Relaxation dynamics of isolated many-body systems

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Dieter Vollhardt Kazumi Maki

APS March Meeting, San Diego, 1977

Kazumi Maki

APS March Meeting, Chicago,1979

Kurt Scharnberg Richard A. Klemm
Dieter Vollhardt Kazumi Maki

Outline

1. Quantum time evolution

   vs. predictions of statistical mechanics

2. Exact real-time dynamics after an interaction quench

   - Falicov-Kimball model in DMFT [1]
   - $1/r$ Hubbard chain [2]

3. Validity of generalized Gibbs ensembles [2]

— in collaboration with Martin Eckstein (Augsburg) —

[1] Eckstein & Kollar, Phys. Rev. Lett. **100**, 120404 (2008)
[2] Kollar & Eckstein, Phys. Rev. A **78**, 013626 (2008)

1. Quantum time evolution vs. predictions of statistical mechanics

Time evolution of isolated quantum systems

"Quantum quench":

- start with $|\psi_0\rangle$ and switch to new Hamiltonian H at $t = 0$
- time evolution for $t \geq 0$:

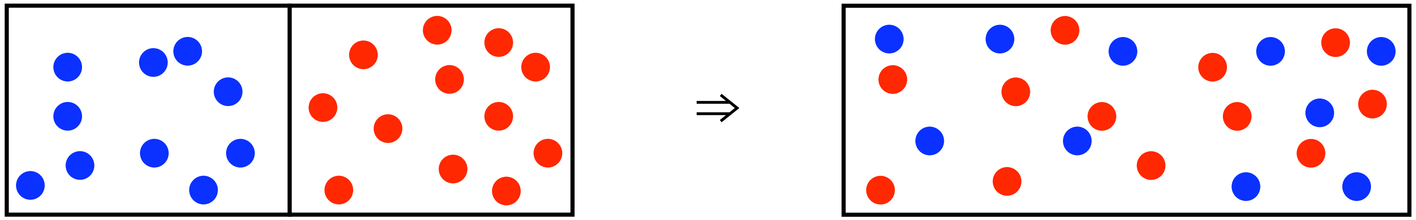
$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle = \sum_\alpha \overbrace{c_\alpha}^{=\langle\alpha|\psi_0\rangle} e^{-iE_\alpha t}|\alpha\rangle$$

components of wave function oscillate forever!

$\Rightarrow$ $\langle A\rangle_t = \mathrm{Tr}[A\rho(t)]$ with $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$

Relaxation to new equilibrium state?

- expected for simple observables and complicated Hamiltonian



Quenched Bose condensate

Abrupt increase of interaction:

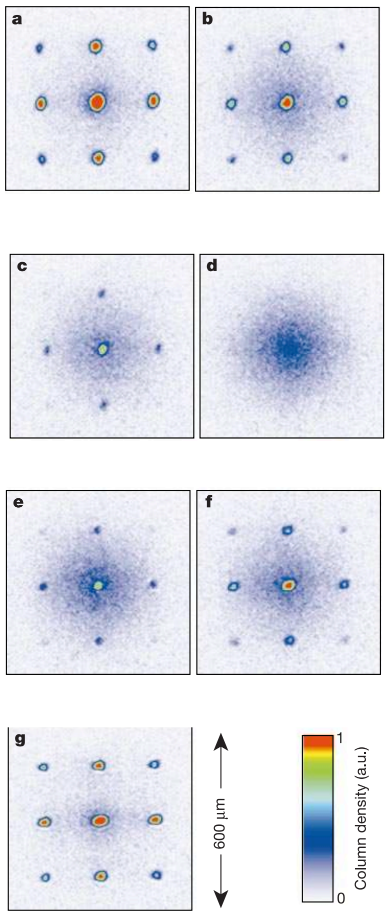
Greiner, Mandel, Hänsch, Bloch ’02

$t\!=\!0\mu s$ $t\!=\!100\mu s$

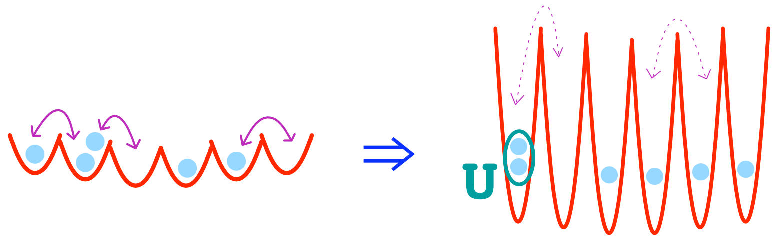
$t\!=\!150\mu s$ $t\!=\!250\mu s$

$t\!=\!350\mu s$ $t\!=\!400\mu s$

$t\!=\!550\mu s$



collapse and revival



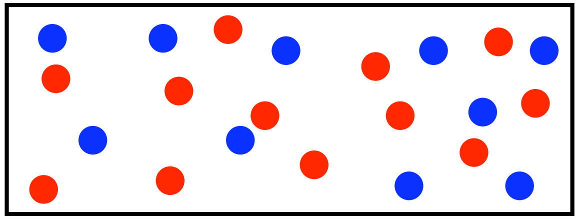
$|\psi(0)\rangle$ = Bose condensate

$$t \geq 0: \quad H \approx U \sum_i n_i(n_i - 1)$$

$$\Rightarrow \quad |\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle$$

oscillates!

