# Flow Equations and Non-Equilibrium Quantum Many-Body Systems

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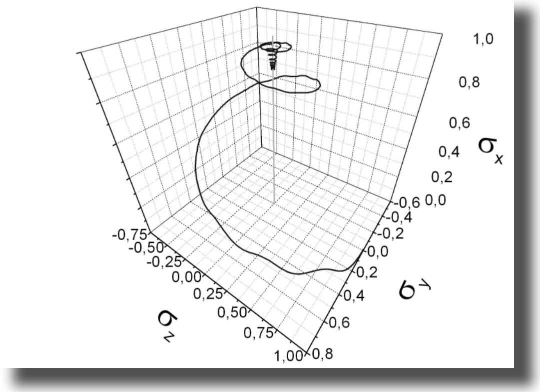
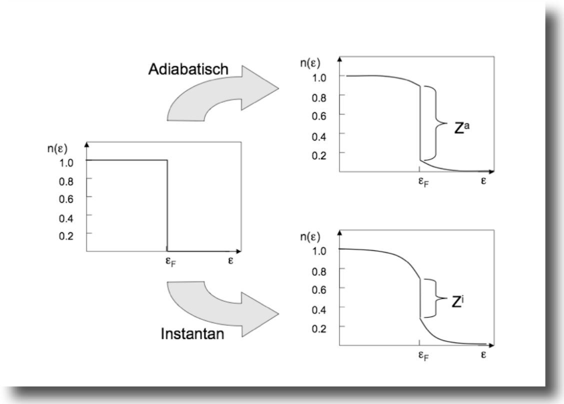
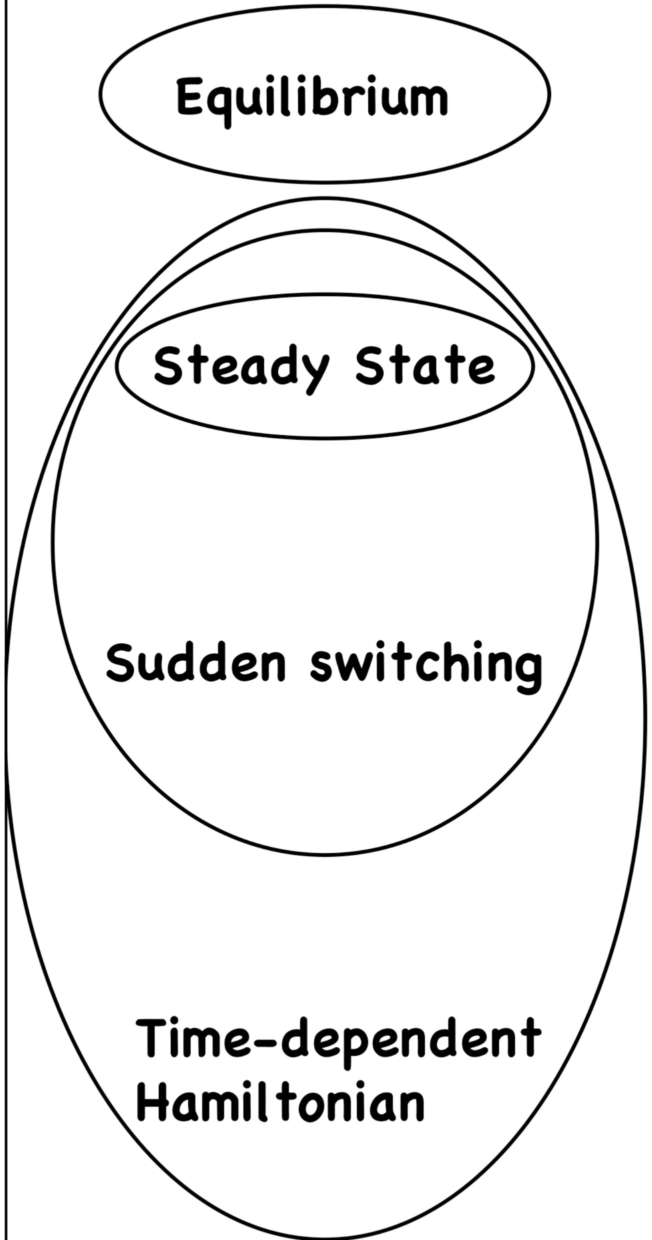



**ERG 2008 Heidelberg**
**July 4, 2008**

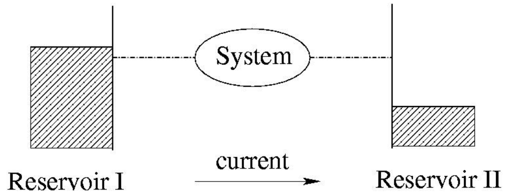
# Non-Equilibrium Problems: Classification




**Equilibrium:** Properties of ground state |GS> or thermal state $\rho \propto \exp(-\beta H)$

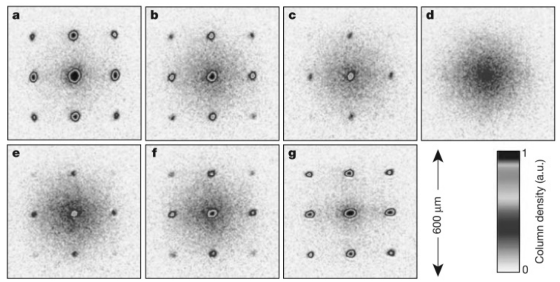
Translation invariance in time

**Steady State:** Transport driven by external potential bias ⇒ non-thermal steady state




Asymptotic steady state (with transl. invariance in time)

