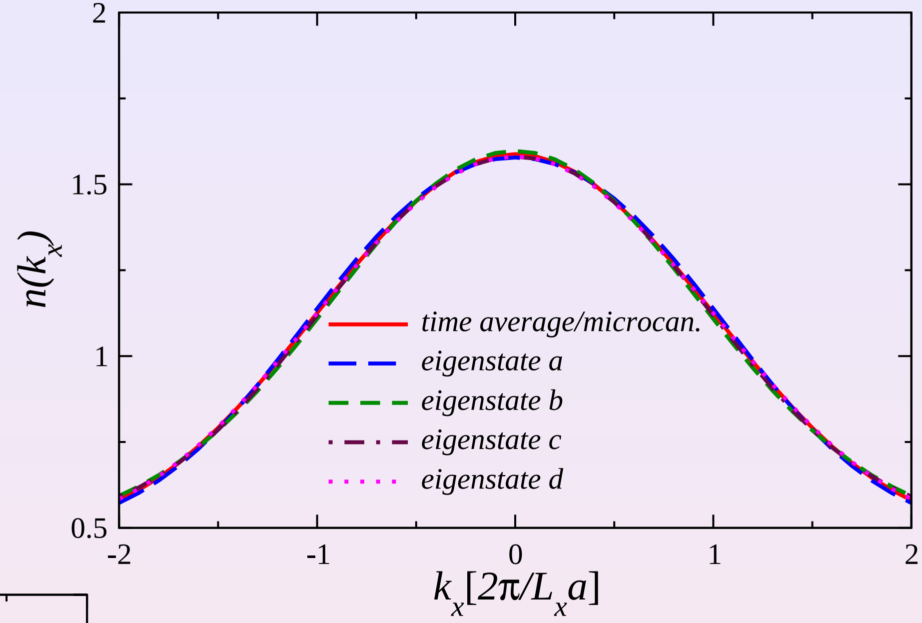
Left hand side: Depends on the initial conditions through $C_\alpha = \langle \Psi_\alpha | \psi_I \rangle$
Right hand side: Depends only on the initial energy

Eigenstate thermalization hypothesis (ETH)
M. Srednicki, PRE **50**, 888 (1994).

> The expectation value $\langle \Psi_\alpha | \hat{A} | \Psi_\alpha \rangle$ of a few-body observable $\widehat{A}$ 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 $\widehat{A}$ at the mean energy E_α:

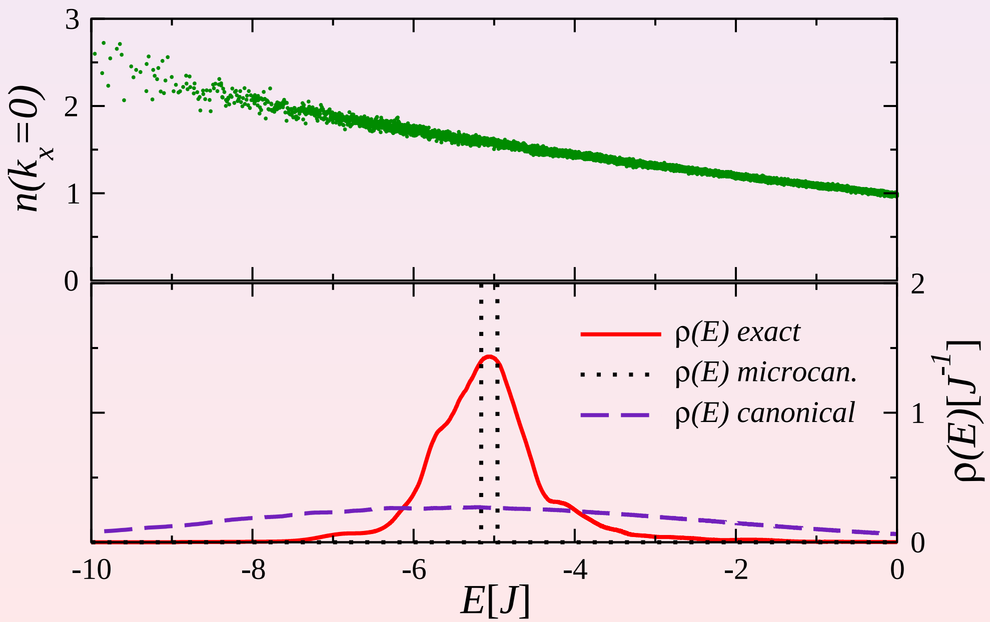
$$\langle \Psi_\alpha | \hat{A} | \Psi_\alpha \rangle = \langle A \rangle_{\text{microcan.}}(E_\alpha)$$