Equilibrium statistical mechanics



Ensemble description:

- $\langle A \rangle = \mathrm{Tr}[\rho_{\mathrm{ens}} A]$ in equilibrium
- All accessible microstates equally probable in ρ_{ens} — "fundamental postulate"
- $S = \mathrm{Tr}[\rho \ln \rho]$ maximized by ρ_{ens}
- A_i conserved $\Rightarrow$ fix $\mathrm{Tr}[\rho_{\mathrm{ens}} A_i] = \langle A_i \rangle_{t=0}$

  $\Rightarrow$ $\rho_{\mathrm{ens}} \propto \exp(-\sum_i \lambda_i A_i)$ — Boltzmann-Gibbs ensemble

Maxwell 1866, Boltzmann 1872, Gibbs 1878
von Neumann 1927, Jaynes 1957, ..., Balian 1991

Thermal ensembles:

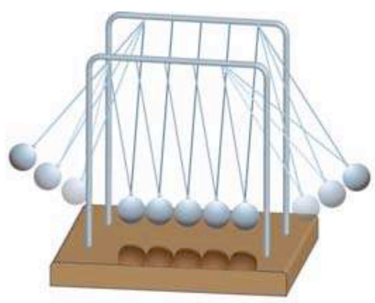
- microcanonical, canonical, grand-canonical
- e.g., $\rho_{\mathrm{gran}} \propto \exp(-\beta(H - \mu N))$ with $\langle H \rangle$, $\langle N \rangle$ fixed

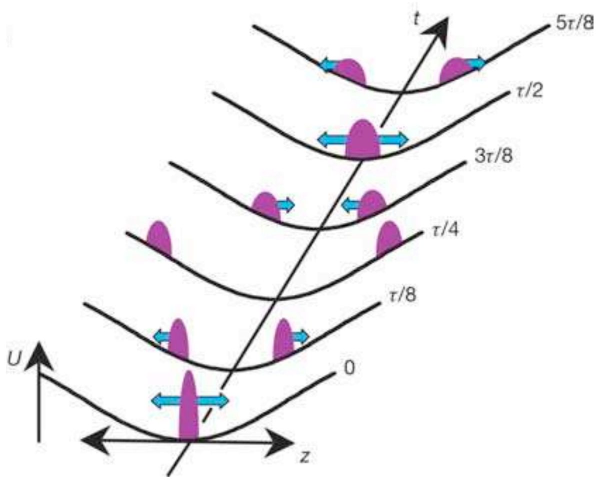
Quantum Newton's cradle

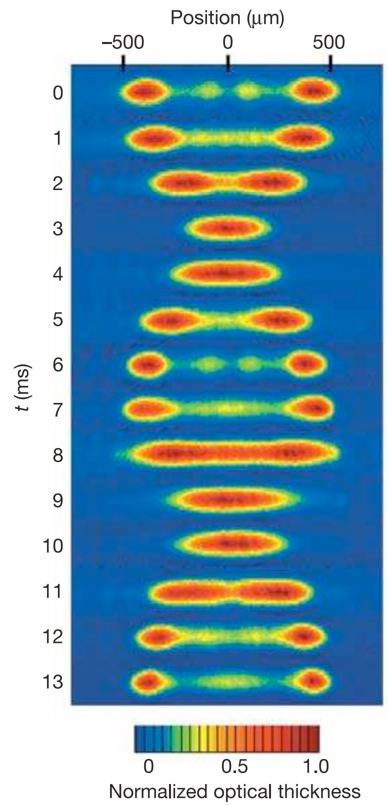
Oscillations of trapped ^{87}Rb atoms:

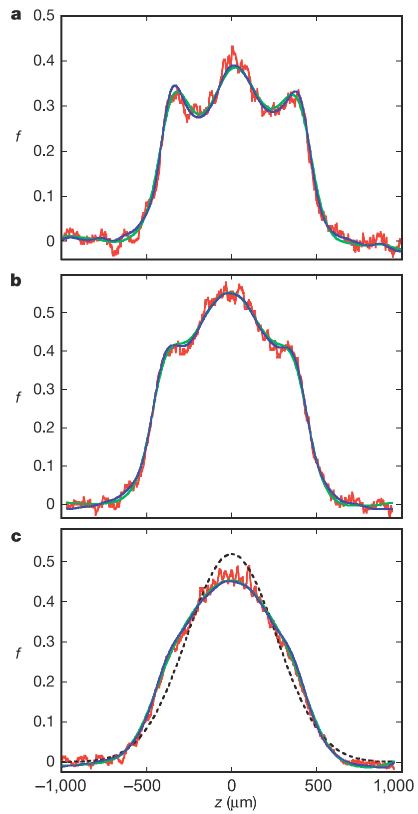
Kinoshita, Wenger, Weiss '06

$\langle b_k^\dagger b_k \rangle$ reaches steady state, but not thermal state









lack of thermalization
due to (near-)integrability

Generalized Gibbs ensembles

Statistical description with generalized Gibbs ensembles

$$H_{\text{eff}} = \sum_\alpha \epsilon_\alpha n_\alpha \;\Rightarrow\; \rho_{\text{GGE}} \propto \exp(-\textstyle\sum_\alpha \lambda_\alpha n_\alpha)$$

$$\Rightarrow\; \text{Tr}[\rho \ln \rho] = \max \text{ with fixed } \langle n_\alpha \rangle$$

Jaynes '57
Girardeau '69
Rigol, Muramatsu, Olshanii '06
Rigol, Dunjko, Yurowski, Olshanii '07
Gangardt & Pustilnik '08
Barthel & Schollwöck '08

General questions for isolated many-body systems:

- Relaxation of $\langle A \rangle_t$? Mott gap?
- Memory of initial state? $c_\alpha = \langle \alpha | \psi_0 \rangle$
- Final steady state? Thermalization?

Cazalilla '06
Mehta & Andrei '06, '07
Brody et al. '07
Kollath, Läuchli, Altman '07
Rigol, Dunjko, Yurovsky, Olshanii '07
Manmana, Wessel, Noack, Muramatsu '07
Cramer, Dawson, Eisert, Osborne '08
Rigol, Dunjko, Olshanii '08
F. Heidrich-Meisner et al. '08
Moeckel & Kehrein '08
Polkovnikov & Gritsev '08
Gutmann, Gefen, Mirlin '08
Barmettler et al. '08
Rossini et al. '08
...

Here:

- Relaxation dynamics for two models of interacting fermions
- Criteria for validity of GGEs

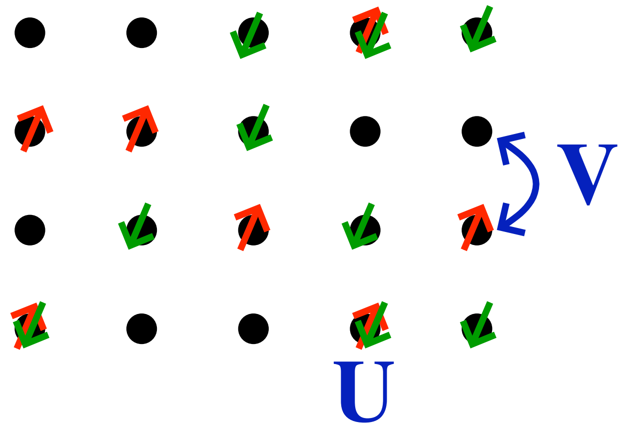
2. Exact dynamics after an interaction quench

- Falicov-Kimball model in DMFT
- $1/r$ Hubbard chain

Exact dynamics after an interaction quench

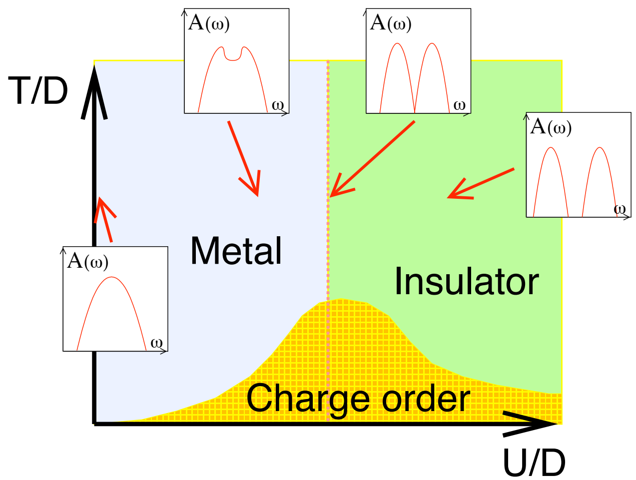
- Fermionic Hubbard model:

$$H = \underbrace{\sum_{ij\sigma} V_{ij\sigma}\, c^\dagger_{i\sigma} c_{j\sigma}}_{= \sum_{\boldsymbol{k}\sigma} \epsilon_{\boldsymbol{k}\sigma}\, c^\dagger_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma}} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$



- Falicov-Kimball model:
  - ✓-particles immobile, $V_{ij\downarrow} = 0$
  - Equilibrium: annealed disorder
  - Nonequilibrium: DMFT, exact in $d = \infty$

