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Thermalization of Quantum Gas upon Free Expansion

Jae Dong Noh (University of Seoul)

The 5th East Asian Joint Seminar on Statistical Physics
(22-25 OCT 2019, ITP/CAS, Beijing)

Overview

- Thermalization of isolated quantum systems
  - from (nonequilibrium initial state) to (equilibrium state) via unitary time evolution
  - Eigenstate Thermalization Hypothesis

- Quantum thermalization upon eigenstate Joule (free) expansion

- Reference :
  "Heating and Cooling of Quantum Gas by Eigenstate Joule Expansion",
  JD Noh, Eiki Iyoda, and Takahiro Sagawa, PRE **100**, 010106(R) (2019)

Quantum Thermalization

pedagogical lecture by D. Huse
https://www.youtube.com/watch?v=GBxtgyqvZz0

D'Alessio, L., Kafri, Y., Polkovnikov, A., & Rigol, M. (2016)
From quantum chaos and eigenstate thermalization to statistical mechanics and thermodynamics
Advances in Physics, **65**(3), 239–362

isolated quantum many-body system

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

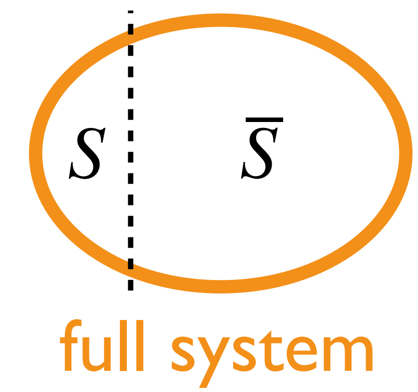
to thermalize

or not to thermalize

integrable
many-body localization
…

Statistical Mechanics vs Quantum Mechanics

for the full system, $|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle = \sum_n C_n e^{-iE_n t}|n\rangle$



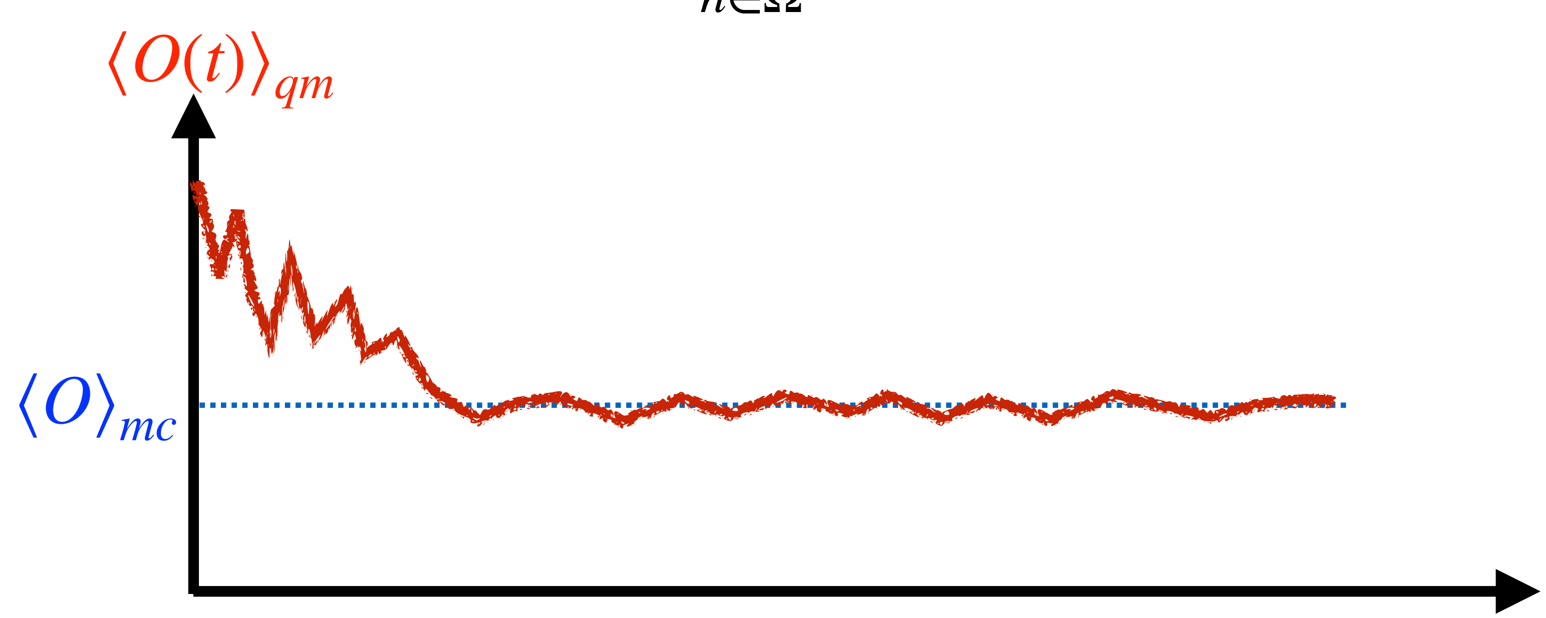
in terms of a local observable O in S

quantum mech.

$$\langle O(t)\rangle_{qm} = \langle \Psi(t)|O|\Psi(t)\rangle = \sum_n |C_n|^2 O_{nn} + \sum_{n\neq m} C_m^* C_n e^{i(E_m - E_n)t} O_{mn}$$

statistical mech.

$$\langle O\rangle_{mc} = \mathrm{Tr} O\rho_{mc} = \frac{1}{|\Omega|}\sum_{n\in\Omega} O_{nn}$$

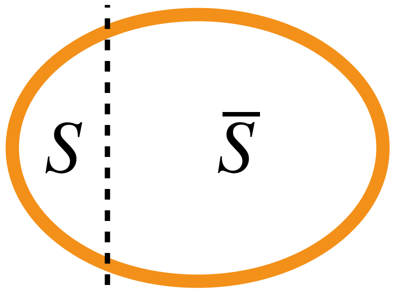


Eigenstate Thermalization Hypothesis

Eigenstate Thermalization Hypothesis

J. M. Deutsch, Phys. Rev. A 43, 2046 (1991)
M. Srednicki, Phys. Rev. E 50, 888 (1994)

ansatz in the basis of eigenstates of H



full system

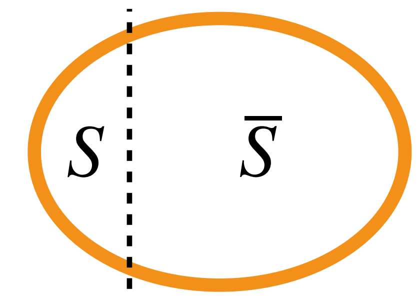
$$O_{mn} = \langle m | O | n \rangle = O(\bar{E})\delta_{m,n} + e^{-S(\bar{E})/2} f_O(\bar{E}, \omega) R_{m,n}$$

- diagonal components : depends only on E_n not explicitly on n
- $S(E)$: thermodynamic entropy
- f_O : smooth function of $\bar{E} = (E_n + E_m)/2$, $\omega = E_m - E_n$
- $R_{m,n}$ = O(1) "random" variables

Density operator

full system $\rho(t)$

subsystem S, reduced density operator $\rho_S(t) = \mathrm{Tr}_{\overline{S}}\,\rho(t)$



full system

$$H = H_S + H_{\overline{S}} + H_{int}$$

ETH

$$\lim_{|\overline{S}|\to\infty} \mathrm{Tr}_{\overline{S}} |E_n\rangle\langle E_n| = \rho_{S,eq}$$

single eigenstate ensemble

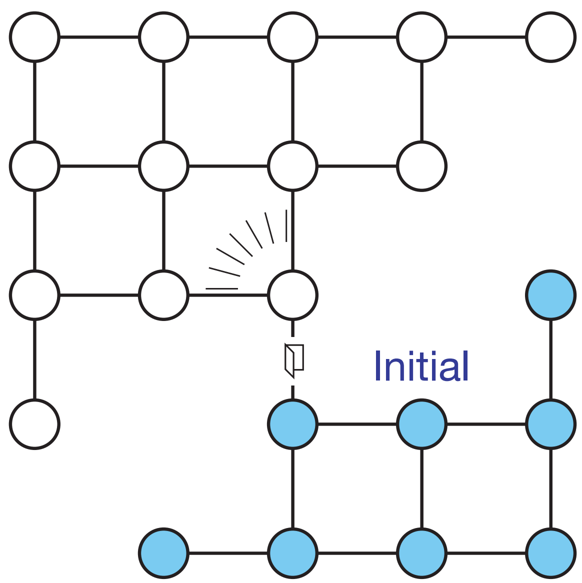
"The full system acts as a thermal reservoir to its subsystems."

nature Vol 452|17 April 2008|doi:10.1038/nature06838

LETTERS

Thermalization and its mechanism for generic isolated quantum systems

Marcos Rigol[1,2], Vanja Dunjko[1,2] & Maxim Olshanii[2]



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

hard-core bosons

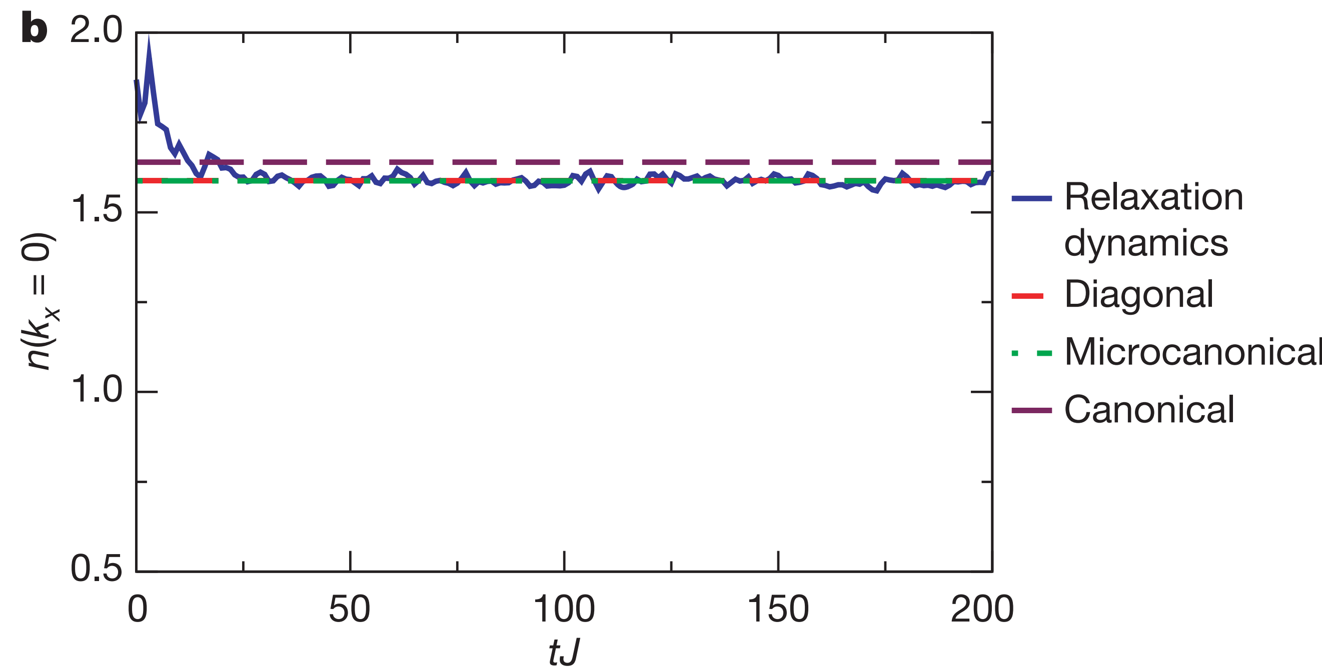
=

spin-1/2 Pauli spins

$D = 20{,}349$ (5 bosons on 21 sites)