**Sudden switching:** Real time evolution of non-thermal initial state




Explicit dependence on waiting time

**Time-dependent Hamiltonian:** Most general class of non-equilibrium problems

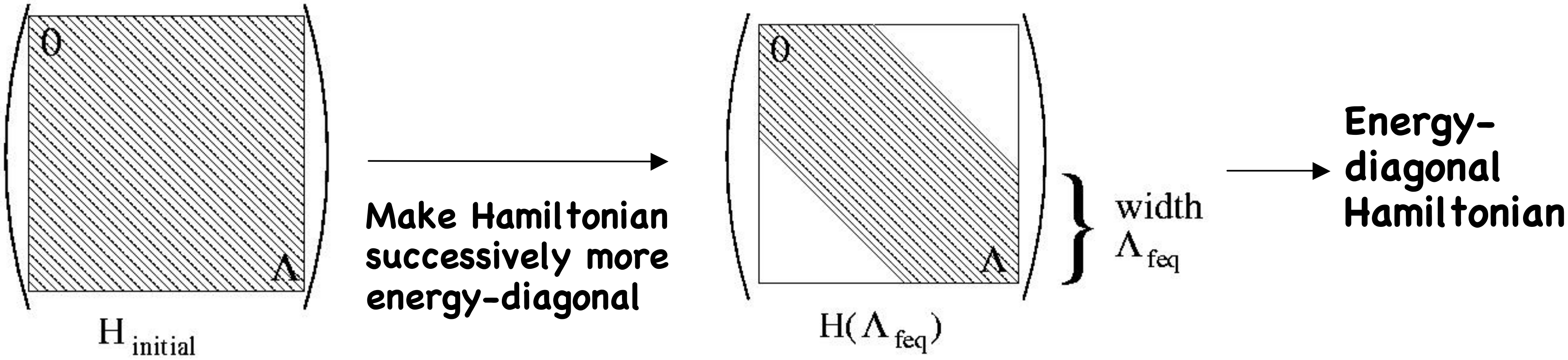
Example: Landau-Zener model

$$H(t) = -\alpha t \sigma_z + g \sigma_x$$

1. Flow Equation Method
2. Application I (steady state):
   Kondo Model with Voltage Bias
3. Application II (real time evolution):
   Sudden Interaction Fermi Liquid

# Flow Equation Method

F. Wegner (1994)
S.K., *The Flow Equation Approach to Many-Body Problems* (Springer 2006)




Implementation of flow: Sequence of infinitesimal unitary transformations

One-parameter family of unitarily equivalent Hamiltonians generated by solving the differential equation ("flow equations")

$$\frac{dH}{dB} = [\eta(B), H(B)]$$

with H(B=0) the initial Hamiltonian and an anti-hermitean generator $\eta$(B).

**Canonical choice of generator (Wegner 1994):**

$$H(B) = H_0(B) \text{ [diagonal part] } + H_{int}(B) \text{ [interaction part]}$$

$\rightarrow$ **define anti-hermitean generator** $\eta(B) = [H_0(B), H_{int}(B)]$

$$\frac{d}{dB} \,\mathrm{Tr}\, H^2_{\mathrm{int}}(B) \leq 0$$

$\rightarrow$ **generates band-diagonal Hamiltonians H(B) with** $B^{-1/2} = \Lambda_{feq}$

**Challenge: Generation of higher and higher order interaction terms**
**→ need suitable expansion parameter (typically running coupling)**

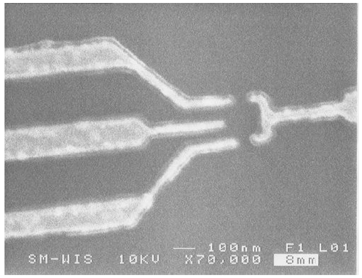
**Advantages:**

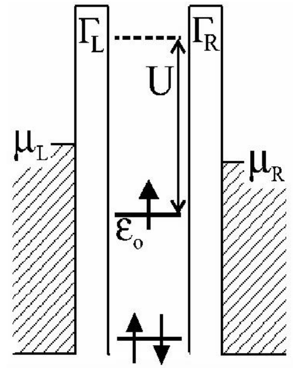
- **RG-like analytical method**
- **Controlled solution in certain strong-coupling problems (e.g., Kondo model, Sine-Gordon model)**
- **Keeps all states in Hilbert space!**
  **→ correlation functions on all energy scales**
  **→ important in non-equilibrium (real time evolution, steady states)**
- **Avoids secular terms in real time evolution!**

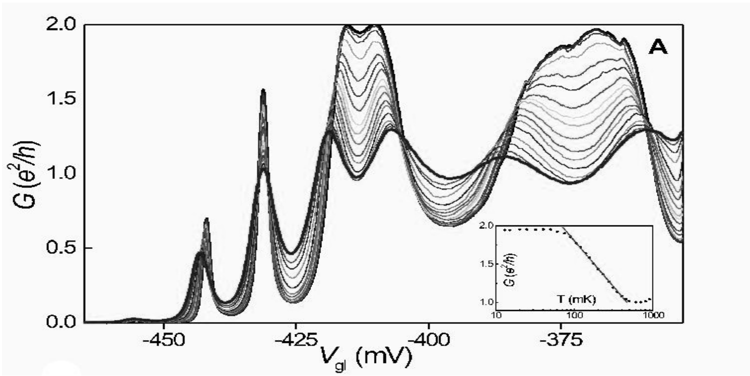
# Application I: Kondo Model with Voltage Bias

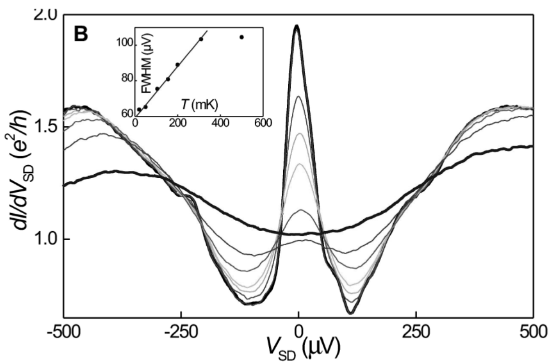
Quantum dots in the Coulomb blockade regime

from Goldhaber-Gordon et al. 1998




from van der Wiel et al. 2000

Kondo model:

$$H = \sum_{a=l,r}\sum_{k,\alpha}\epsilon_k\, c^\dagger_{ak\alpha}c_{ak\alpha} + J_t\,\vec{S}\cdot\sum(c^\dagger_{lk\alpha}\vec{\sigma}_{\alpha\beta}c_{rk'\beta} + c^\dagger_{rk\alpha}\vec{\sigma}_{\alpha\beta}c_{lk'\beta})$$ transport scattering