    Metzner & Vollhardt '89, Brandt & Mielsch '89, ...
    Schmidt & Monien '02, Turkowski & Freericks '05
    Freericks, Turkowski & Zlatić '06



$$n_c = n_f = \frac{1}{2}$$

Nonequilibrium: interaction quench

$$U(t) = \begin{cases} U_- & t < 0 \quad \Rightarrow \quad \text{initial state with } T, \mu, \epsilon_f \\ U_+ & t \geq 0 \quad \Rightarrow \quad \text{time evolution } \exp(-iHt) \end{cases}$$

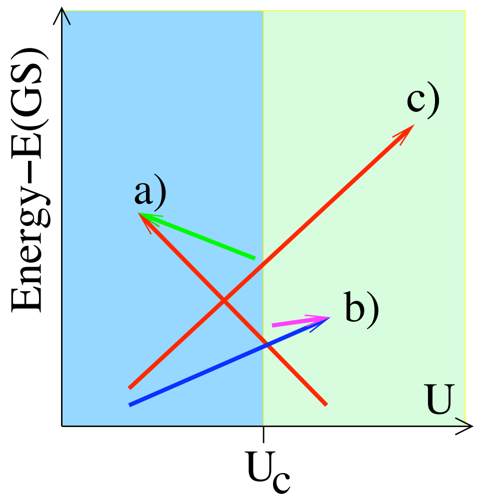
Interaction quench for Falicov-Kimball model

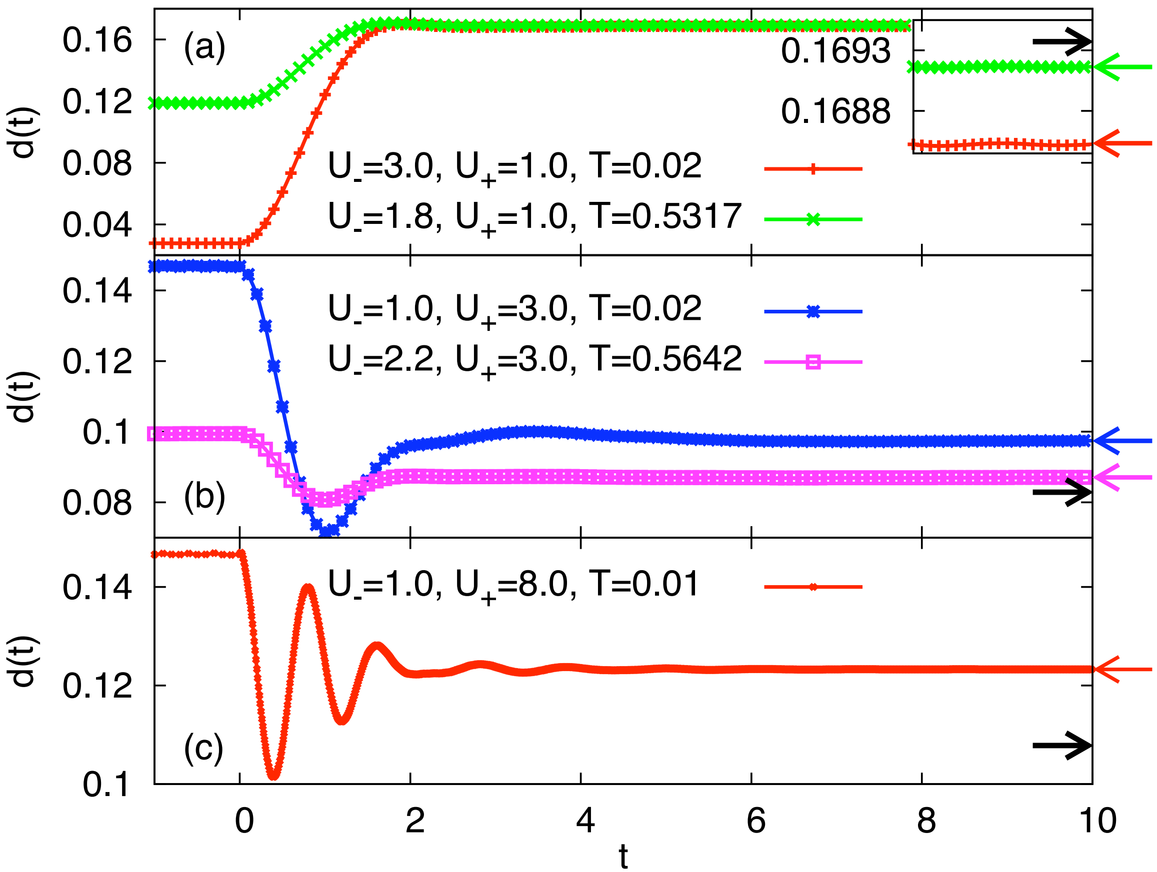
Relaxation of the double occupation: $d(t) = \langle f_i^\dagger f_i c_i^\dagger c_i \rangle_t$