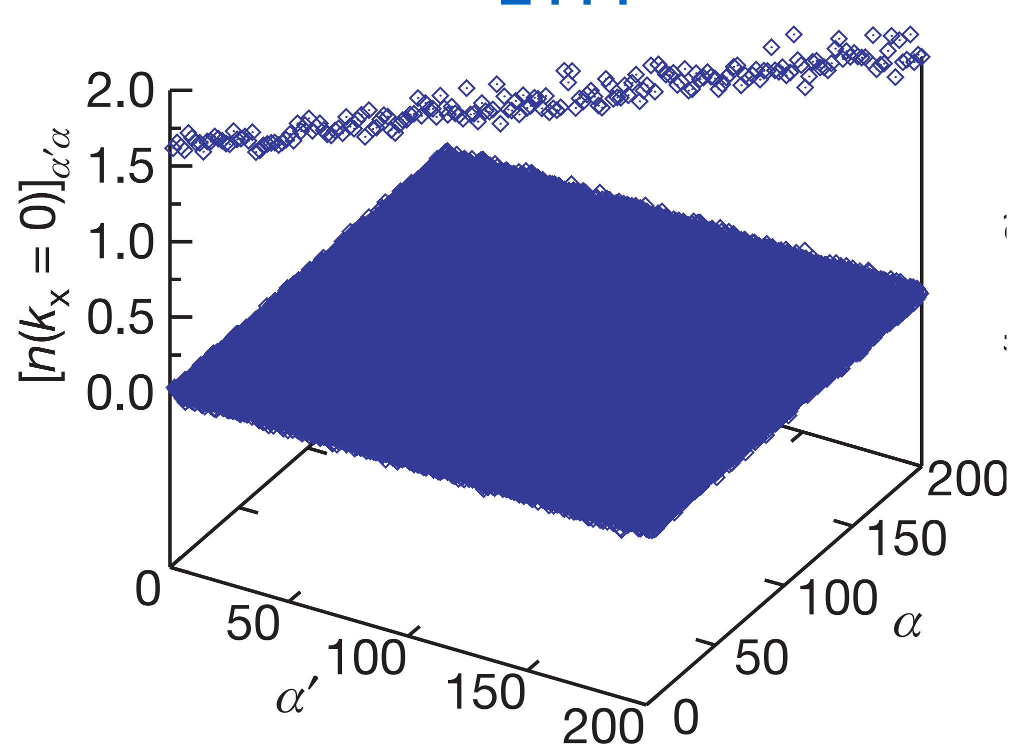
$$n(k_x, k_y) = 1/L^2 \sum_{i,j} e^{-i2\pi \mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)/L} \langle \hat{b}_i^\dagger \hat{b}_j \rangle$$

thermalization



a

ETH



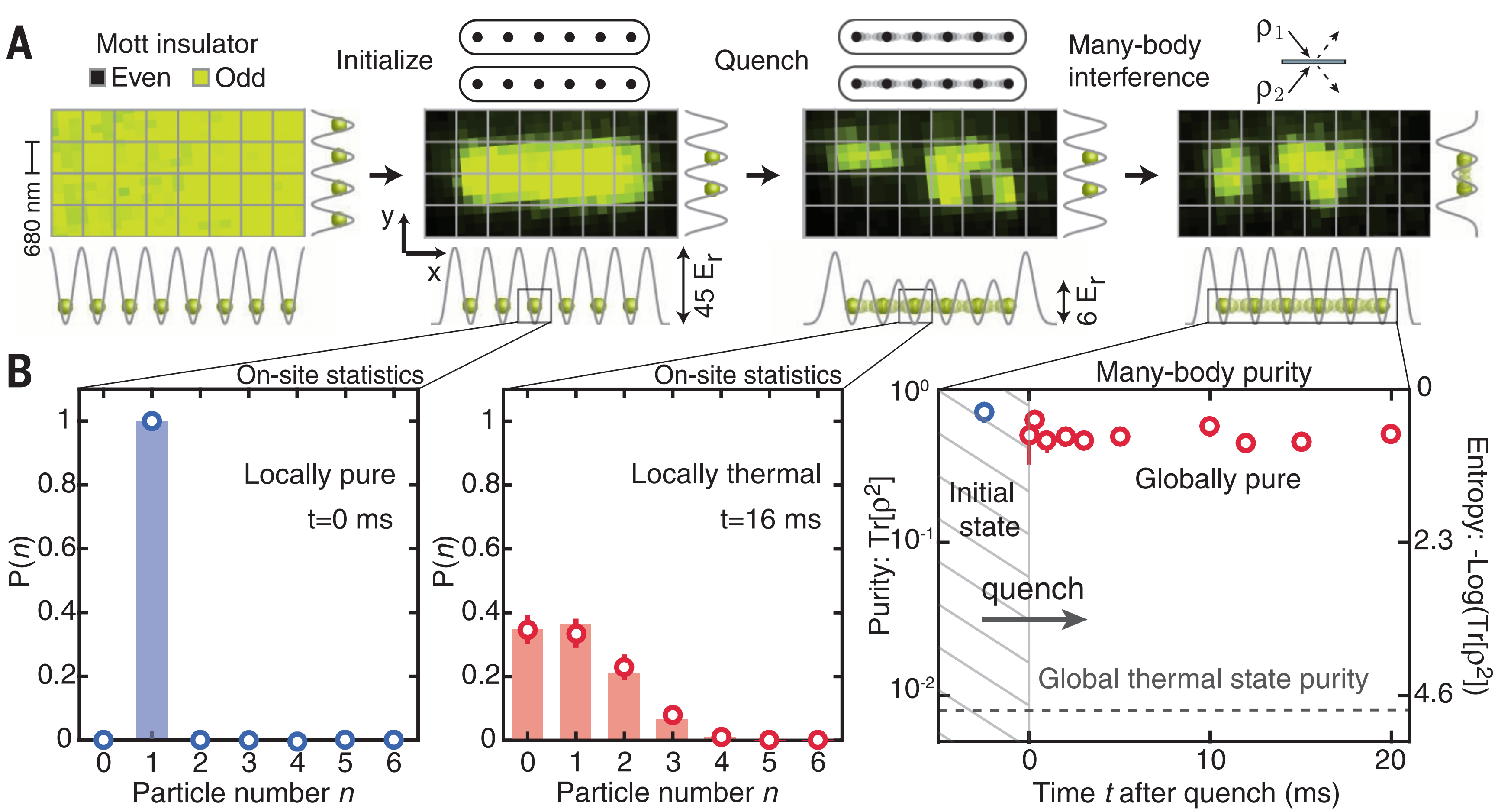
Experiments on Quantum Thermalization

Quantum thermalization through entanglement in an isolated many-body system

Adam M. Kaufman, M. Eric Tai, Alexander Lukin, Matthew Rispoli, Robert Schittko, Philipp M. Preiss, Markus Greiner*

794 19 AUGUST 2016 • VOL 353 ISSUE 6301 sciencemag.org SCIENCE

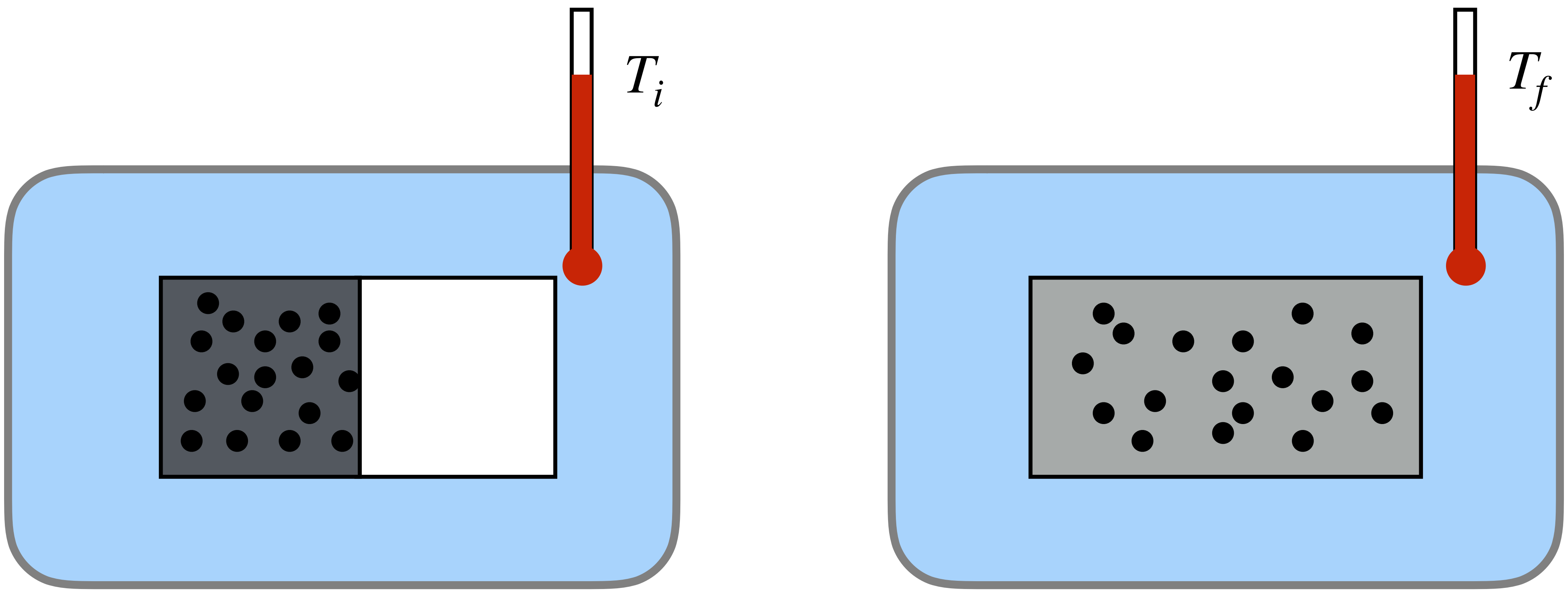
ultra-cold ^{87}Rb atoms



Eigenstate
Joule Expansion

Joule Expansion (classical)

