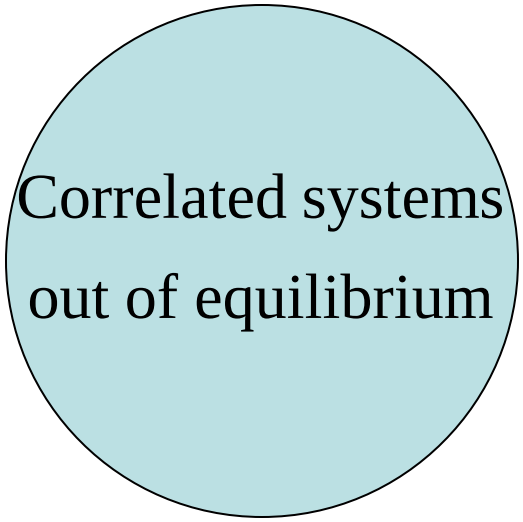
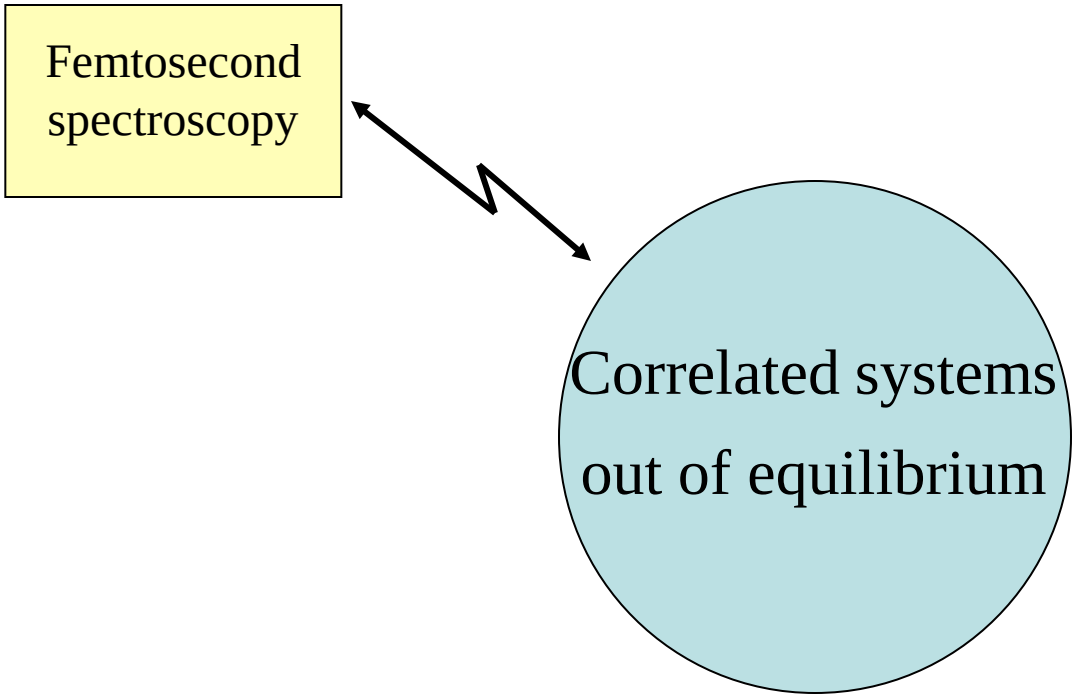
Far-from-Equilibrium and Time-Dependent Phenomena: Theory