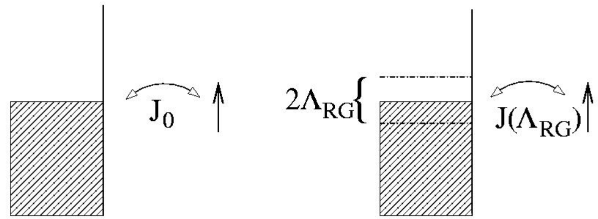
$$+ J_l\,\vec{S}\cdot\sum c^\dagger_{lk\alpha}\vec{\sigma}_{\alpha\beta}c_{lk'\beta} + J_r\,\vec{S}\cdot\sum c^\dagger_{rk\alpha}\vec{\sigma}_{\alpha\beta}c_{rk'\beta}$$

left-left scattering     right-right scattering

# Kondo model: Scaling theory (conventional approach)

Effective Hamiltonians $H(\Lambda_{RG})$ with same low-energy physics:

$$H(\Lambda_{\mathrm{RG}}) = \sum_{|\epsilon_k|<\Lambda_{\mathrm{RG}}} \epsilon_k\, c^\dagger_{k\alpha} c_{k\alpha} + J(\Lambda_{\mathrm{RG}})\, \vec{S}\cdot \sum_{|\epsilon_k|,|\epsilon_{k'}|<\Lambda_{\mathrm{RG}}} c^\dagger_{k\alpha} \vec{\sigma}_{\alpha\beta} c_{k'\beta}$$



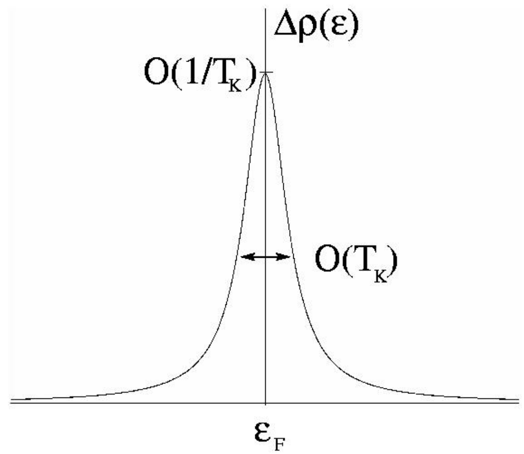

RG-equation:

$$\frac{dJ(\Lambda_{\mathrm{RG}})}{d\Lambda_{\mathrm{RG}}} = -\frac{2J^2}{\Lambda_{\mathrm{RG}}}$$

$$\Rightarrow \quad J(\Lambda_{\mathrm{RG}}) = \frac{1}{2\ln(\Lambda_{\mathrm{RG}}/T_K)} \quad \text{with} \quad T_K = D_0 \exp\left(-\frac{1}{2\rho_F J_0}\right)$$

Divergence for $\Lambda_{RG} = T_K$

Nonperturbative energy scale




Strong-coupling behavior:

→ Formation of bound state (Kondo singlet) / screening of magnetic moment

→ Enhanced density of states pinned at Fermi surface (Kondo peak)

# Kondo model: Flow equation approach

S.K., PRL 95, 056602 (2005)

Flow equations "independent" from equilibrium/non-equilibrium setting:

$$
\begin{aligned}
H(B) \;=\; & \sum_{t,\alpha} \epsilon_t\, c^\dagger_{t\alpha} c_{t\alpha} + \sum_{t',t} J_{t't}(B)\, \vec{S}\cdot\vec{s}_{t't} \\
& + i \sum_{t',t,u',u} K_{t't,u'u}(B)\; :\vec{S}\cdot(\vec{s}_{t't}\times\vec{s}_{u'u}): \\
& + \text{new normal} - \text{ordered interactions in } O(J^3)
\end{aligned}
$$

Initial structure of Hamiltonian

Newly generated terms in $O(J^2)$

Neglected terms in $O(J^3)$

Canonical generator $\eta(B) = [H_0(B), H_{int}(B)]$

Flow equations:

$$
\begin{aligned}
\frac{dJ_{t't}}{dB} \;=\; & -(\epsilon_{t'}-\epsilon_t)^2 J_{t't} \\
& + \sum_v (\epsilon_{t'}+\epsilon_t-2\epsilon_v) J_{t'v} J_{vt}\, (n(v)-1/2) \\
& + \frac{1}{2} \sum_{u',u} (2\epsilon_u - 2\epsilon_{u'} + \epsilon_t - \epsilon_{t'})\, J_{u'u} (K_{u'u,t't} - K_{t't,u'u}) \\
& \quad \times [n(u')\,(1-n(u)) + n(u)\,(1-n(u'))] \\
& + O(J^4) \\
\frac{dK_{t't,u'u}}{dB} \;=\; & -(\epsilon_{t'}+\epsilon_{u'}-\epsilon_t-\epsilon_u)^2 K_{t't,u'u} - (\epsilon_{u'}-\epsilon_u) J_{t't} J_{u'u} \\
& + O(J^3)
\end{aligned}
$$

Occupation number

$$n(u) = \langle c^\dagger_{u\alpha}\, c_{u\alpha} \rangle$$

depends on initial non-interacting ground state (different structure equilibrium vs. non-equilibrium)!