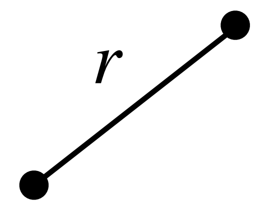
Joule's experiment in 1845

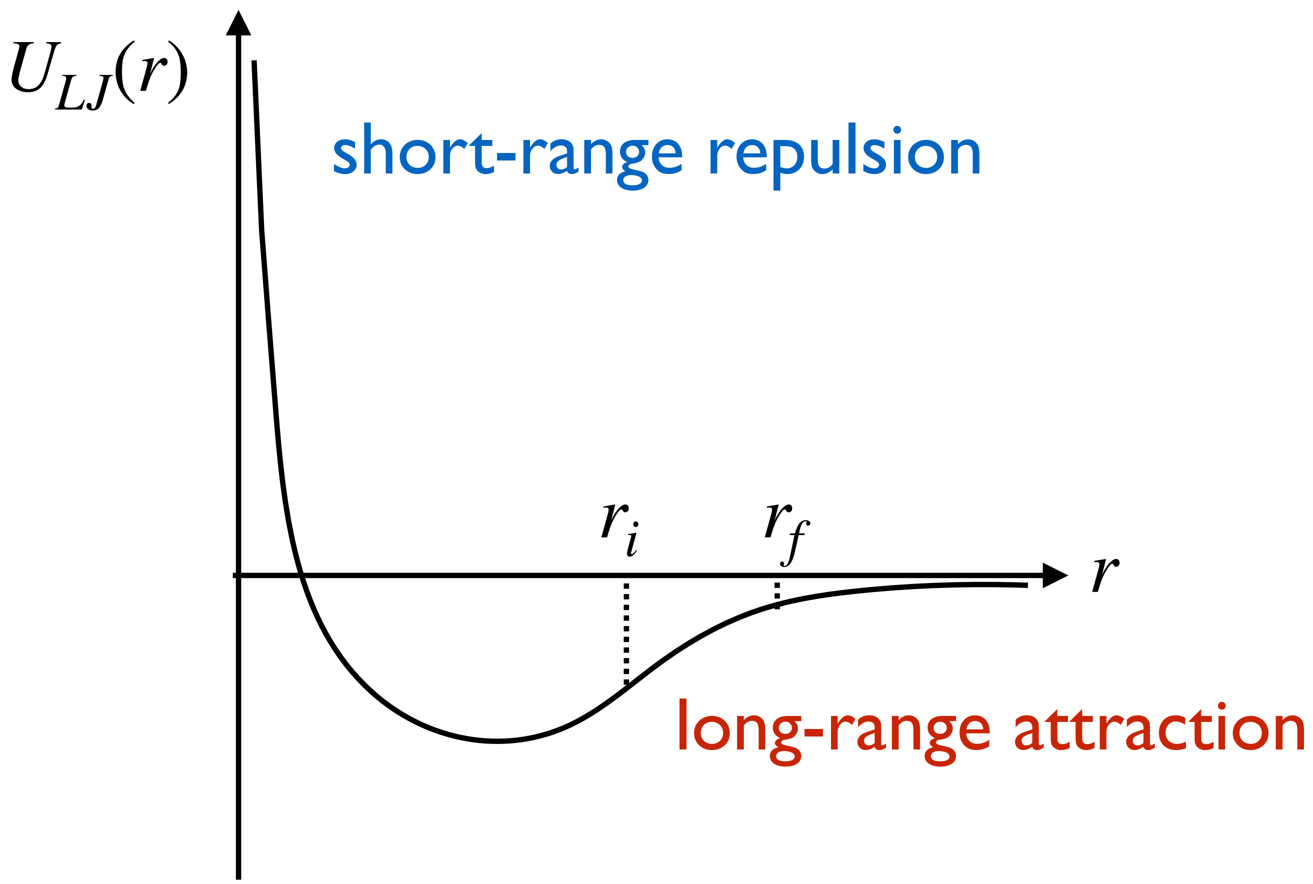


$T_f = T_i$ for the non-interacting ideal gas

Joule expansion of real gas

Lennard-Jones potential





$$E = E_K + E_U$$

upon expansion,

$r \nearrow \quad \Longrightarrow \quad E_U \nearrow$ and $E_K \searrow$

real gases cool down.

Joule expansion of real gas

Free expansion for real gases

Am. J. Phys. 61 (9), September 1993

Jacques-Olivier Goussard
Magistère de Physique, Université Denis Diderot Paris 7, France

Bernard Roulet
Groupe de Physique des Solides, associé au CNRS, URA 17, Université Paris 7 et Paris 6, Tour 23, 2, Place Jussieu, 75251-Paris Cedex 05, France

(Received 15 July 1992; accepted 18 January 1993)

It is sometimes "proved" by simple physical arguments that real gases get cooler when experiencing a free expansion. These arguments are in some way incorrect since the result is in contradiction with experiment, at least for some gases. We show how these arguments can be corrected and find that there is an "inversion temperature" for all real gases. Values of the inversion temperature can be easily estimated and are compared with experiments.

Joule coefficient $J = \left(\frac{\partial T}{\partial V}\right)_E = -\frac{1}{C_V}\left(\frac{\partial E}{\partial V}\right)_T$

$$= -\frac{1}{C_V}\left(\frac{\partial E_U}{\partial V}\right)_T$$

mean field approximation

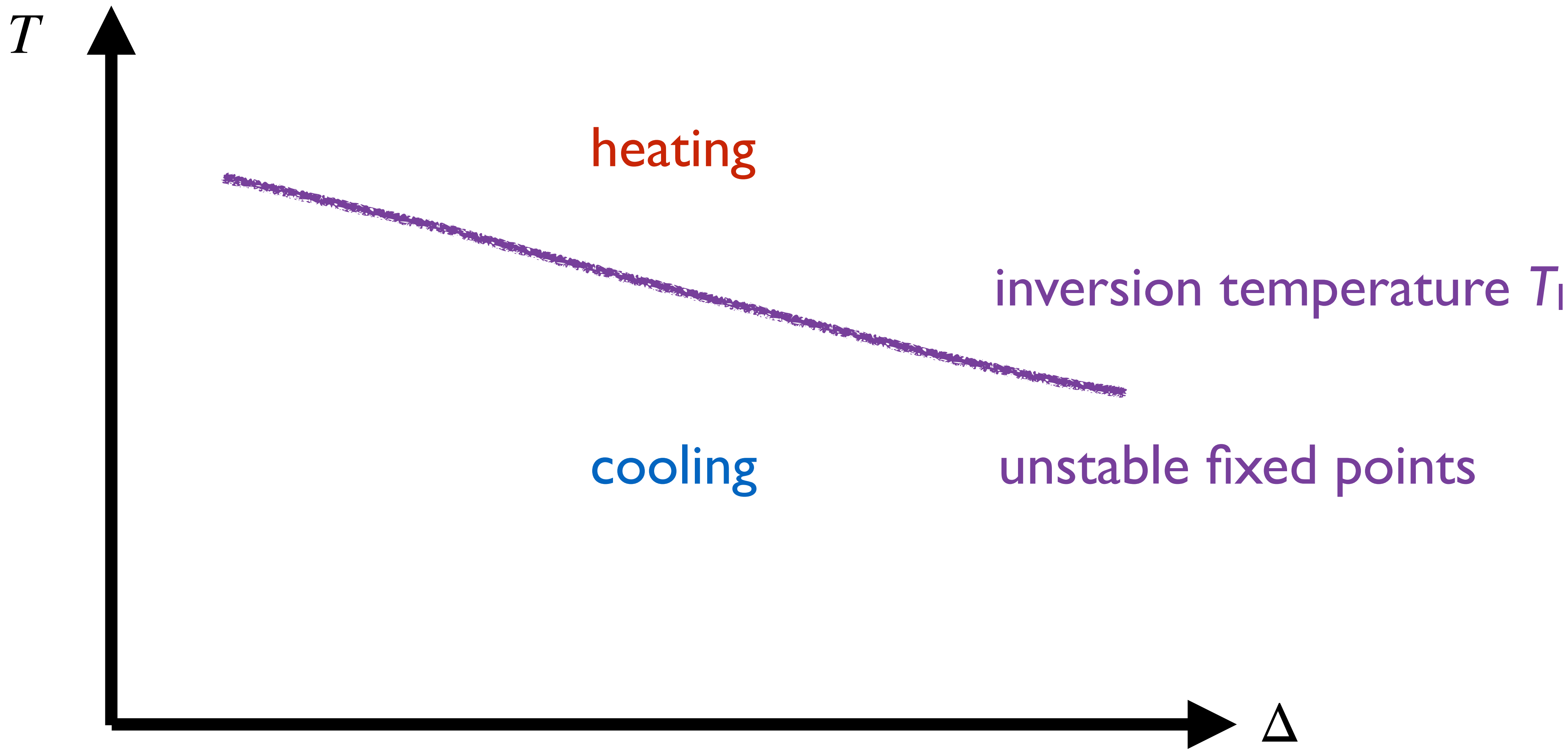
$$E_U = \frac{N(N-1)}{2} \frac{\int_V d^3r\ U_{LJ}(r) e^{-U_{LJ}(r)/T}}{\int_V d^3r\ e^{-U_{LJ}(r)/T}}$$