Statistical description after relaxation



Momentum distribution

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



$n(k_x = 0)$ vs energy

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

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

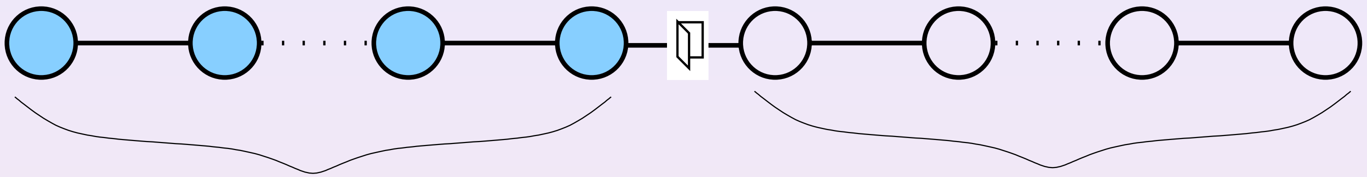
$P(E)_{mic.} \rightarrow \text{constant}$

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

One-dimensional integrable case

Similar experiment in one dimension

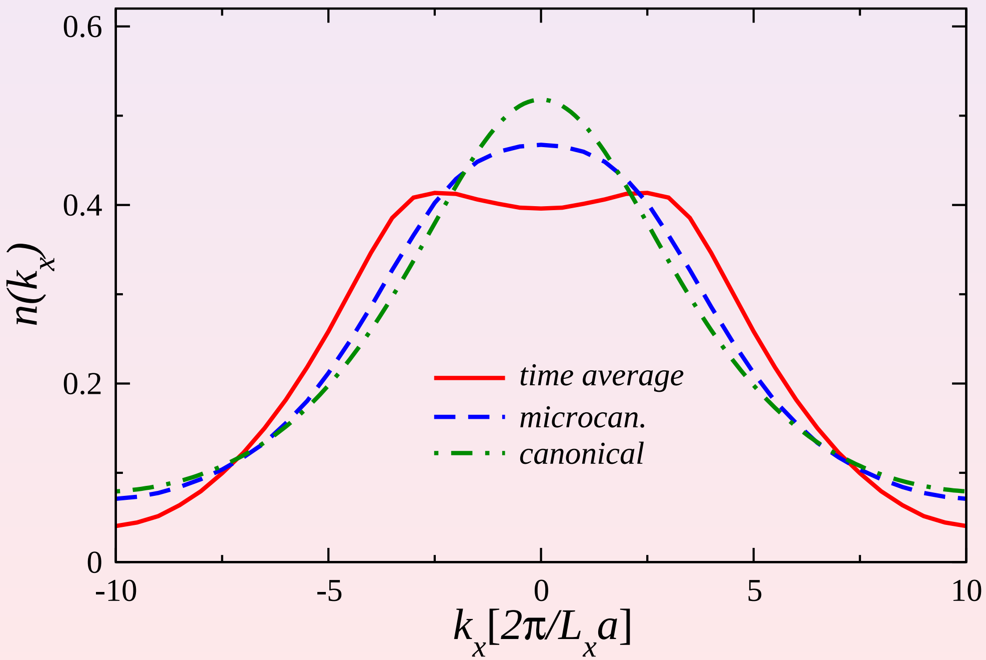
Initial



8 sites **13 sites**

Time average vs Stat. Mech.

No thermalization!