bandwidth = 4

$U_c = 2$

$n_c = n_f = \frac{1}{2}$





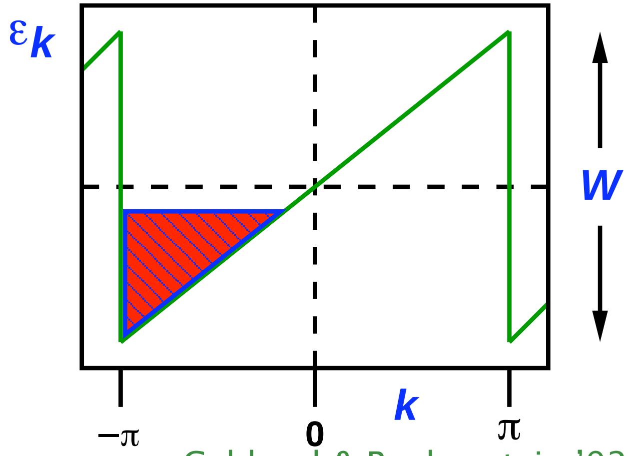
- Fast relaxation to stationary state; similar for $\langle c_{\boldsymbol{k}}^\dagger c_{\boldsymbol{k}} \rangle_t$
- $U_+ \gg V$: h/U-periodic collapse and revival oscillations
- Non-thermal final state, agrees with GGE for $U \to U + \delta U$

Hubbard chain with long-range hopping

Long-range hopping $\sim 1/r$:

$$V_{j\ell} = \frac{-iW}{2\pi}\frac{1}{j-\ell} \quad \Leftrightarrow \quad \underbrace{\epsilon_k = \frac{W}{2\pi}k}_{\text{linear dispersion}}$$

W = bandwidth



Gebhard & Ruckenstein ’92
Gebhard, Girndt, Ruckenstein ’94
Gebhard & Girndt ’94

Hubbard model with $1/r$ hopping:

$$H = \sum_{ij\sigma} V_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad \Rightarrow \quad \text{bosonic } H_{\text{eff}} \quad \Rightarrow \quad \text{solvable}$$

- $n = 1$: Mott metal-insulator transition at $U_c = W$, gap: $\Delta = U - U_c$

- $n = 1, U \to \infty$: Heisenberg chain with $1/r^2$ exchange

  Haldane ’88
  Shastry ’88

  Gutzwiller ground state: fully projected Fermi sea

- Ground state: $\left\{ \begin{array}{ll} |\text{FS}\rangle & \text{for } U = 0 \\ \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) |\text{FS}\rangle & \text{for } U = \infty \end{array} \right\} = |\psi(t=0)\rangle$

Relaxation of the double occupation $\langle n_{i\uparrow} n_{i\downarrow} \rangle$

Time dependence of $d(t) = \langle n_{i\uparrow} n_{i\downarrow} \rangle_t$: bandwidth $W = 1$

$$d(t) = \begin{cases} c_+ + f(t) & \text{“up” quench from } 0 \text{ to } U \\ [c_- - f(t)]/U & \text{“down” quench from } \infty \text{ to } U \end{cases}$$

Long-time limit for $n = 1$:

$$c_\pm = \frac{1}{8} \mp \left[\frac{(1-U)^2}{16U} + \frac{(1-U^2)^2}{16U^2} \ln \left| \frac{1-U}{1+U} \right| \right]$$

regular for $U \to 0, U_c, \infty$

Asymptotics for $n = 1$:

$$f(t) = -\frac{\cos(Ut)\cos(t)}{2Ut^2}$$

damped oscillations with modulation

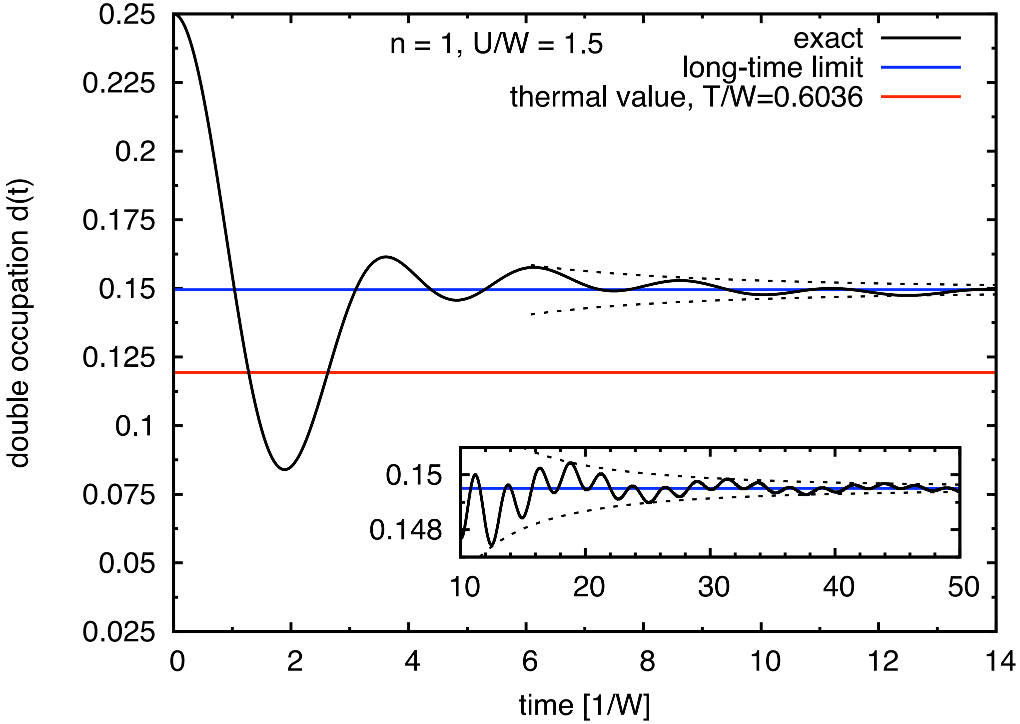
Non-thermal final state: agrees with GGE prediction ✔