$$J = \frac{N^2}{2V^2 C_V} \int_V d^3r\ U_{LJ}(r) e^{-U_{LJ}(r)/T}$$

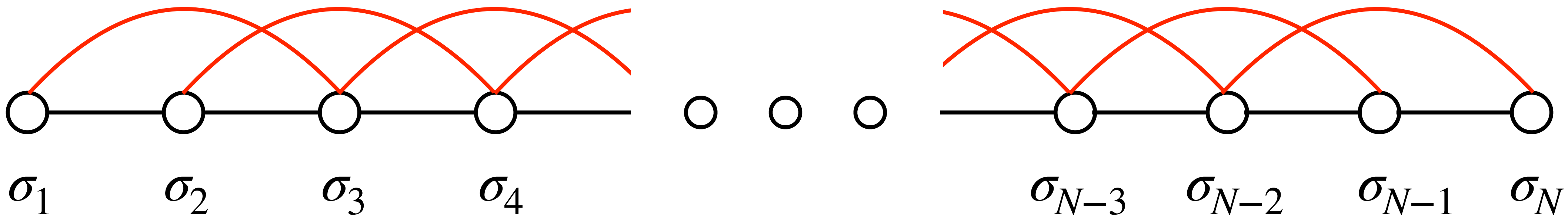
< 0 moderate temperatures

> 0 high temperatures

Inversion temperature



spin-1/2 XXZ chain

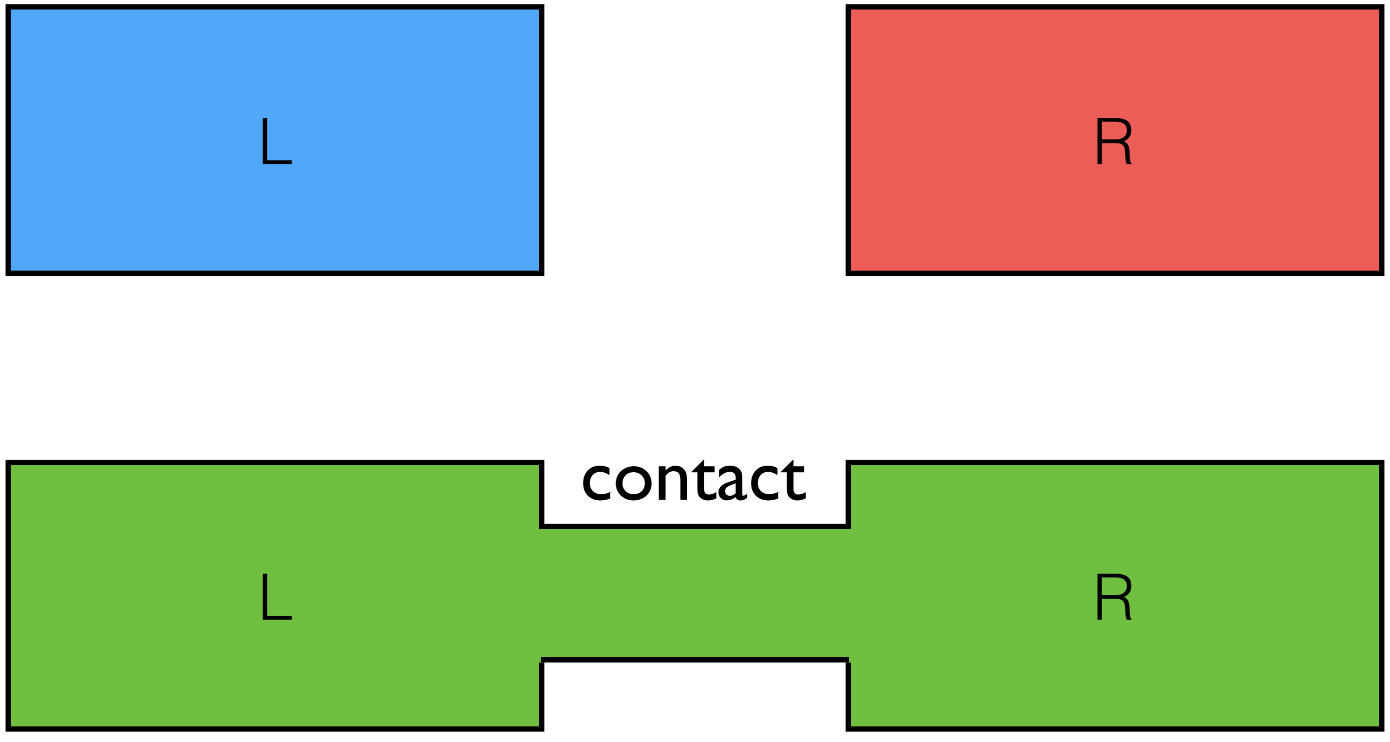


$$H_{XXZ} = \frac{1}{1+\lambda}\left(H_{XXZ1} + \lambda H_{XXZ2}\right)$$

λ : degree of integrability breaking

Eigenstate Thermalization Hypothesis for nonzero λ

spin-1/2 lattice fermions = hardcore bosons


L
R
contact
L
R

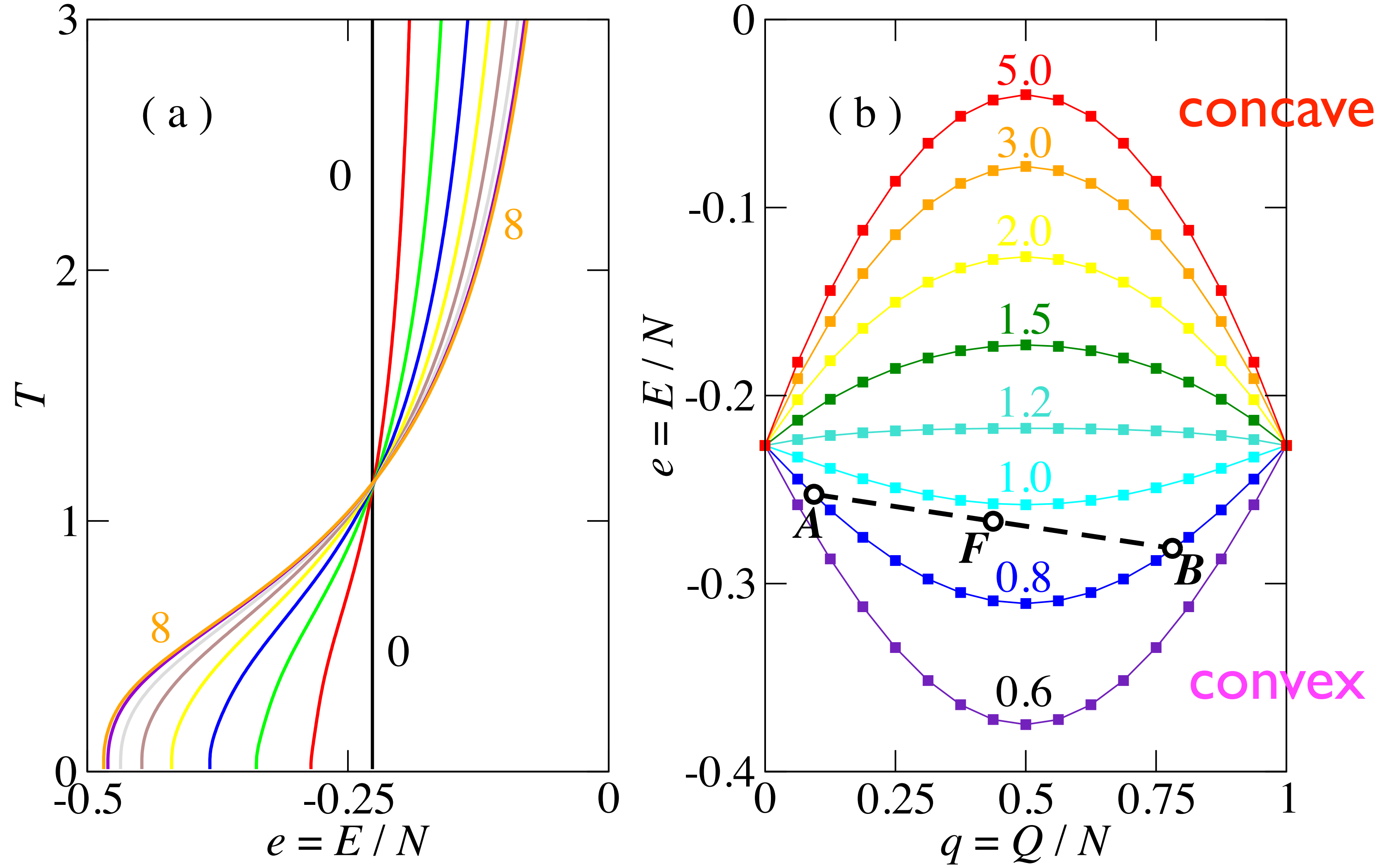
Energy vs Temperature

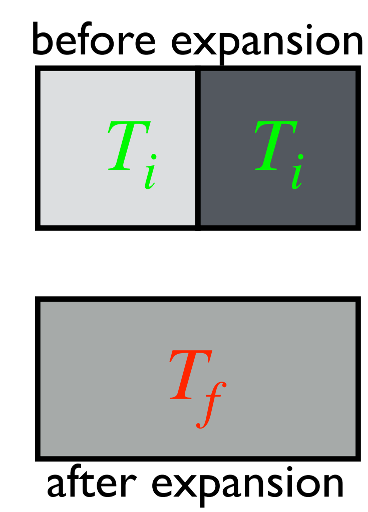
energy eigenstates $H_{XXZ}|Q,n\rangle = E_{Q,n}|Q,n\rangle \qquad n = 0,1,\cdots,\binom{N}{Q}-1$

temperature $T_{Q,n} \leftrightarrow |Q,n\rangle \qquad E_{Q,n} = \frac{1}{Z_Q}\sum_l E_{Q,l}e^{-E_{Q,l}/T_{Q,n}}$

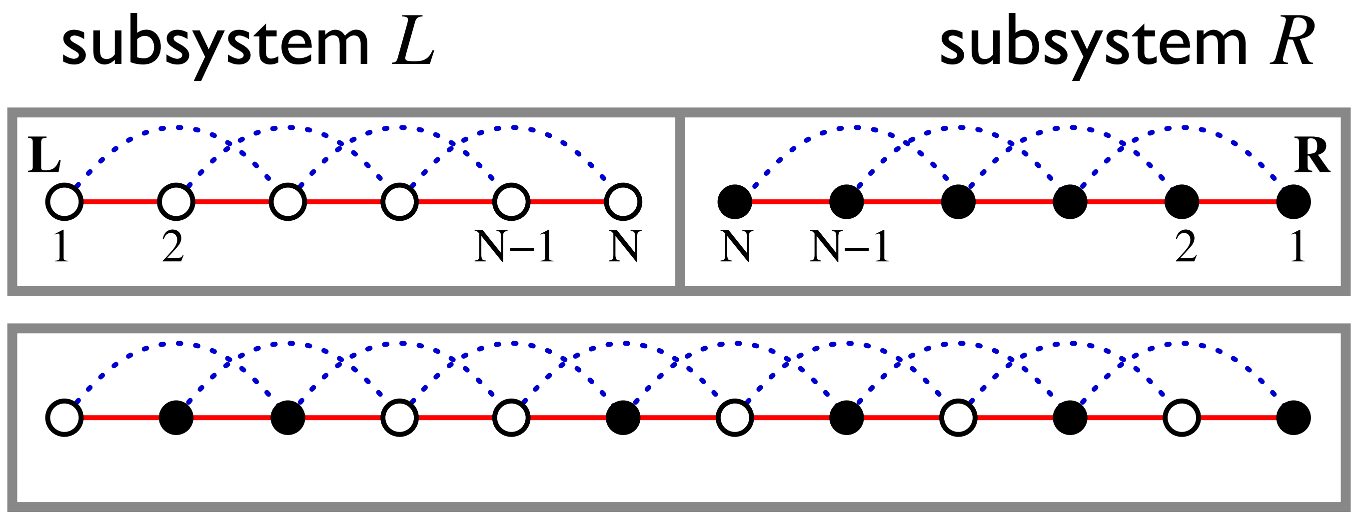
numerical exact diagonalization (D_{max} = 12,870)

$(N = 16,\ \Delta = 1/2,\ \lambda = 1)$





Coupled XXZ chains



Hamiltonian $H = H_L + H_R + H_{int.}$

initial state $|\Psi(0)\rangle = |Q_L, n_L\rangle \otimes |Q_R, n_R\rangle$ pure state