Effective flow equations for

- $J_l$ : Left-left scattering at left Fermi level
- $J_r$ : Right-right scattering at right Fermi level
- $J_t$ : Average over transport couplings over energy window V between left and right Fermi level (relevant for current)

Initial flow for $\Lambda_{feq} > V$ identical to conventional scaling:

$$\frac{dJ_l}{d\Lambda_{\rm feq}} = -\frac{2(J_l^2 + J_t^2)}{\Lambda_{\rm feq}}$$

$$\frac{dJ_r}{d\Lambda_{\rm feq}} = -\frac{2(J_r^2 + J_t^2)}{\Lambda_{\rm feq}}$$

$$\frac{dJ_t}{d\Lambda_{\rm feq}} = -\frac{2J_t(J_l + J_r)}{\Lambda_{\rm feq}}$$

## Later flow for $\Lambda_{feq}$ < V:

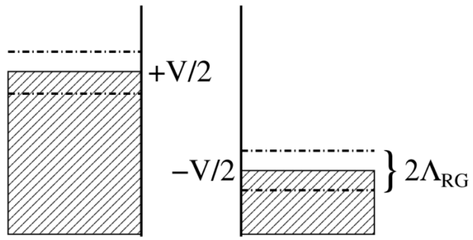
$$\frac{dJ_t}{d\Lambda_{\rm feq}} = \sqrt{2\pi}\,\frac{V}{\Lambda_{\rm feq}^2}\,J_t^3$$

$$\frac{dJ_l}{d\Lambda_{\rm feq}} = -\frac{2J_l^2}{\Lambda_{\rm feq}} + \sqrt{2\pi}\,\frac{V}{\Lambda_{\rm feq}^2}\,J_l\,J_t^2$$

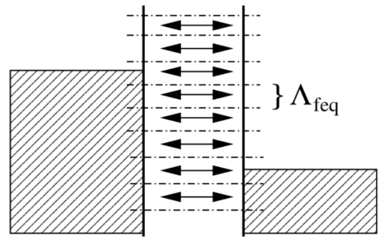
$$\frac{dJ_r}{d\Lambda_{\rm feq}} = -\frac{2J_r^2}{\Lambda_{\rm feq}} + \sqrt{2\pi}\,\frac{V}{\Lambda_{\rm feq}^2}\,J_r\,J_t^2$$

Coherent strong-coupling

Decoherence




Conventional scaling




Flow equation approach

→ **Competition between coherence and decoherence**

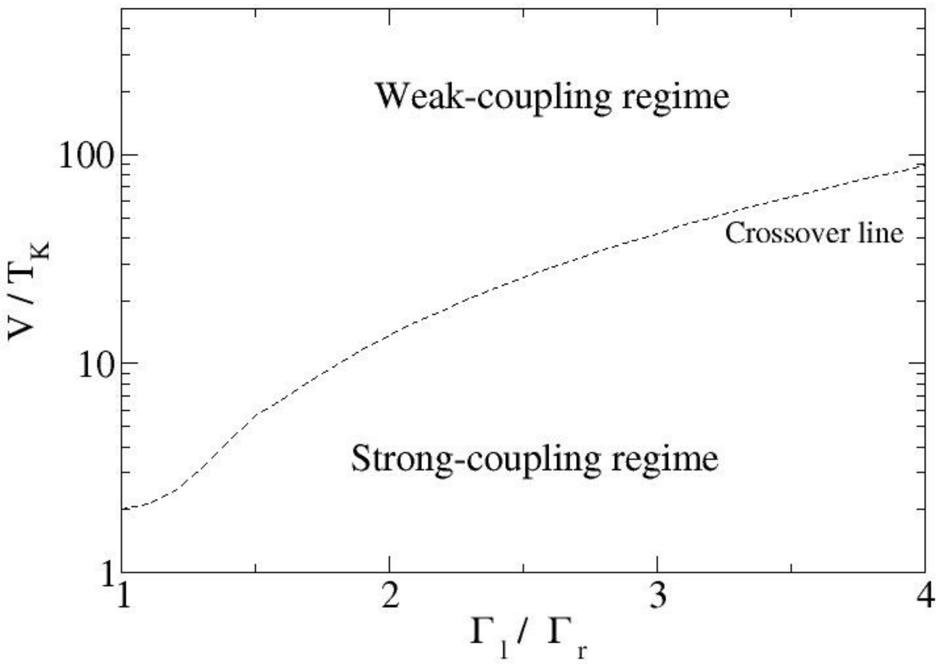
- Decoherence acts different from finite temperature in RG
- Decoherence scale set by spin relaxation rate due to steady current

$$\Gamma_{\rm rel} \propto \frac{4\Gamma_l\Gamma_r}{(\Gamma_l+\Gamma_r)^2}\,\frac{V}{\ln^2(V/T_K)}$$

- Third order terms >> second order terms for $\Lambda_{feq}$ << V
- Flow equations: $1/(\Lambda_{feq})^2$ most IR-singular behavior
- Third order terms in RG β-function for equilibrium impurity model translate into flow equation decoherence term

**Novel structure of scaling equations with respect to $\Lambda_{feq}$**

# Results: Phase diagram in non-equilibrium




from S.K., PRL 95, 056602 (2005)

Symmetric dots

Decoherence prevents 2-channel Kondo physics

Asymmetric dots

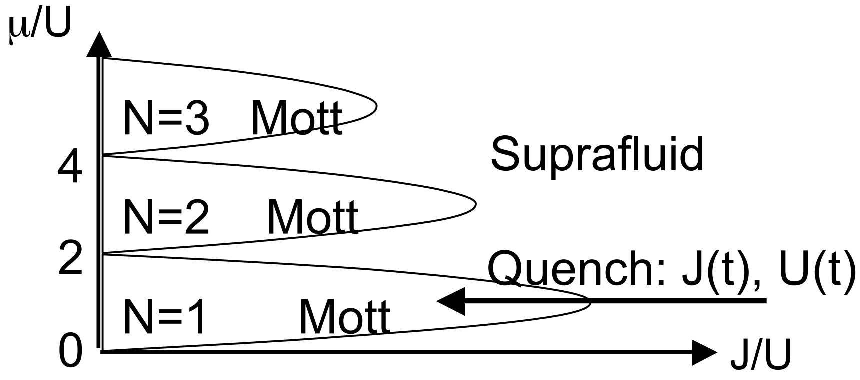
Strong-coupling regime extends to very large ratios $V/T_K$
$\rightarrow$ 1-channel Kondo physics