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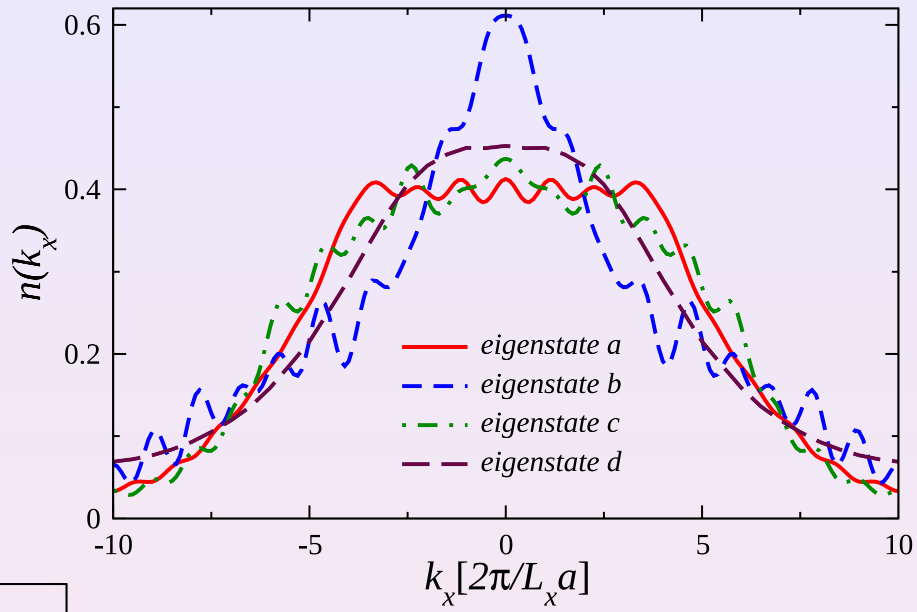

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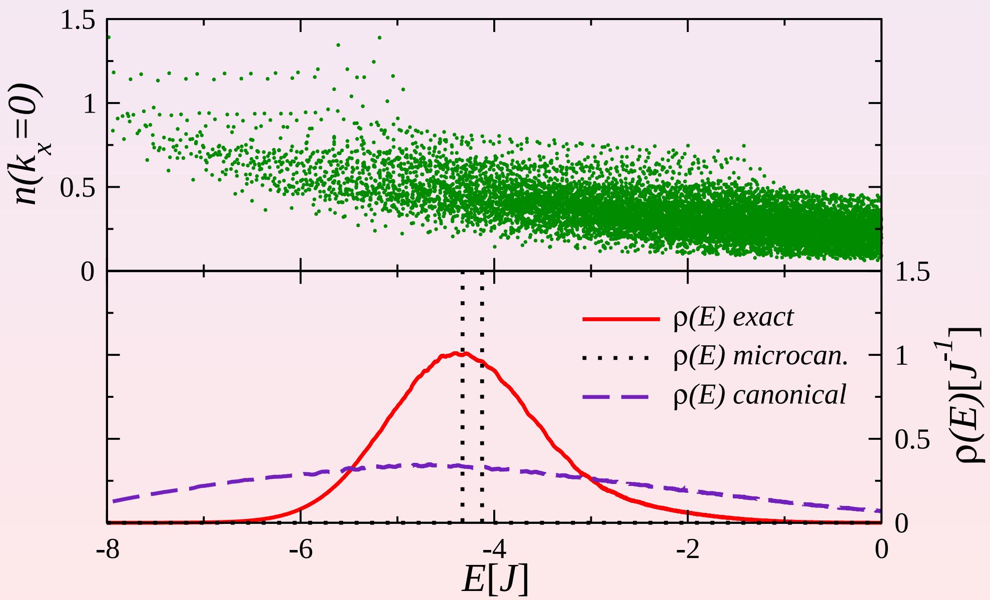