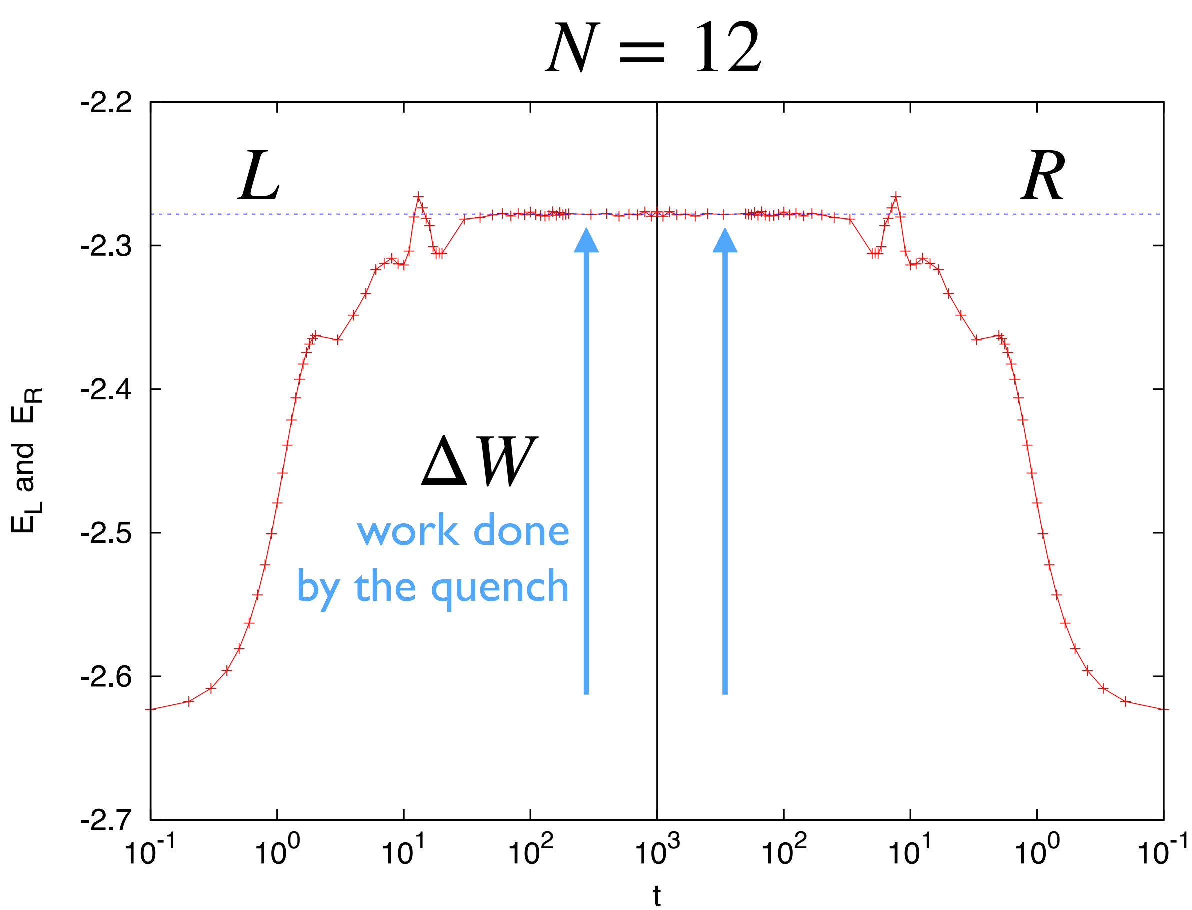
unitary time evolution after quenching $|\Psi(t)\rangle = e^{-iHt}|\Psi(0)\rangle$ full diaginalization of H or Lie-Suzuki-Trotter decomposition

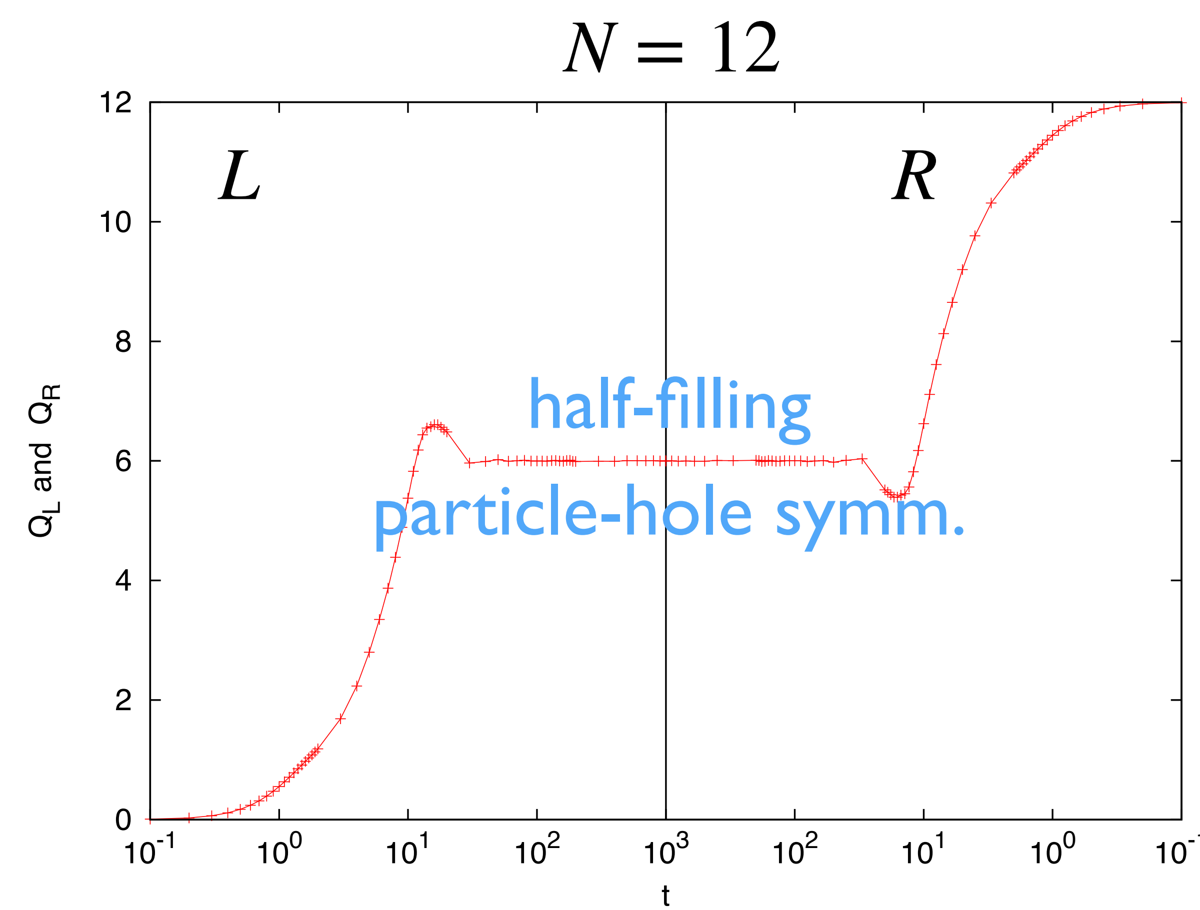
reduced density matrix $\rho_L = \mathrm{Tr}_R|\Psi(t)\rangle\langle\Psi(t)|$ singular value decomposition

Joule expansion into vacuum

Initial condition : Subsystem L is empty, while subsystem R is fully occupied.

$$|\Psi(0)\rangle = |0\rangle \otimes \cdots \otimes |0\rangle \otimes |1\rangle \cdots \otimes |1\rangle \Rightarrow |\Psi(t)\rangle$$

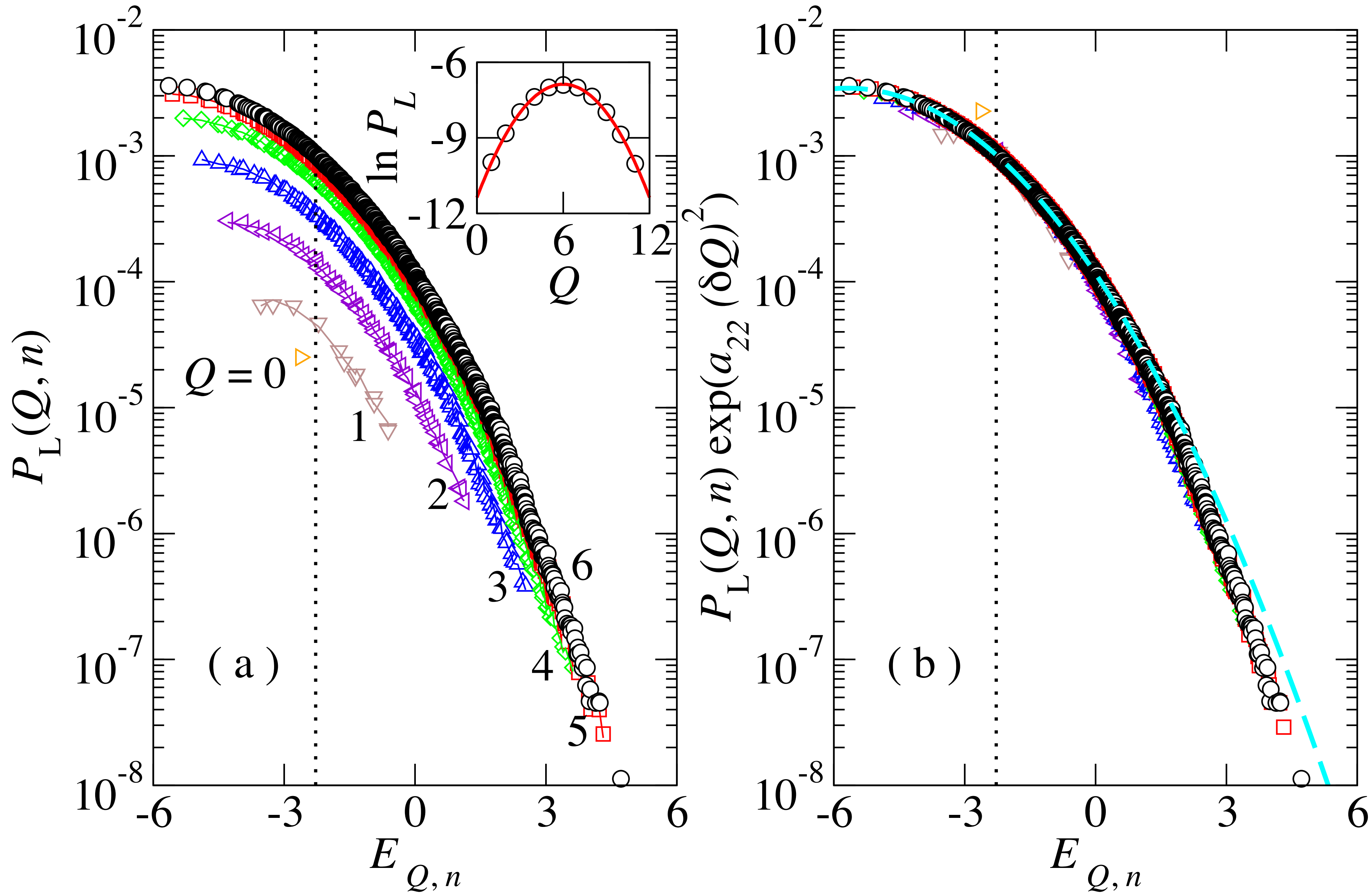




homogeneous steady state

Joule expansion into vacuum

probability distribution $P_L(Q,n) = \langle Q,n|\rho_L|Q,n\rangle$



Probability distribution

quantum thermalization

$$P_L(Q,n) \propto \exp\left[S_R(E_{tot} - E_{Q,n}, Q_{tot} - Q)\right]$$ (weak coupling limit)