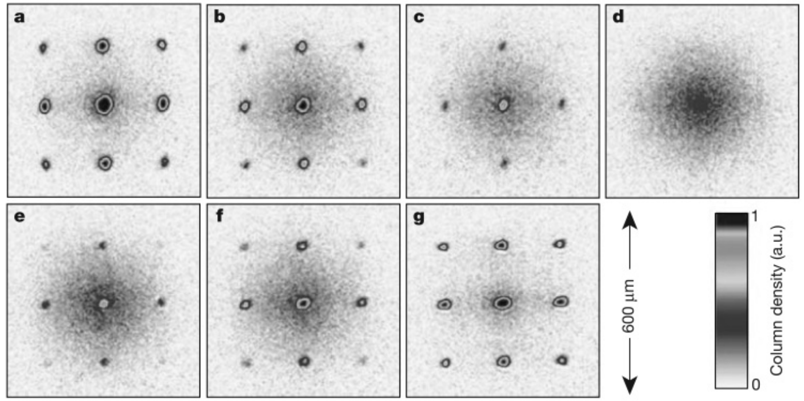
Reasons:

Current ($\rightarrow$ noise) suppressed for asymmetric dots

# Real Time Dynamics in Ultracold Atomic Gases

**M. Greiner et al.; Nature 419, 51 (2002)**



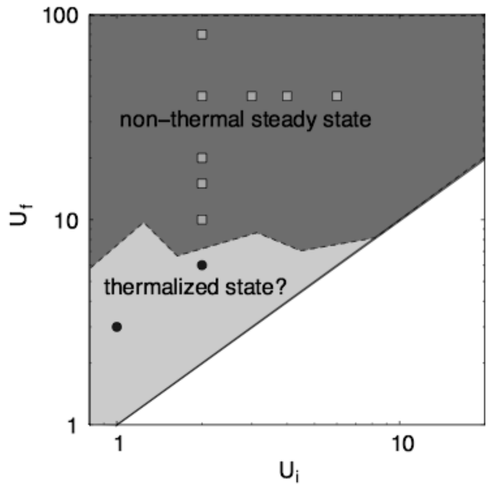




**"Collapse and Revival"**

**C. Kollath, A. Läuchli, E. Altman; Phys. Rev. Lett. 98, 180601 (2007)**

**Time-dependent DMRG for 1d system**

$\boxed{\textbf{Ergodicity?}}$



# Classical Mechanics: Perturbation Theory

**"Real time evolution" with small anharmonic terms**

$$H = \frac{1}{2}p^2 + \frac{1}{2}q^2 + \frac{g}{4}q^4$$

**Ansatz:** $q(t) = q^{(0)}(t) + g\,q^{(1)}(t) + O(g^2)$ (initial condition: $q(t=0)=0$)

$$\Rightarrow \quad q^{(0)}(t) = c\,\sin t$$

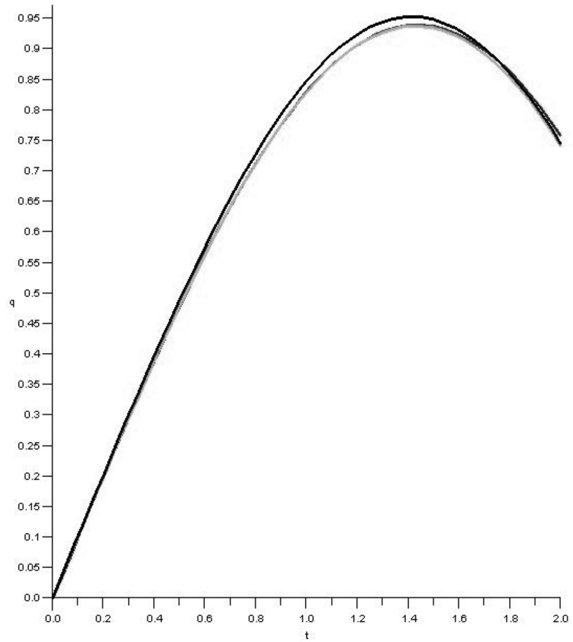
$$\Rightarrow \quad \ddot{q}^{(1)}(t) = -q^{(1)}(t) - c^3\,\sin^3 t$$

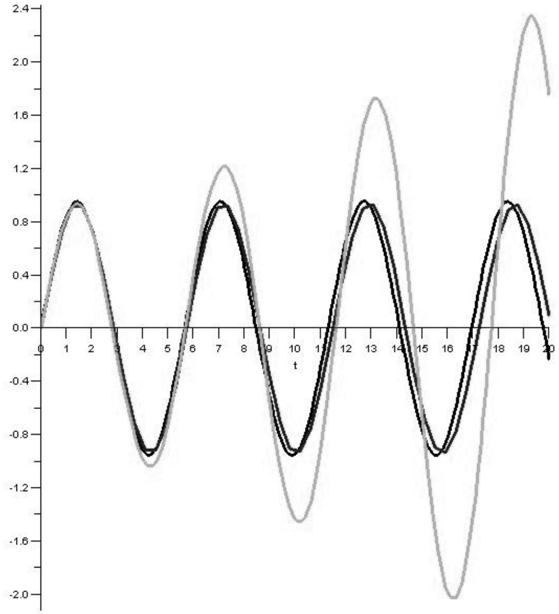
$$\Rightarrow \quad q^{(1)}(t) = \sin t - \frac{c^3}{8}\left(\sin t\,\cos^2 t + 2\,\sin t - 3t\,\cos t\right)$$

"Secular term"