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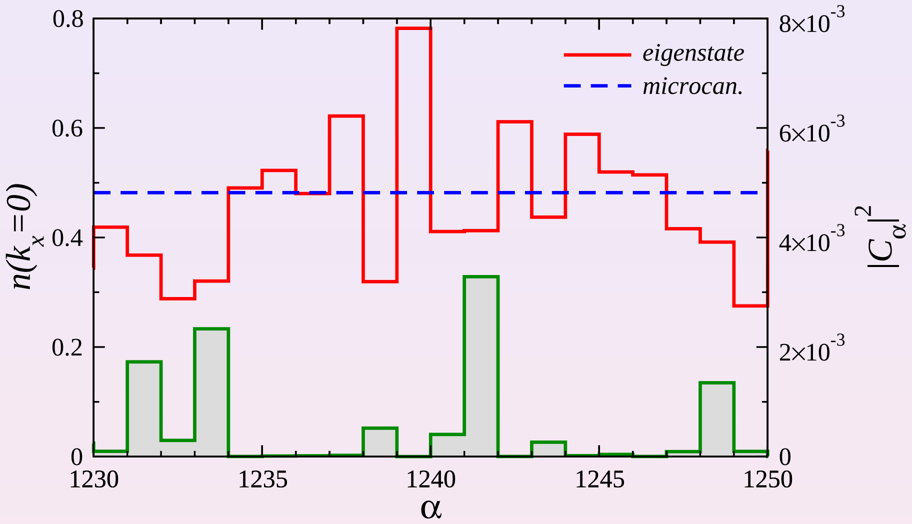
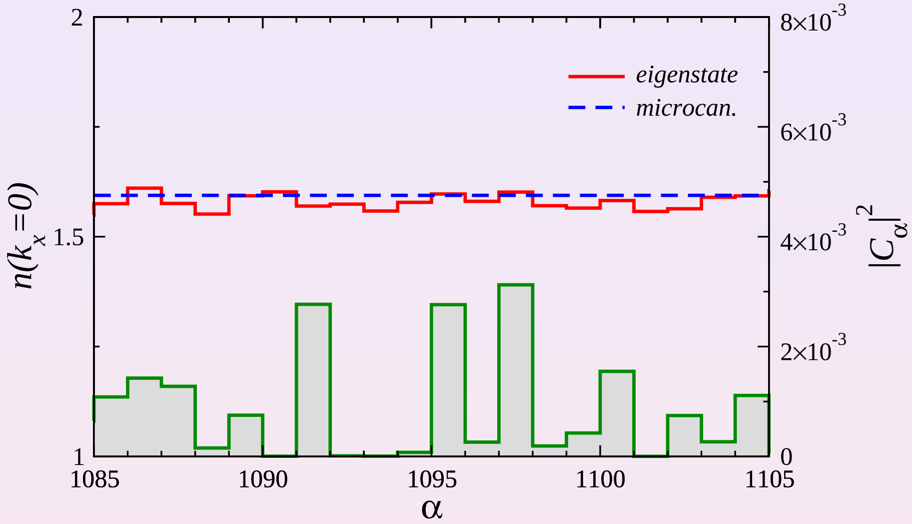
Integrable vs Nonintegrable cases

Correlations between $n(k)$ and C_α

1D (integrable) case



2D (nonintegrable) case



$\Downarrow$

Conservation laws play an important role in integrable models (Talk later today by Anibal Iucci).

$\Downarrow$

Correlations are not relevant, and they are not present!

Outline

Relaxation dynamics of hard-core boson in 2D

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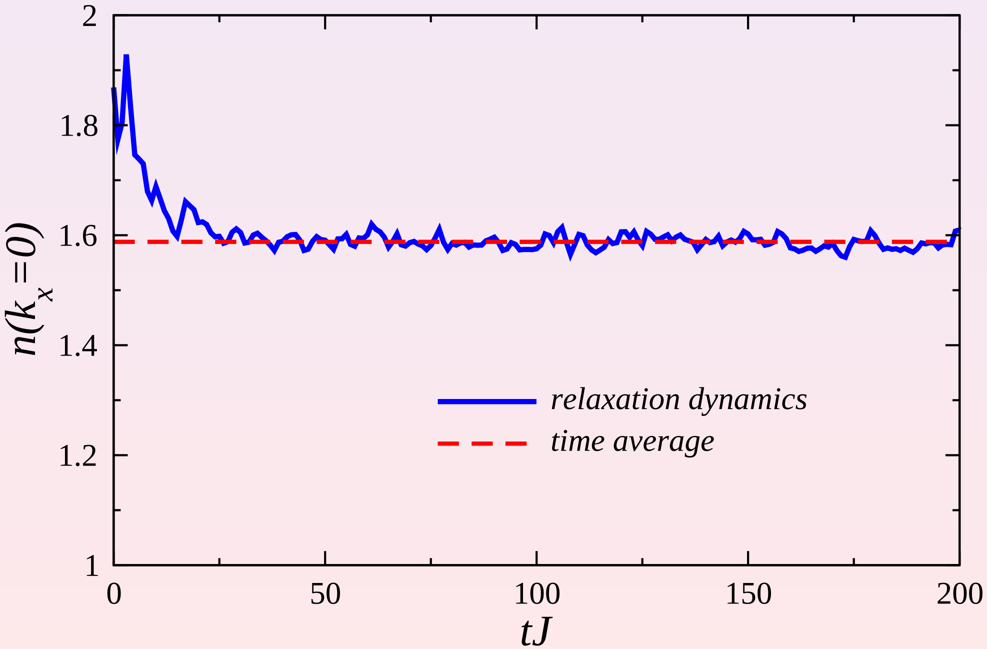
$$\widehat{H} = -J \sum_{\langle i,j \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right) + U \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j, \qquad \hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

MR, V. Dunjko, and M. Olshanii, arXiv:0708.1324 (2007).