let $\delta E = E_{Q,n} - \bar{E}_L$ and $\delta Q = Q_L - \bar{Q}_L$

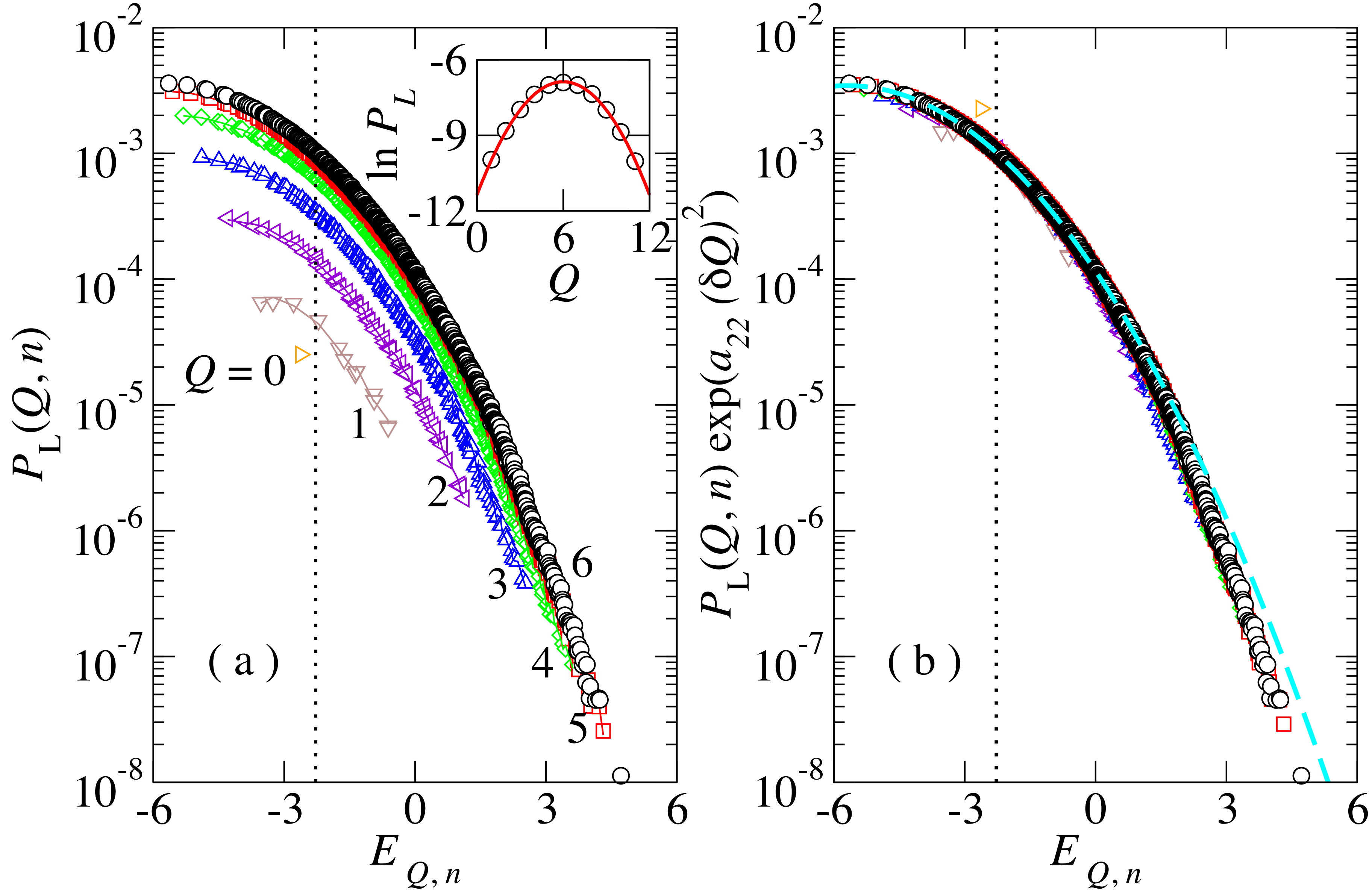
grand canonical ensemble (like) distribution

$$P_L(Q,n) \propto \exp\left[-(\delta E - \mu \delta Q)/T - a_{11}(\delta E)^2 - 2a_{12}(\delta E)(\delta Q) - a_{22}(\delta Q)^2 + \cdots\right]$$

Probability distribution

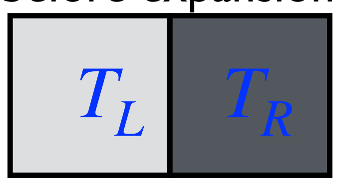
$$P_L(Q,n) \propto \exp\left[-(\delta E - \mu\delta Q)/T - a_{11}(\delta E)^2 - 2a_{12}(\delta E)(\delta Q) - a_{22}(\delta Q)^2 + \cdots\right]$$

particle-hole symmetry ($\mu = a_{12} = 0$)