**Well known:**

**Secular terms invalidate naive perturbation theory for large times!**




**red line: exact**

**green line: naive pert. theory**

**black line: canonical pert. theory**

**Much better … Canonical perturbation theory**

**Find canonical transformation (q,p) → (Q,P) that brings H to normal form:**

$$\tilde{H}(Q,P) = H_0 + g\,\alpha H_0^2 + O(g^2) \quad \text{with} \quad H_0 = \frac{1}{2}P^2 + \frac{1}{2}Q^2$$

**Transformation of variables:**

$$\Rightarrow \quad q(t) = Q(t) - \frac{3}{32}g\left(3P^2(t)\,Q(t) + \frac{5}{3}Q^3(t)\right) + O(g^2)$$
$$= c\,\sin(\omega t) - \frac{3}{32}g\,c^3\left(3\cos^2(\omega t)\,\sin(\omega t) + \frac{5}{3}\sin^3(\omega t)\right) + O(g^2) \quad \text{with} \quad \omega = 1 + \frac{3}{4}g\,E_0$$

Problem of naive perturbation theory:

naive expansion in coupling constant produces secular terms

$$\sin(\omega t) = \sin\left((1+\frac{3}{4}g E_0)\,t\right)$$
$$= \sin t + \frac{3}{4} g E_0 t \cos t + O(g^2)$$

canoncial perturbation theory

naive perturbation theory in coupling

Likewise: Secular terms in perturbative evaluation for real time evolution of interacting quantum many-body system

$\Rightarrow$ Same recipe: Perturbation theory based on unitary transformations instead of “naive” perturbation expansion

Additional complications:
- Continuum of energy scales
- Nonperturbative effects in coupling constant

# Forward-Backward Transformation

A. Hackl and S.K., arXiv:0709.2100

$$\begin{tikzcd}[column sep=huge, row sep=huge]
\mathrm{B} = 0 & \mathrm{B} = \infty \\
H, O, |\Psi_i\rangle \arrow[r, "\mathrm{U}"] \arrow[d, dashed, "\substack{\text{Non-perturbative solution}\\ \text{of Heisenberg equations of}\\ \text{motion for operator O(t)}}"] & \tilde{H}, \tilde{O}, |\tilde{\Psi}_i\rangle \arrow[d, "\text{Time evolution}"] \\
O(t), |\Psi_i\rangle & \tilde{O}(t) = e^{i\tilde{H}t}\tilde{O}e^{-i\tilde{H}t}, |\tilde{\Psi}_i\rangle \arrow[l, "\mathrm{U}^{\dagger}"']
\end{tikzcd}$$

No secular terms!

## Equilibrium Dynamics (T=0)

$$\begin{array}{ccc} \mathrm{B}=0 & & \mathrm{B}=\infty \\ H,\ O,\ |\Psi_i\rangle & \xrightarrow{\ \mathrm{U}\ } & \tilde{H},\ \tilde{O},\ |\tilde{\Psi}_i\rangle \\ \downarrow & & \downarrow \\ O(t),\ |\Psi_i\rangle & \xleftarrow{\ \mathrm{U}^\dagger\ } & \tilde{O}(t) = e^{i\tilde{H}t}\tilde{O}e^{-i\tilde{H}t},\ |\tilde{\Psi}_i\rangle \end{array}$$

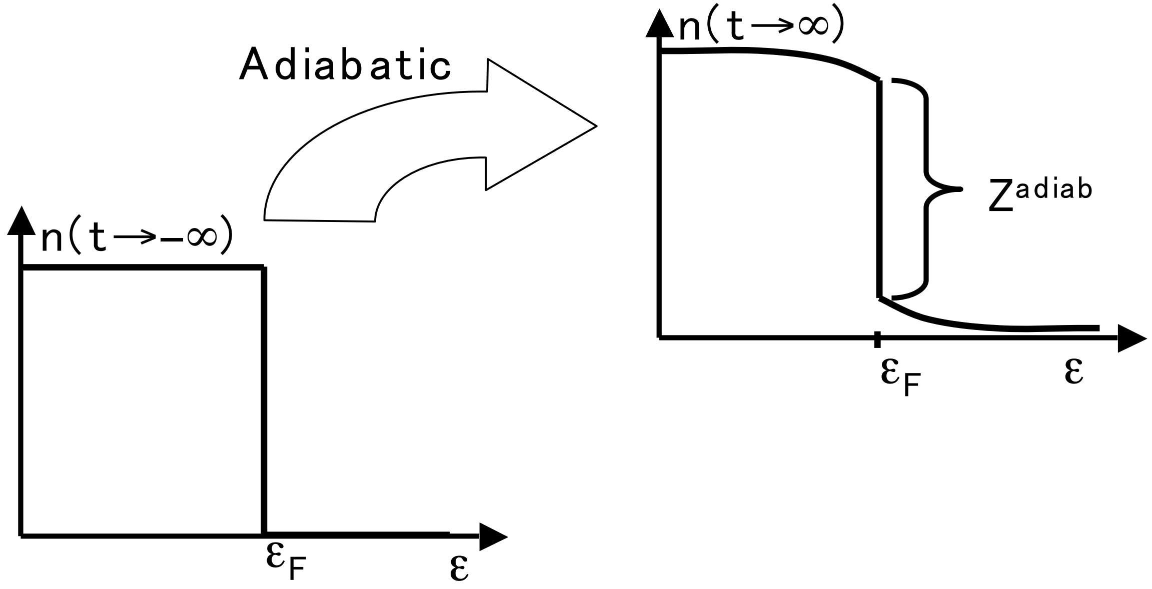
Non-perturbative solution of Heisenberg equations of motion for operator O(t)