Nonequilibrium dynamics in 2D



Weak n.n. $U = 0.1J$

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Hilbert space: $D = 20349$

All states are used!

Time fluctuations

Are they small because of dephasing?

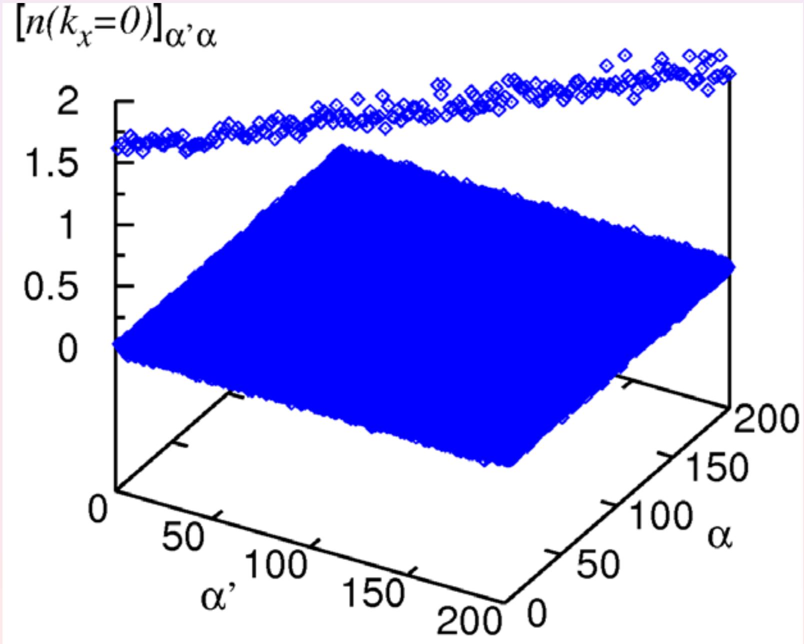
$$\langle \hat{A}(t)\rangle - \overline{\langle \hat{A}(t)\rangle} = \sum_{\substack{\alpha',\alpha \\ \alpha'\neq\alpha}} C^{\star}_{\alpha'} C_{\alpha} e^{i(E_{\alpha'}-E_{\alpha})t} A_{\alpha'\alpha} \sim \sum_{\substack{\alpha',\alpha \\ \alpha'\neq\alpha}} \frac{e^{i(E_{\alpha'}-E_{\alpha})t}}{N_{\text{states}}}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

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

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

$$\overline{\langle \hat{A}\rangle} = \sum_{\alpha} |C_{\alpha}|^2 A_{\alpha\alpha}$$

$$\sim \sum_{\alpha} \frac{1}{N_{states}} A_{\alpha\alpha} \sim A^{\text{typical}}_{\alpha\alpha}$$