Relaxation of the double occupation $\langle n_{i\uparrow} n_{i\downarrow} \rangle$

$n = 1$, quench to insulator with $U = 1.5W$

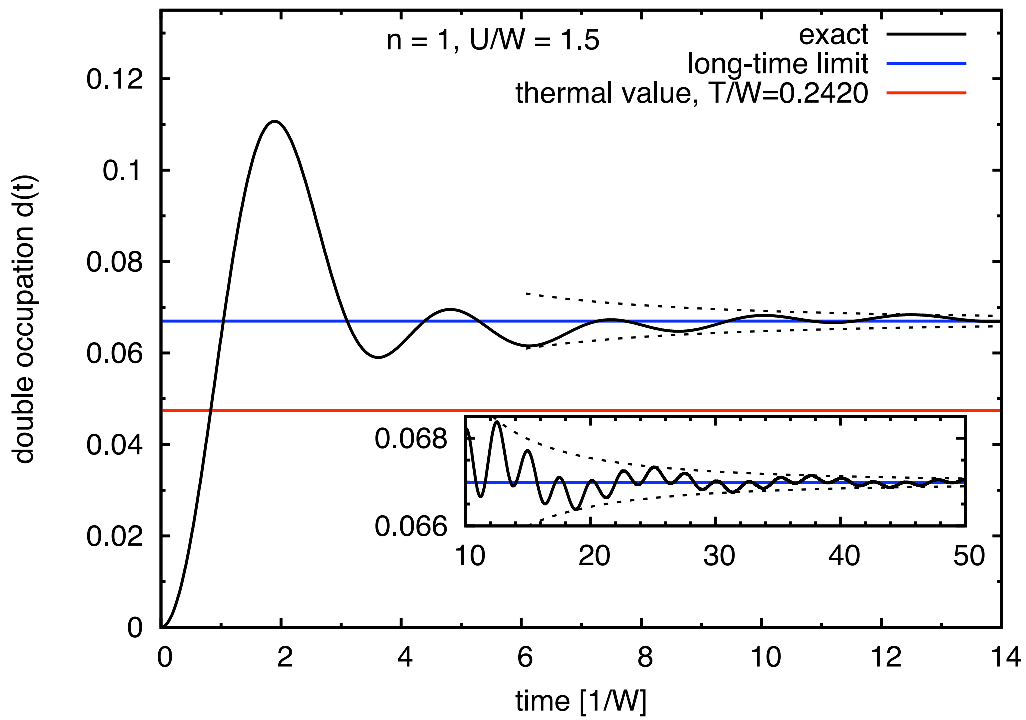
from $U = 0$

$$|\psi(0)\rangle = |\mathrm{FS}\rangle$$



from $U = \infty$

$$|\psi(0)\rangle = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) |\mathrm{FS}\rangle$$



relaxation ✔ but no thermalization ✘

Relaxation of the double occupation $\langle n_{i\uparrow} n_{i\downarrow} \rangle$

Time dependence of $d(t)$ for arbitrary $n \le 1$

$$d(t) = \begin{cases} c_+ + f(t) & \text{“up” quench from } 0 \text{ to } U \\ [c_- - f(t)]/U & \text{“down” quench from } \infty \text{ to } U \end{cases}$$

Long-time limit:

$$c_\pm = \frac{n^2}{8} \mp \frac{\Delta^2}{32U^2}\left[2nU + \Omega^2 \ln\frac{\omega}{\Omega}\right]$$

$$W \equiv 1$$
$$\Delta = U - 1$$
$$\Omega = U + 1$$
$$\omega = \sqrt{\Omega^2 - 4Un}$$

Asymptotics:

$$f(t) = -\frac{n(1-n)}{2}\overbrace{\frac{\sin(\omega t)}{t}}^{\text{slow!}} - \frac{\cos(\Omega t)}{4Ut^2} + \frac{(1-3n)\omega^2 + (1-n)\Omega^2}{2\omega^2}\frac{\cos(\omega t)}{4Ut^2} + O\left(\frac{1}{t^3}\right)$$