Time evolution

# Application II: Sudden Interaction Fermi Liquid

**Landau Fermi liquid theory:**

**Adiabatic switching on of interaction**
**→ 1 to 1 correspondence between physical electrons and quasiparticles**




**What happens for sudden switching?**

**Translation-invariant closed system + nonzero excitation energy**

**⇒ Thermalization?**

M. Möckel and S.K., PRL 100, 175702 (2008)

**Hubbard model in d≥2 dimensions**

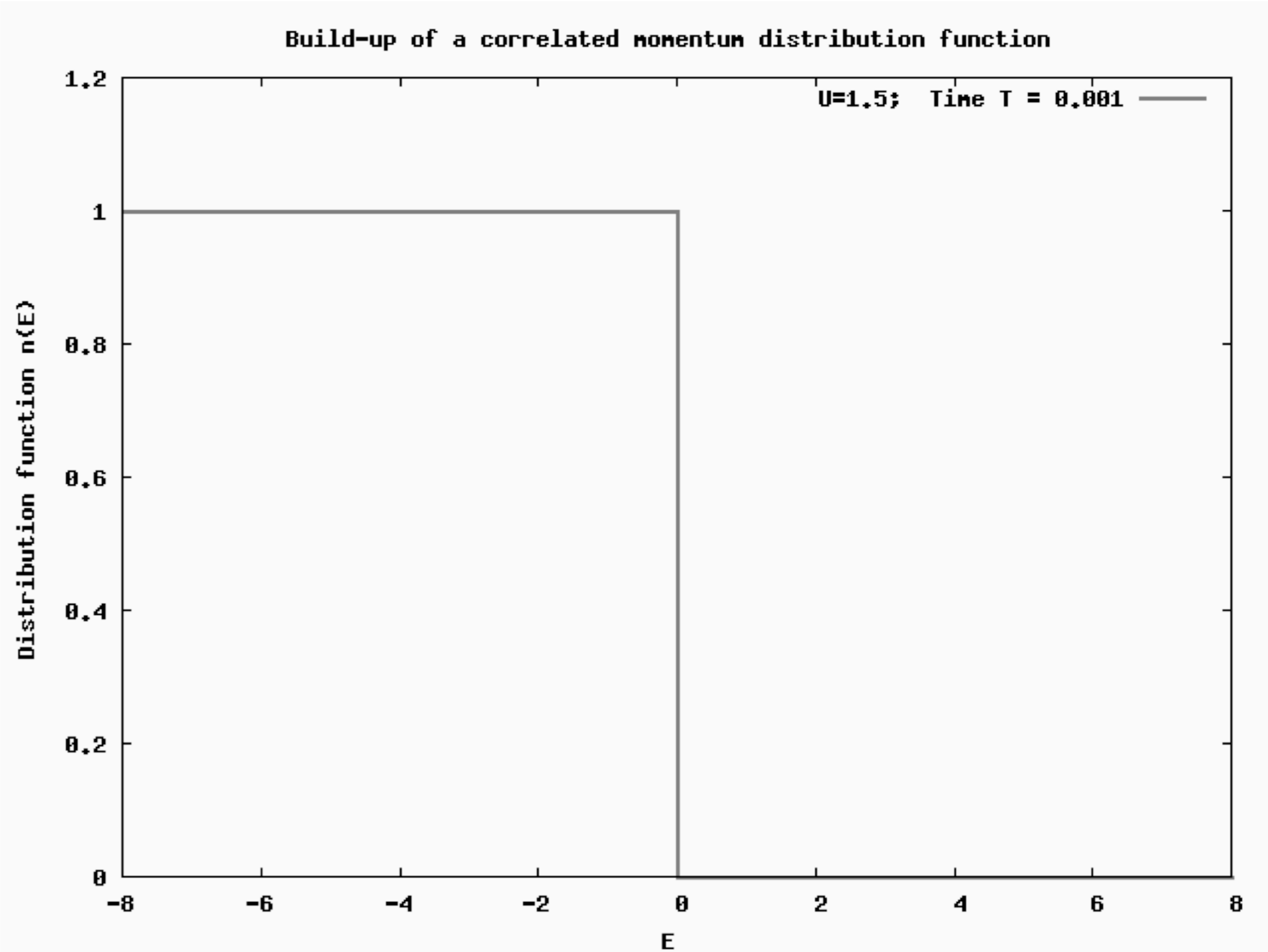
$$H = \sum_{k,\alpha} \varepsilon_k c^\dagger_{k\alpha} c_{k\alpha} + U\,\Theta(t) \sum_i \left(n_{i\uparrow} - \frac{1}{2}\right)\left(n_{i\downarrow} - \frac{1}{2}\right)$$