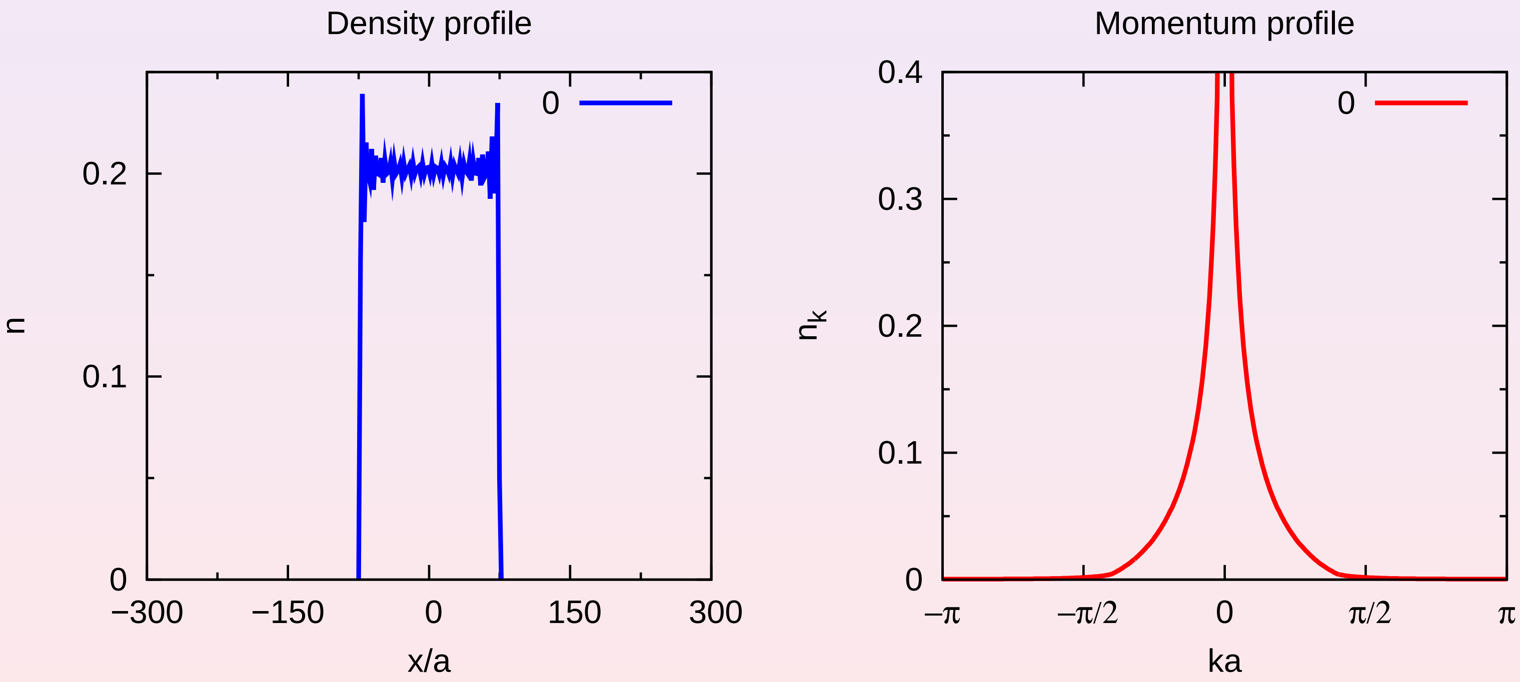
Outline

Relaxation dynamics

HCB Hamiltonian

$$H = -t \sum_i \left(b_i^\dagger b_{i+1} + h.c. \right), \qquad b_i^{\dagger 2} = b_i^2 = 0$$