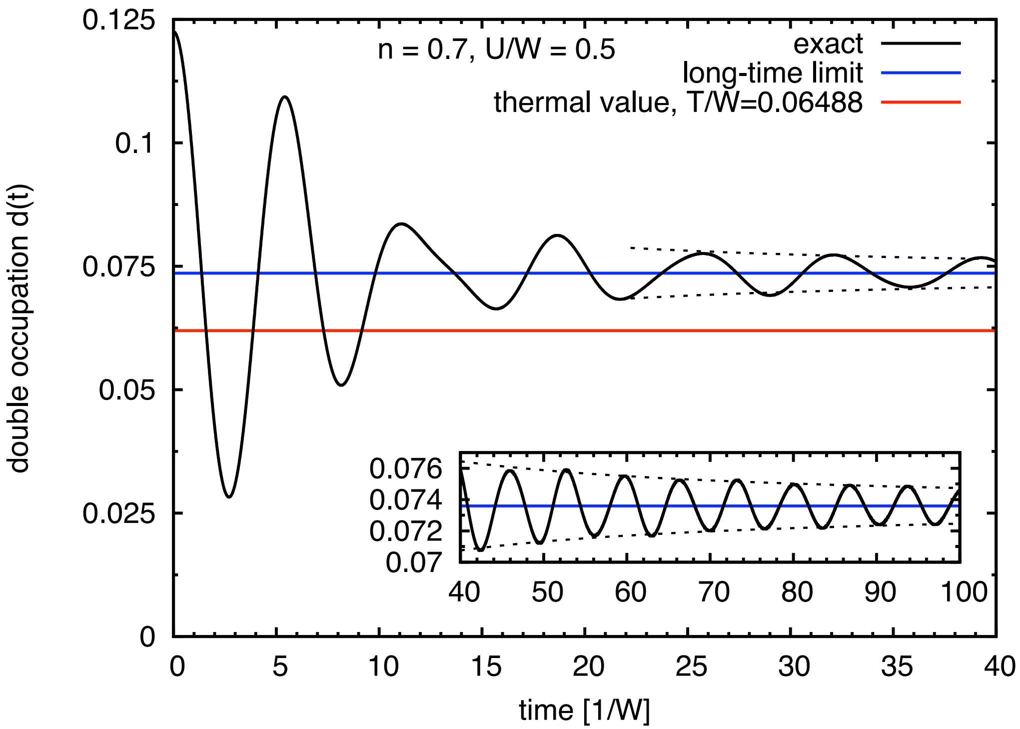
Non-thermal final state: agrees with GGE prediction ✔

Relaxation of the double occupation $\langle n_{i\uparrow} n_{i\downarrow} \rangle$

$n = 0.7$, quench to metal with $U = 0.5W$

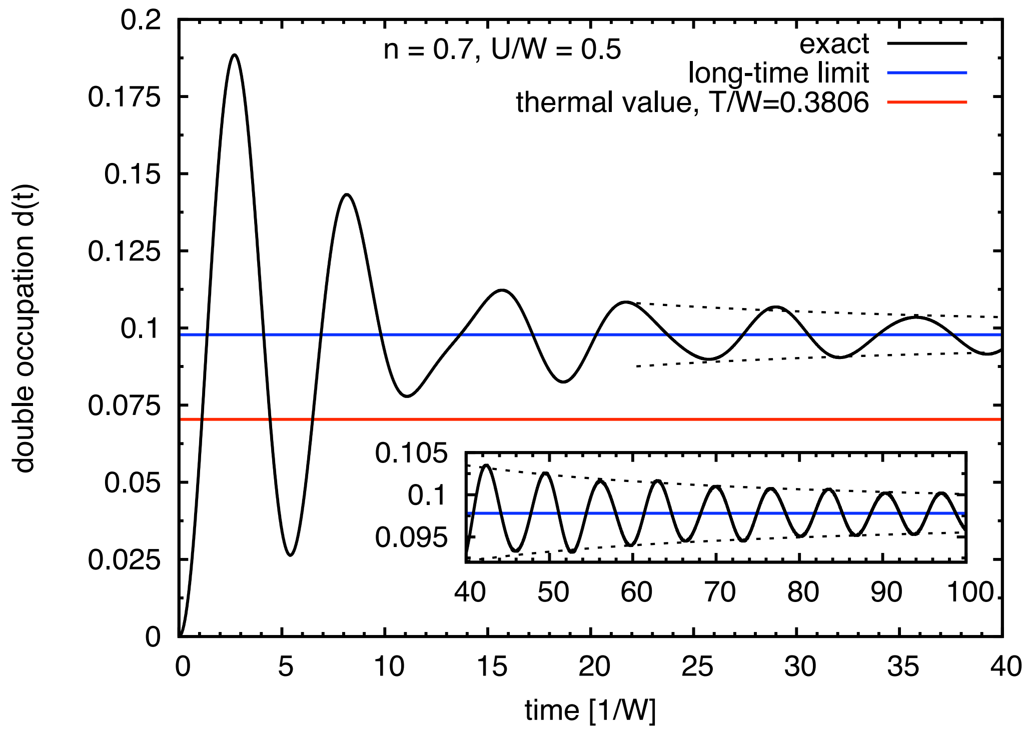
from $U = 0$

$$|\psi(0)\rangle = |\mathrm{FS}\rangle$$



from $U = \infty$

$$|\psi(0)\rangle = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) |\mathrm{FS}\rangle$$