**Forward transformation:**

$$\frac{dO(B)}{dB} = [\eta(B), O(B)] \quad , \quad O(B=0) = O$$

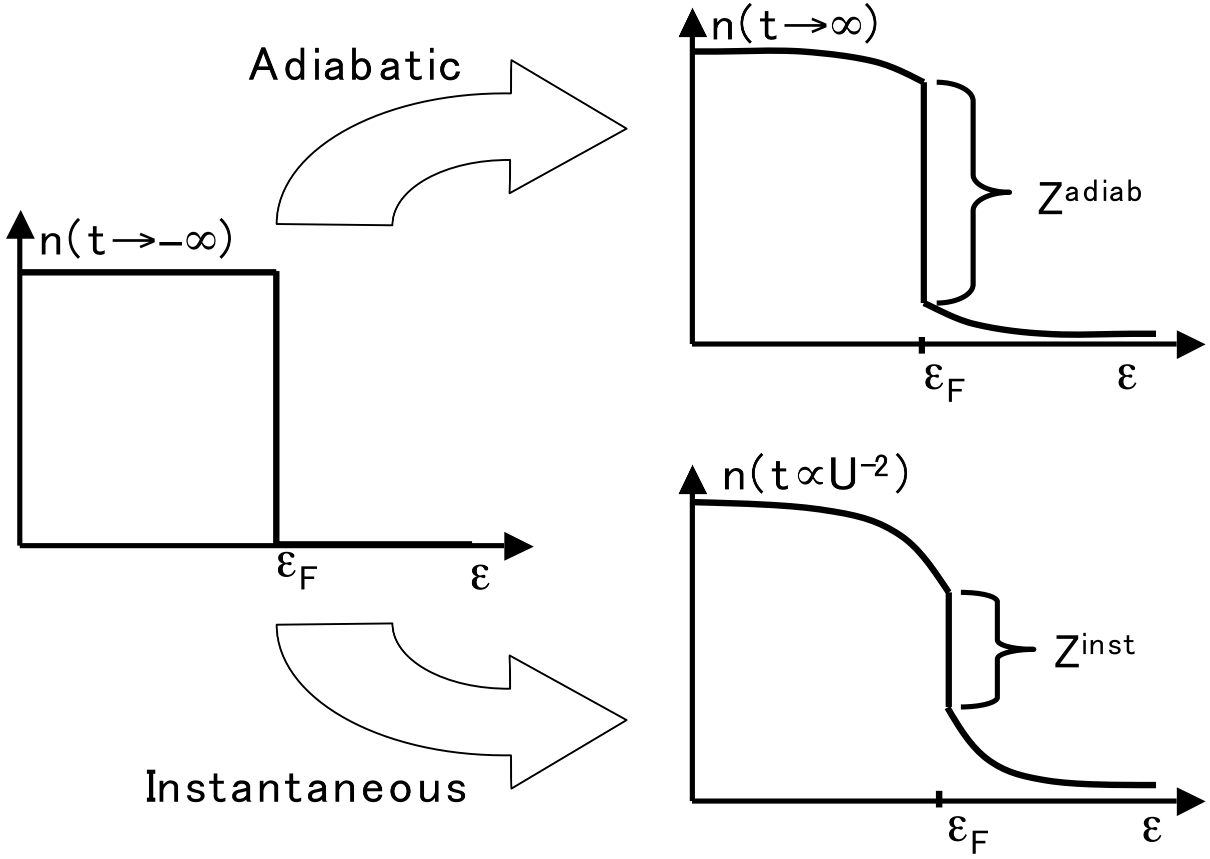
$$c^\dagger_{k\uparrow}(B=\infty) = h_k\, c^\dagger_{k\uparrow} + \sum_{k'_1,k'_2,k_1} M^k_{k'_1 k'_2 k_1} \; : c^\dagger_{k'_1\uparrow} c^\dagger_{k'_2\downarrow} c_{k_1\downarrow} : + \text{higher order terms}$$

- $h_k$ only nonzero at Fermi surface for zero temperature
- Quasiparticle residue (equilibrium) $Z = h^2_{k_F}$


Build-up of a correlated momentum distribution function
U=1.5;  Time T = 0.001
Distribution function n(E)
E
1.2
1
0.8
0.6
0.4
0.2
0
-8
-6
-4
-2
0
2
4
6
8

# Real Time Evolution

**Calculation to order $U^2$**




**Sudden switching looks like T=0 Fermi liquid with "wrong" quasiparticle residue:**

$$1 - Z^{inst} = 2\,(1 - Z^{adiab})$$

## Partial calculation to order $U^4$ :

Electron at Fermi surface decays into particle-hole excitations on time scale $t \propto U^{-4}$

Consistent with quantum Boltzmann equation for quasiparticle distribution

[illegible]

$\propto U^2$

phase space $\propto U^2$ available ("wrong" quasiparticle distribution after time $t \propto U^{-2}$)

$\Rightarrow$ leads to thermalization (Fermi-Dirac distribution) after time scale $t \propto U^{-4}$ with temperature $T_{eff} \propto U$

$\Rightarrow$ consistent with excitation energy

# Sudden switching (generic weak interaction g)

Time scale

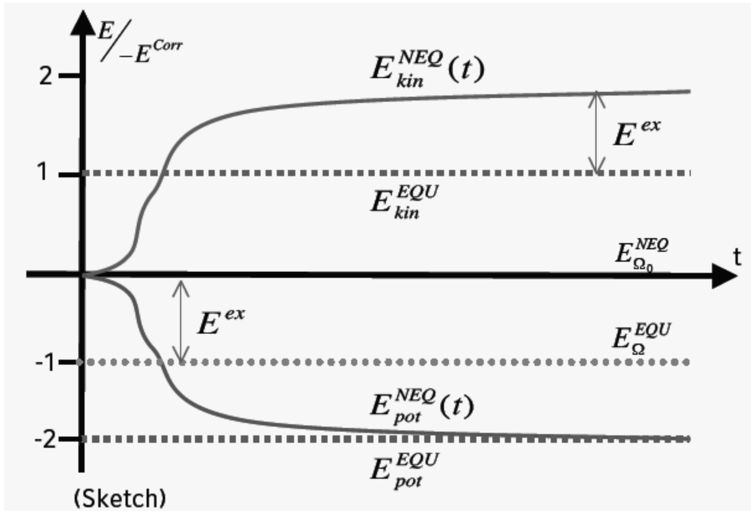
$0 < t < g^{-2}$ • Formation of quasiparticles

$t \approx g^{-2}$ • T=0 Fermi liquid with "wrong" quasiparticle residue:

$$1-Z^{inst} = 2\,(1-Z^{adiab})$$

$g^{-2} < t < g^{-4}$ • Quasi-steady state

• Prethermalization (Berges et al. 2004)




$g^{-4} < t$ • Quantum Boltzmann equation (Quasiparticles explore available phase space):

Thermalization with $T \propto g$

## Thanks to collaborators on flow equations & non-equilibrium

- D. Lobaskin: Time-dependent Kondo model
  [ D. Lobaskin and S.K., PRB 71, 193303 (2005);
  J. Stat. Phys. 123, 301 (2006) ]
- A. Hackl: Forward-backward transformation (Spin-boson model)
  [ A. Hackl and S.K., arXiv:0709.2100 ]
- M. Möckel: Sudden interaction Hubbard model
  [ M. Möckel and S.K., PRL 100, 175702 (2008) ]
- P. Fritsch: Kondo model with voltage bias and magnetic field
  [ Preprint in August 2008 ]
- M. Heyl, A. Hoffmann, P. Wang