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



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

Statistical description after relaxation

Thermal equilibrium

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

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

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

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

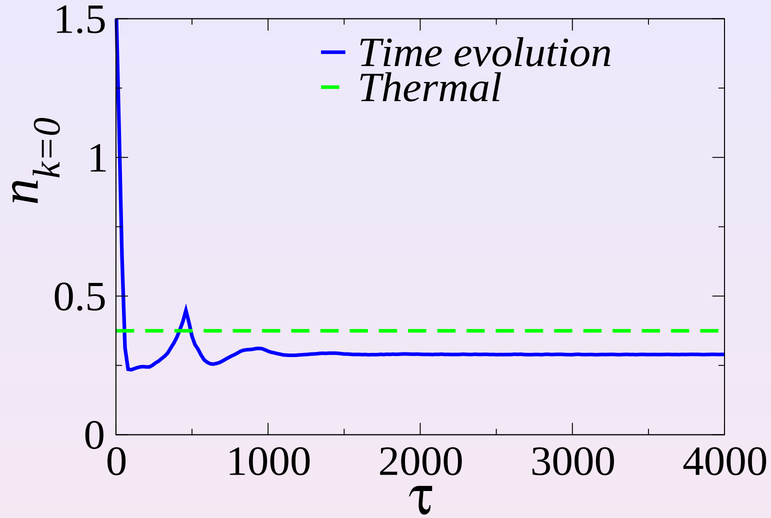
Constrained equilibrium

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

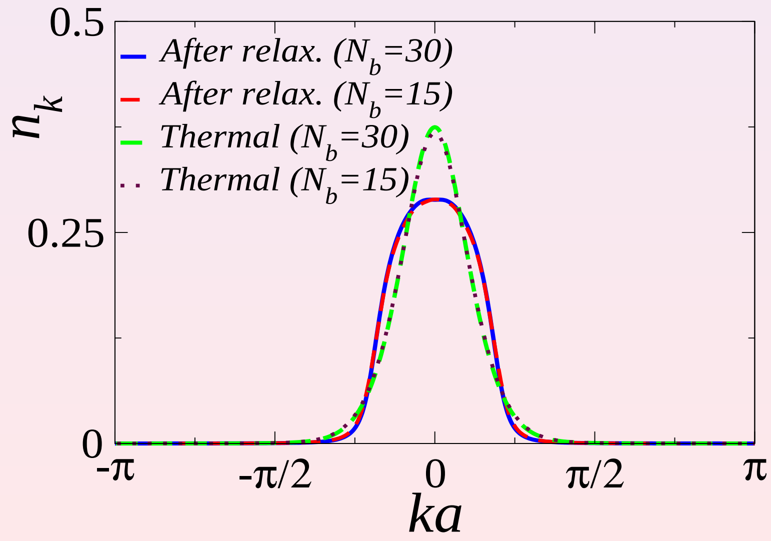
$$Z_c = \text{Tr}\left\{\exp\left[-\sum_m \lambda_m \hat{I}_m\right]\right\}$$

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

Evolution of $n_{k=0}$



n_k after relaxation



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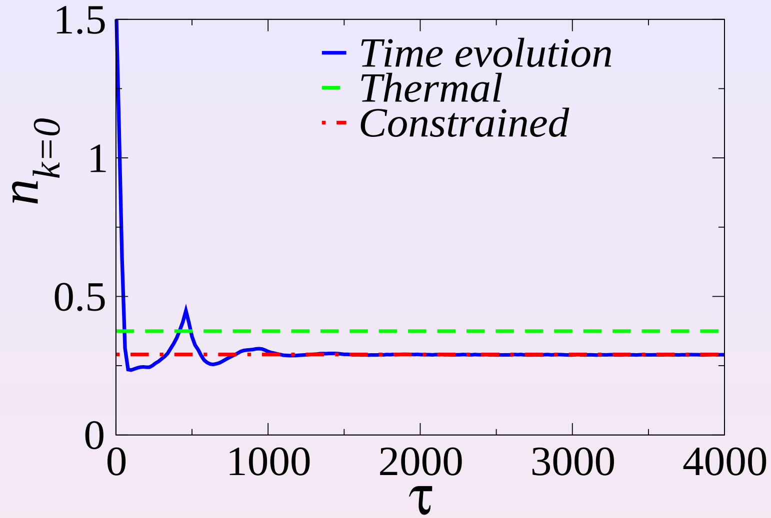

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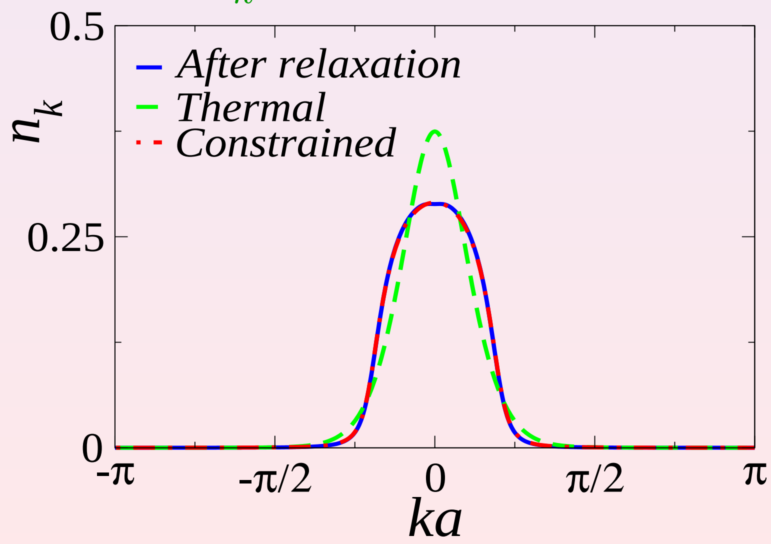
n_k after relaxation



Statistical description after relaxation

Integrals of motion

(underlying noninteracting fermions)

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

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

Lagrange multipliers

$$\lambda_k = \ln\left[\frac{1-\langle\hat{I}_k\rangle_{\tau=0}}{\langle\hat{I}_k\rangle_{\tau=0}}\right]$$

PRL 97, 156403 (2006) PHYSICAL REVIEW LETTERS week ending 13 OCTOBER 2006

Effect of Suddenly Turning on Interactions in the Luttinger Model

M. A. Cazalilla

Donostia International Physics Center (DIPC), Manuel de Lardizabal 4, 20018-Donostia, Spain

(Received 19 June 2006; published 12 October 2006)

The evolution of correlations in the *exactly* solvable Luttinger model (a model of interacting fermions in one dimension) after a suddenly switched-on interaction is *analytically* studied. When the model is defined on a finite-size ring, zero-temperature correlations are periodic in time. However, in the thermodynamic limit, the system relaxes algebraically towards a stationary state which is well described, at least for some simple correlation functions, by the generalized Gibbs ensemble recently introduced by Rigol *et al.* (cond-mat/0604476). The critical exponent that characterizes the decay of the one-particle correlation function is different from the known equilibrium exponents. Experiments for which these results can be relevant are also discussed.