relaxation ✔ but no thermalization ✘

3. Validity of generalized Gibbs ensembles

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Integrable system: $H_{\text{eff}} = \sum_\alpha \epsilon_\alpha n_\alpha$ with $[n_\alpha, n_\beta] = 0$

$\Rightarrow$ $\rho_{\text{GGE}} \propto \exp(-\sum_\alpha \lambda_\alpha n_\alpha)$ = generalized Gibbs ensemble

Works in many cases, but not all:

✔ $\langle b_k^\dagger b_k \rangle$ for hard-core bosons, n_α = JW fermions

✘ but not unit-cell-averaged $\langle b_i^\dagger b_j \rangle$

Rigol, Muramatsu, Olshanii '06
Rigol, Dunjko, Yurowski, Olshanii '07

✔ $\langle c_k^\dagger c_k \rangle$ for Luttinger model, n_α = bosons — Cazalilla '06

✘ misses correlations between conserved quantities — Gangardt & Pustilnik '08

✔ finite-range observables, Gaussian initial states — Barthel & Schollwöck '08

✔ Falicov-Kimball model & Hubbard chain with long-range hopping

Role of observables and initial states

Integrable system: $H_{\text{eff}} = \sum_{\alpha} \epsilon_\alpha n_\alpha$ with $[n_\alpha, n_\beta] = 0$ and $n_\alpha = c^\dagger_\alpha c_\alpha = 0, 1$

General observable: $A = \sum_{\alpha\beta} A_{\alpha\beta}\, c^\dagger_{\alpha_1} \cdots c^\dagger_{\alpha_m} c_{\beta_m} \cdots c_{\beta_1}$

- Ensemble average:

$$\langle A \rangle_{\text{GGE}} = \sum_{\{\alpha_i\},P} (\pm 1)^P A_{\alpha,P\alpha}\ \langle n_{\alpha_1} \rangle_{t=0} \cdots \langle n_{\alpha_m} \rangle_{t=0}$$

- Stationary value for nondegenerate spectrum:

$$\langle A \rangle_{\text{final}} = \sum_{\{\alpha_i\},P} (\pm 1)^P A_{\alpha,P\alpha}\ \langle n_{\alpha_1} \cdots n_{\alpha_m} \rangle_{t=0}$$

Validity of statistical prediction: $\langle A \rangle_{\text{GGE}} = \langle A \rangle_{\text{final}}$?

- depends on observable, initial state, system size, . . .
- $1/r$ Hubbard chain: $A = \sum_i n_{i\uparrow} n_{i\downarrow} = \sum_{\alpha\beta} A_{\alpha\beta} c^\dagger_\alpha c_\beta$ ✔

Combinations of constraints

Important ambiguity:

- If n_α conserved, then also $n_\alpha n_\beta$ and $n_\alpha n_\beta n_\gamma$ etc.
- Include products in ρ ?
  - Fix some products $\Rightarrow$ ensemble predicts them correctly
  - Fix all products $\Rightarrow$ yields all stationary values correctly

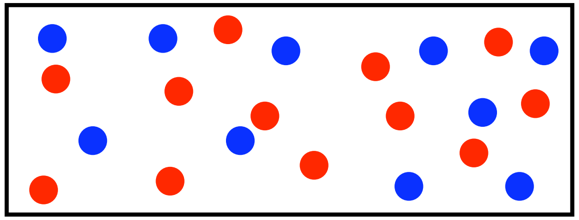
Brody et al. '07, Manmana et al. '07, Rigol et al. '08

Disadvantages for interacting integrable systems:

- Products of constants of motion

  $\Rightarrow$ complicated correlators, not measurable in practice
- Detailed information as input

  $\Rightarrow$ not a statistical description



Conclusion

Relaxation of isolated many-body systems:

- Constraints can prevent thermalization
- Mott insulators can relax to new steady state

Generalized Gibbs ensembles for integrable systems:

- Correct for sufficiently uncorrelated observables / initial states
- Can be improved with combinations of constraints

Further applications of DMFT for nonequilibrium:

- Slow parameter changes
  $\longrightarrow$ poster on Thursday by Martin Eckstein
- Pump-probe spectroscopy

  Eckstein & Kollar 0808.1005, 0809.4282