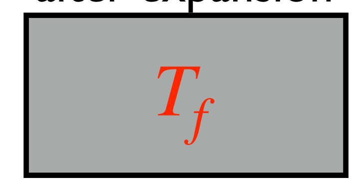


Heating/Cooling by Joule expansion

before expansion

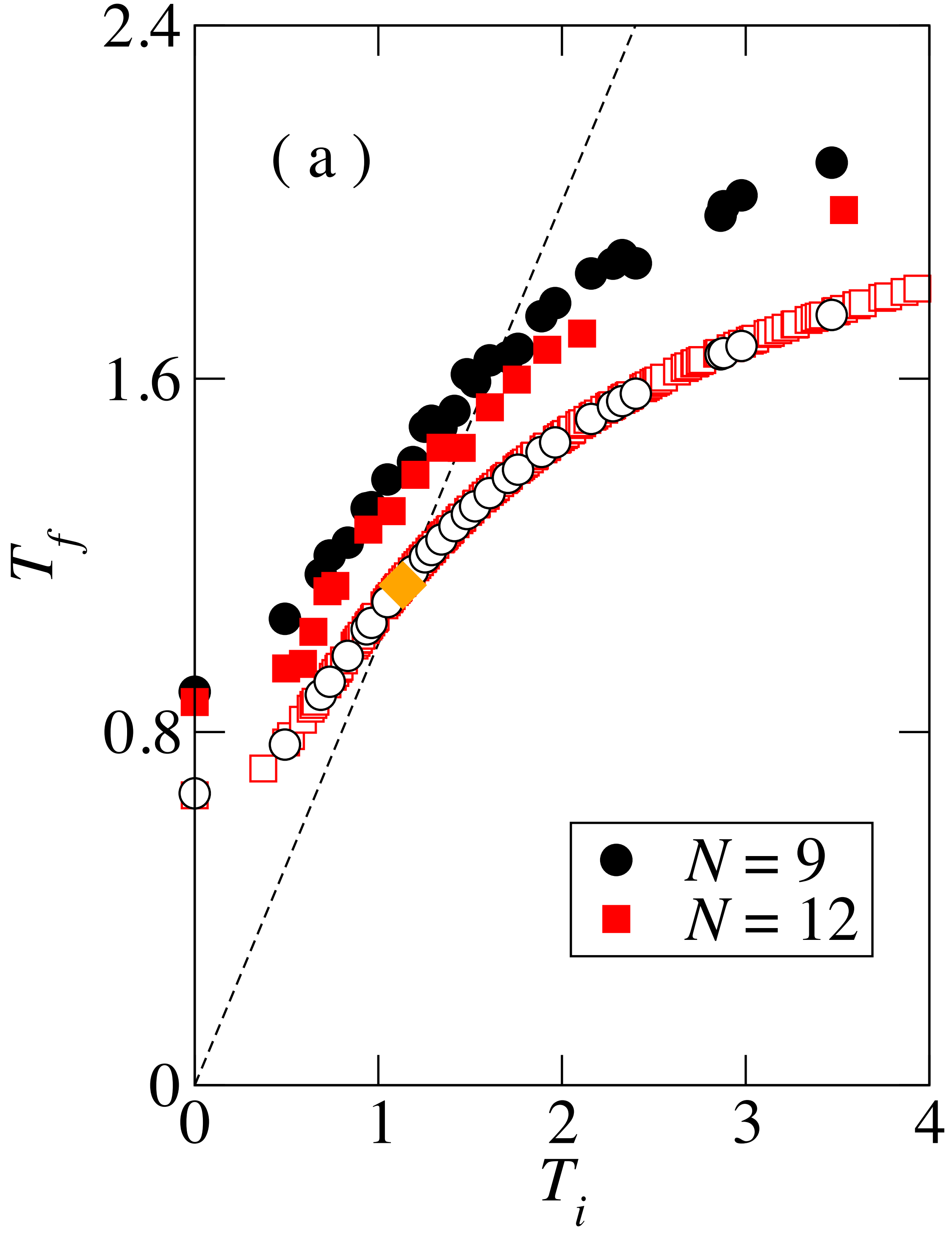


after expansion

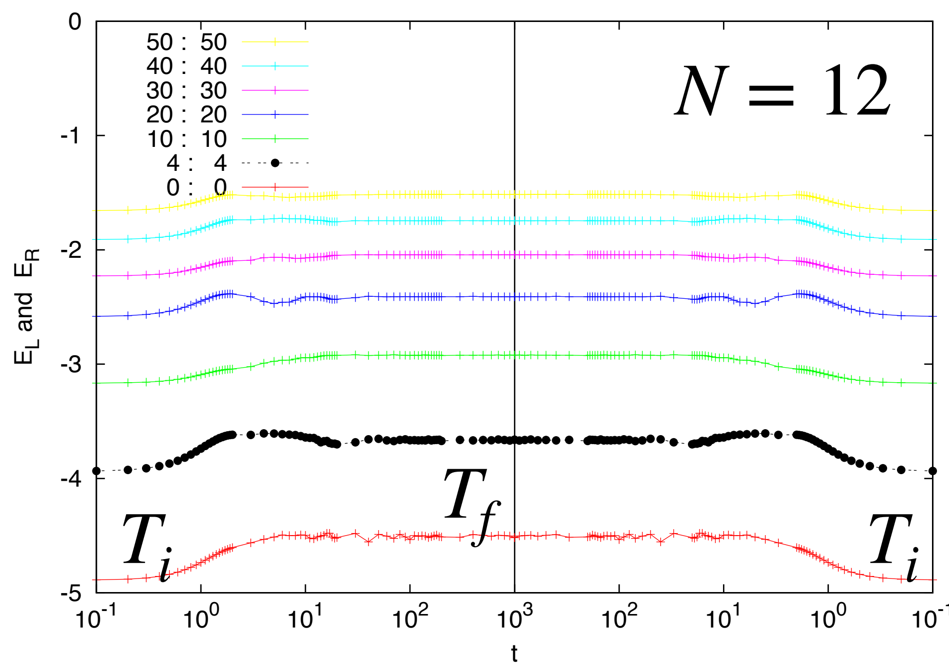


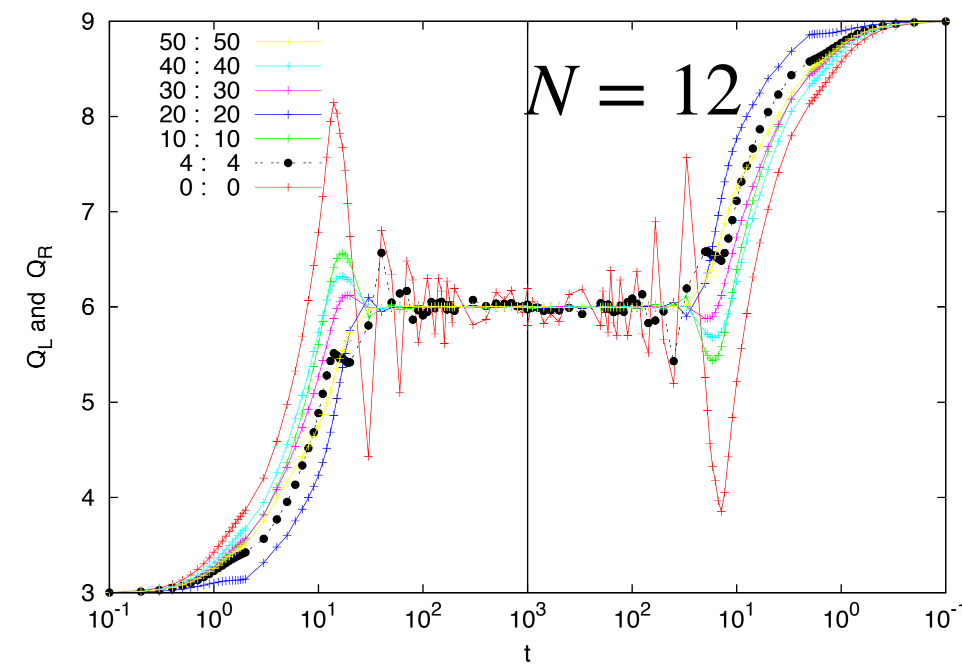
$(q_L = Q_L/N, q_R = Q_R/N)$	particle density	$q = (Q_L + Q_R)/(2N)$
$\lvert Q_L, n_L\rangle \otimes \lvert Q_R, n_R\rangle$	wave function	$e^{-iHt}\lvert\Psi(0)\rangle$
$T_L = T(Q = Q_L, E = E_{Q_L,n_L})$	temperature	$T_f = T\left(\dfrac{Q_L + Q_R}{2}, \dfrac{E_{Q_L,n_L} + E_{Q_R,n_R}}{2}\right)$
$T_R = T(Q = Q_R, E = E_{Q_R,n_R})$		$P_L(Q,n) \propto \exp\left\{-\dfrac{\delta E}{T_f} - \dfrac{(\delta E)^2}{2T_f^2 C_v}\right\}$