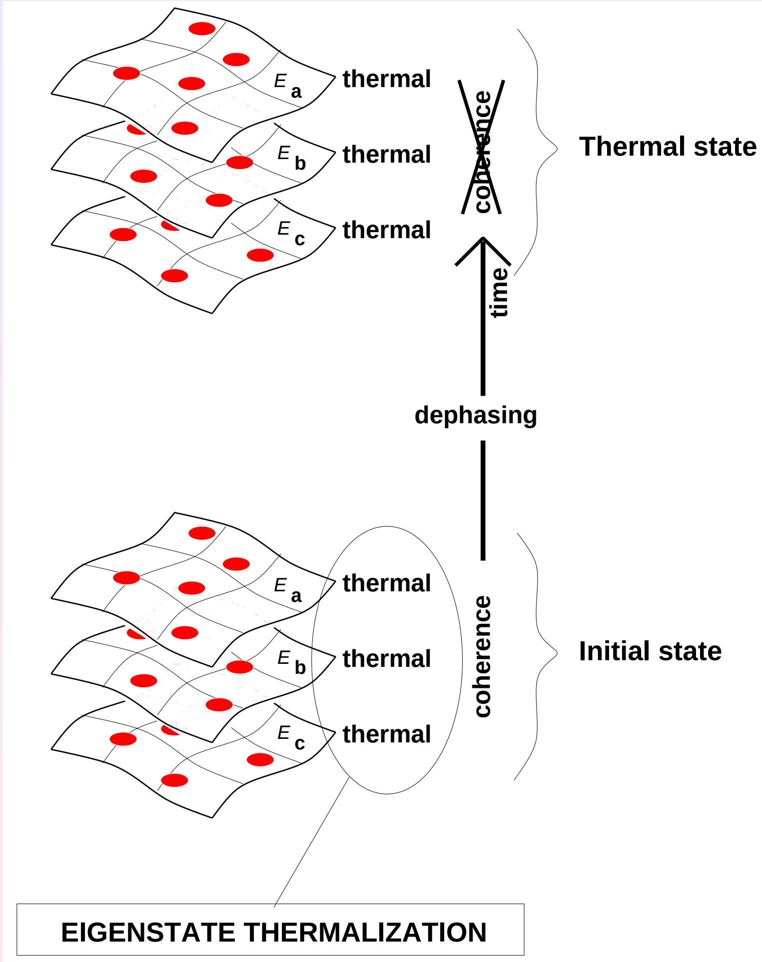
DOI: 10.1103/PhysRevLett.97.156403 PACS numbers: 71.10.Pm, 02.30.Ik, 03.75.Ss, 05.70.Ln

P. Calabrese and J. Cardy, J. Stat. Mech. 0706, P008 (2007).

M. Eckstein and M. Kollar, arXiv:0707.2789.

Summary

- Statistical mechanics works for generic isolated systems
  ★ Finite size effects
- Eigenstate thermalization hypothesis (ETH)
  ★ $\langle \Psi_\alpha | \hat{A} | \Psi_\alpha \rangle = \langle A \rangle_{\text{microcan.}}(E_\alpha)$
- Time plays only an auxiliary role
- Integrable systems are different (ETH does not hold!)
- Small time fluctuations $\longleftarrow$ smallness of off-diagonal elements



Open questions

- What happens when one moves away from an integrable point?
- Is there a quantum equivalent of the KAM theorem?

Collaborators

- Vanja Dunjko (U Mass Boston)

- Maxim Olshanii (U Mass Boston)

Open positions

Looking for a postdoc?

- Solve the exercises and send me an email. We may be starting together at Georgetown University (Washington, DC) in September 2008!

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Looking for a postdoc right away?

- Send an email to Corinna Kollath. You may be joining École Polytechnique (Paris) as early as December 2007!