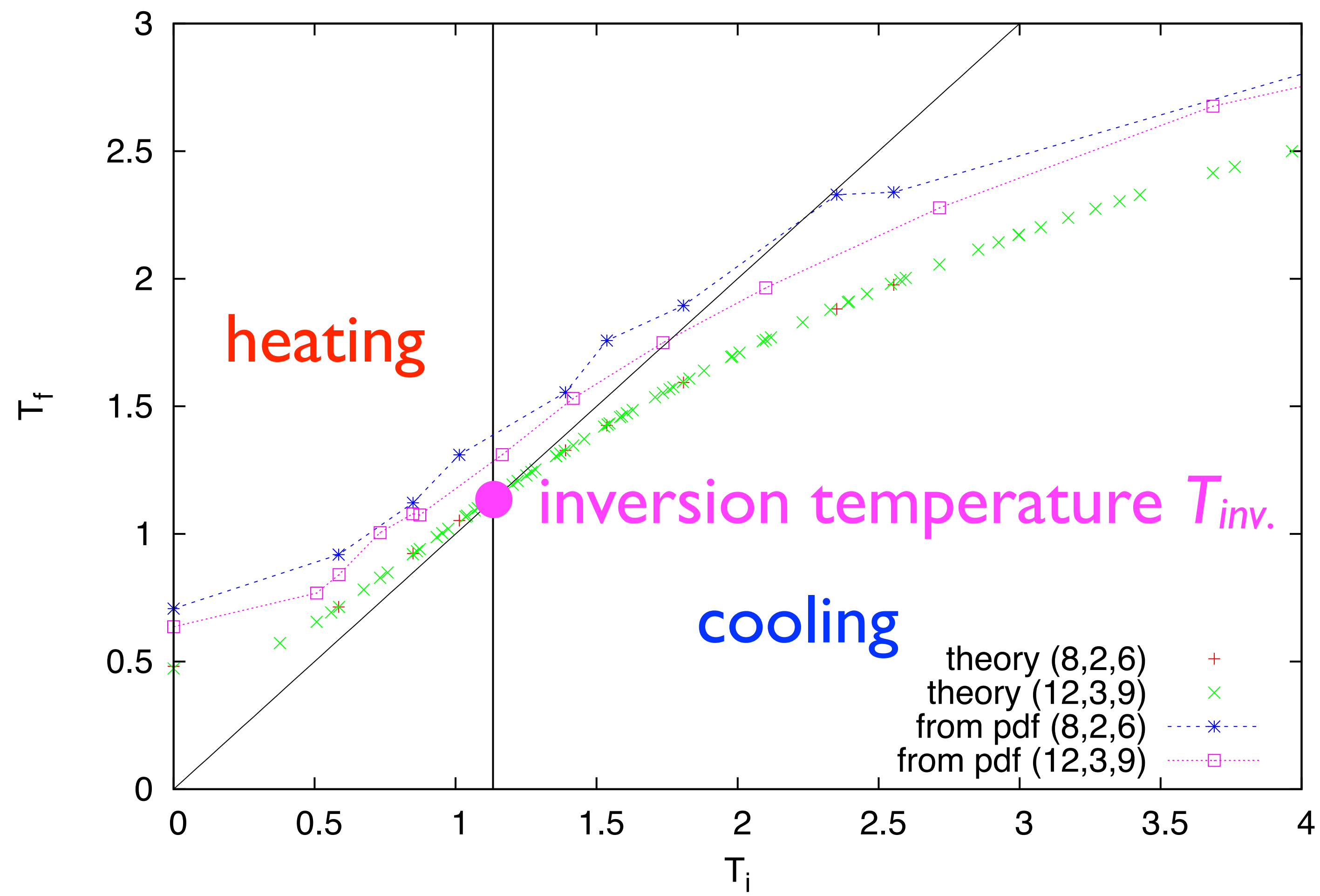
$q_L = 0, q_R = 1$



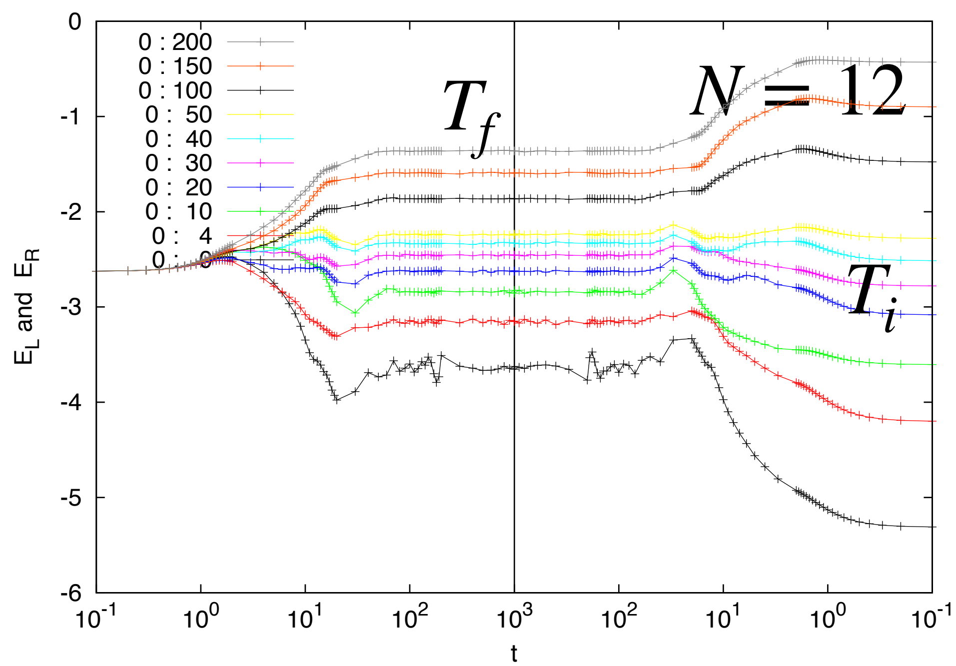
$q_L = 1/4, q_R = 3/4, n_L = n_R$



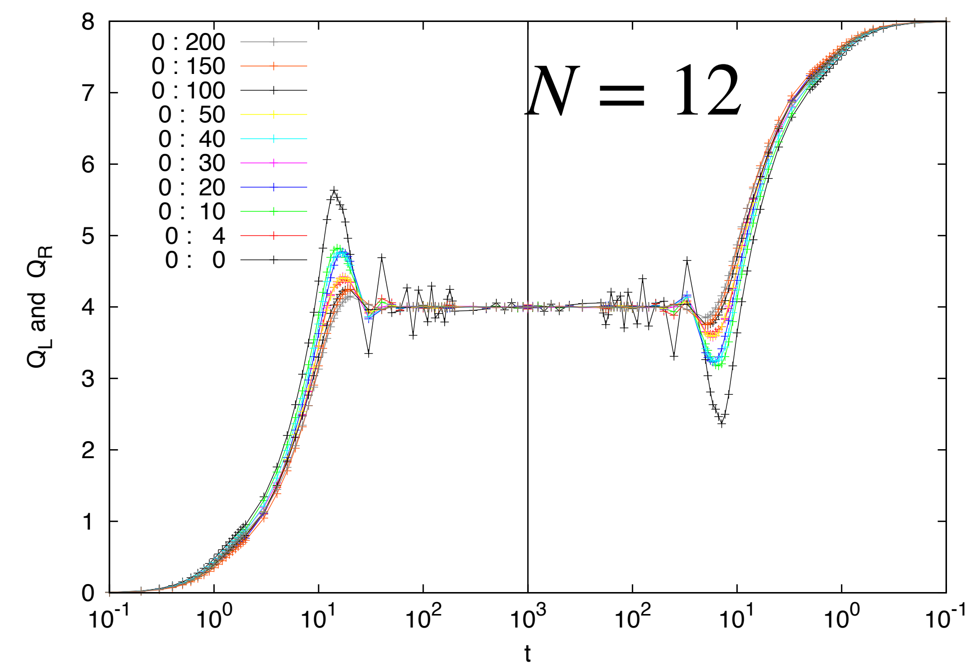




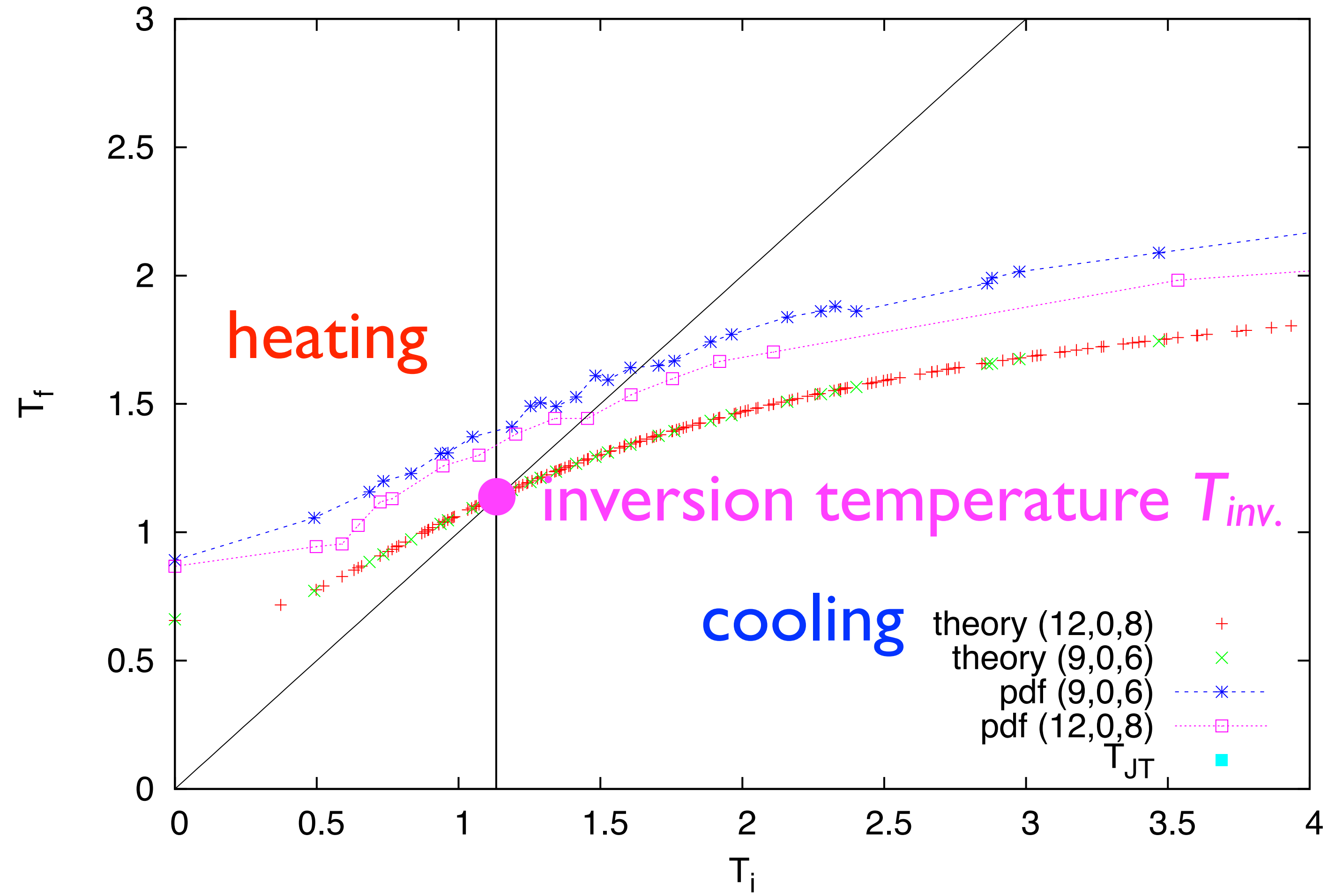
$q_L = 0, q_R = 2/3, n_L = 0$



0 : 200
0 : 150
0 : 100
0 : 50
0 : 40
0 : 30
0 : 20
0 : 10
0 : 4
0 : 0
T_f
$N = 12$
T_i
E_L and E_R
t

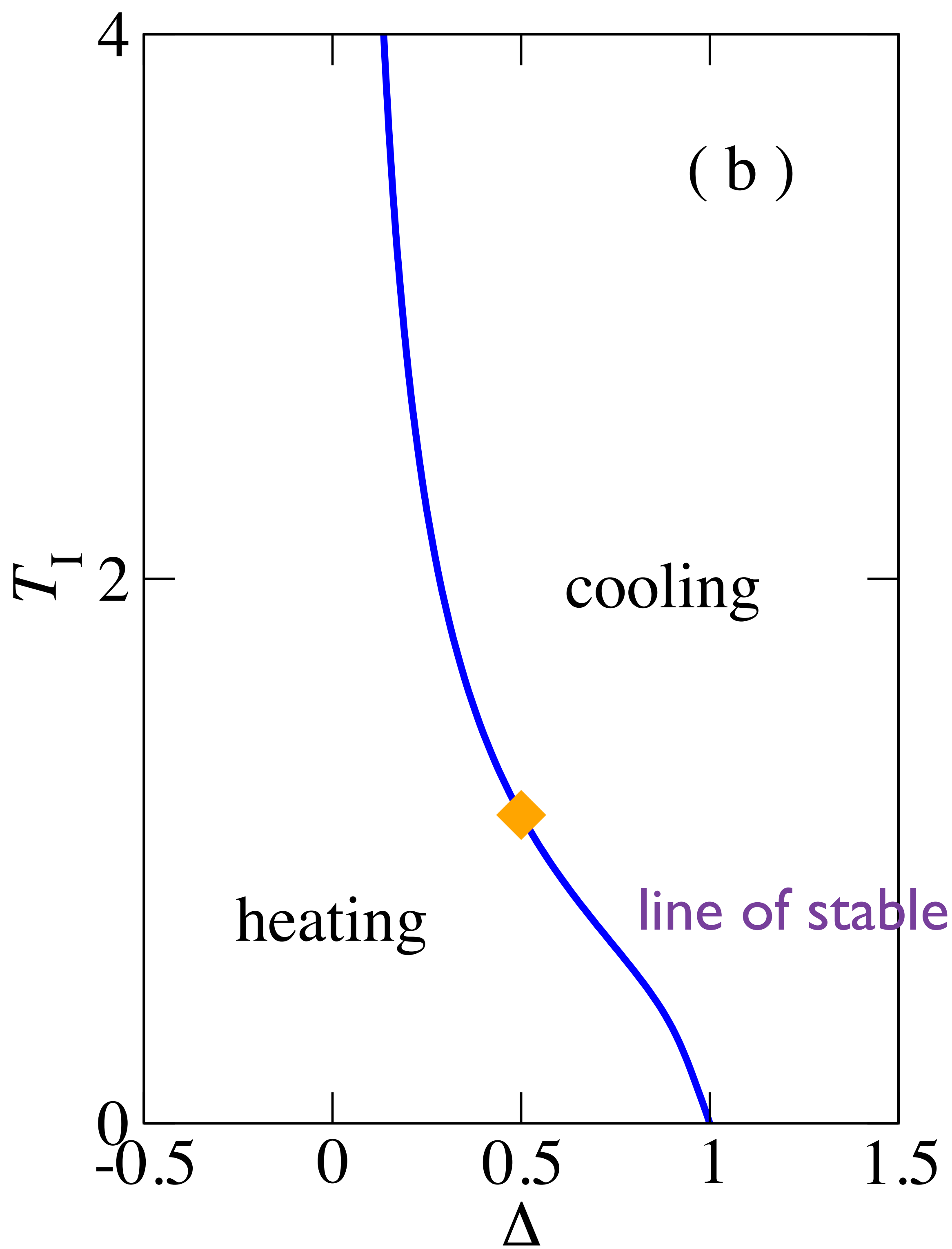


0 : 200
0 : 150
0 : 100
0 : 50
0 : 40
0 : 30
0 : 20
0 : 10
0 : 4
0 : 0
$N = 12$
Q_L and Q_R
t



heating
inversion temperature $T_{inv.}$
cooling
theory (12,0,8)
theory (9,0,6)
pdf (9,0,6)
pdf (12,0,8)
T_{JT}
T_f
T_i

Inversion Temperature



line of stable fixed points

temperature control
of ultracold atoms

nature physics
ARTICLES
PUBLISHED ONLINE: 15 JANUARY 2012 | DOI: 10.1038/NPHYS2205

Fermionic transport and out-of-equilibrium dynamics in a homogeneous Hubbard model with ultracold atoms

Ulrich Schneider[1,2]*, Lucia Hackermüller[1,3], Jens Philipp Ronzheimer[1,2], Sebastian Will[1,2], Simon Braun[1,2], Thorsten Best[1], Immanuel Bloch[1,2,4], Eugene Demler[5], Stephan Mandt[6], David Rasch[6] and Achim Rosch[6]

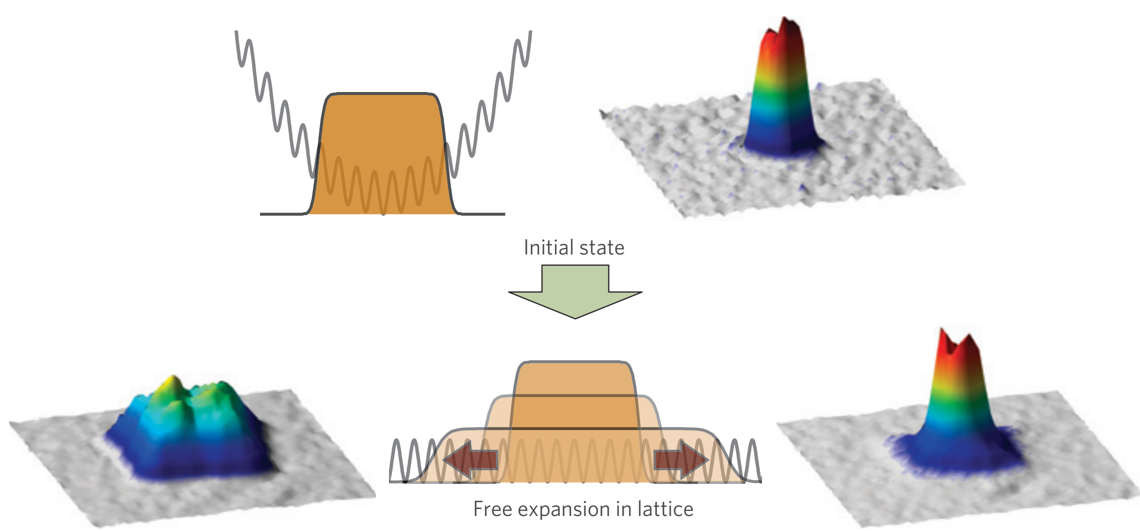


Figure 1 | Expansion of fermionic atoms after a quench of the trapping potential. First a dephased band-insulator is created in the combination of an optical lattice and a strong harmonic trap. Subsequently the harmonic confinement is switched off and the cloud expands in a homogeneous Hubbard model. The observed *in situ* density distributions demonstrate the strong effects of interactions on the evolution.

Summary and Future Works

- Thermalization of coupled systems in general thermal contact
- Cooling/heating of a quantum gas by the eigenstate Joule expansion

- Nonequilibrium dynamics
- Transport
- Quantum entanglement