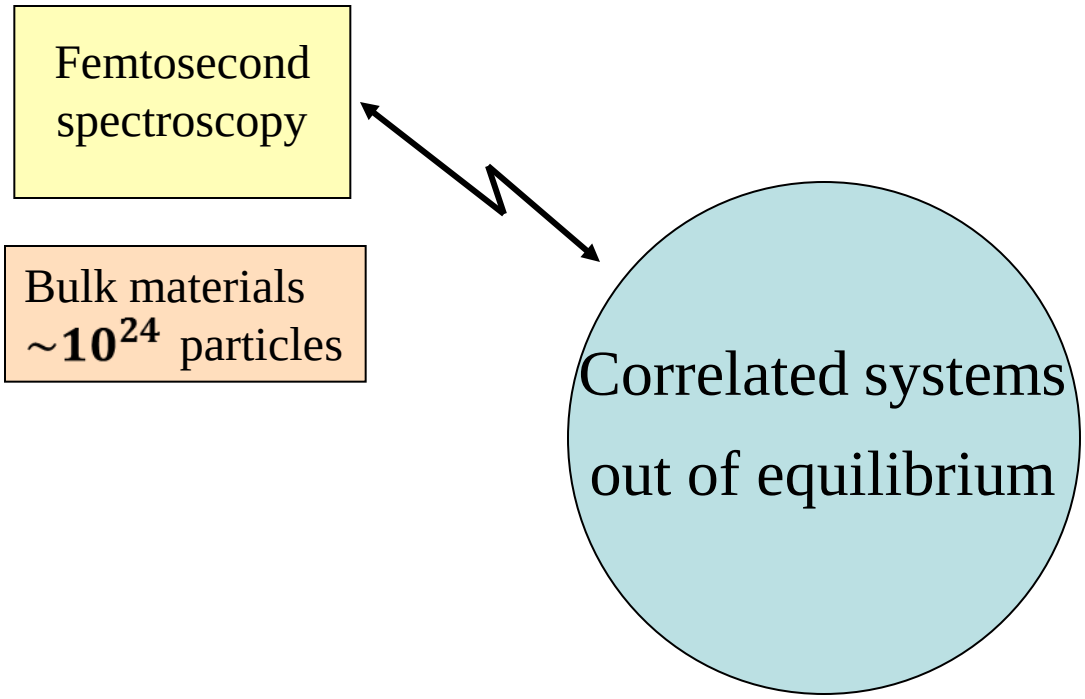
Avraham Schiller

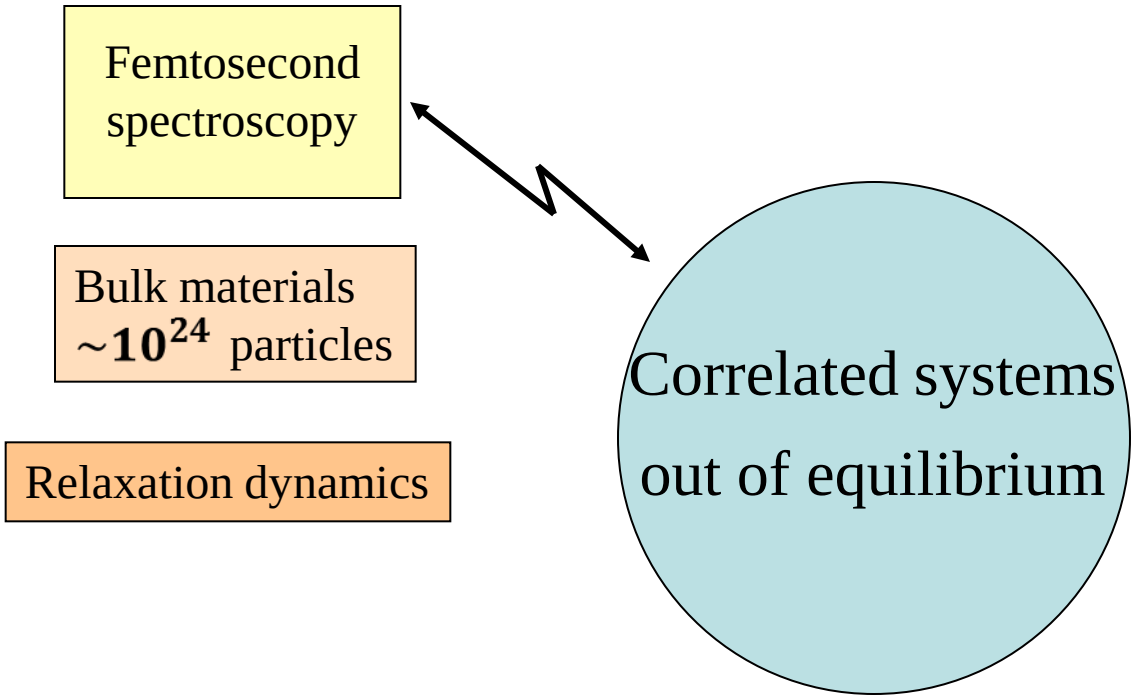
Racah Institute of Physics,

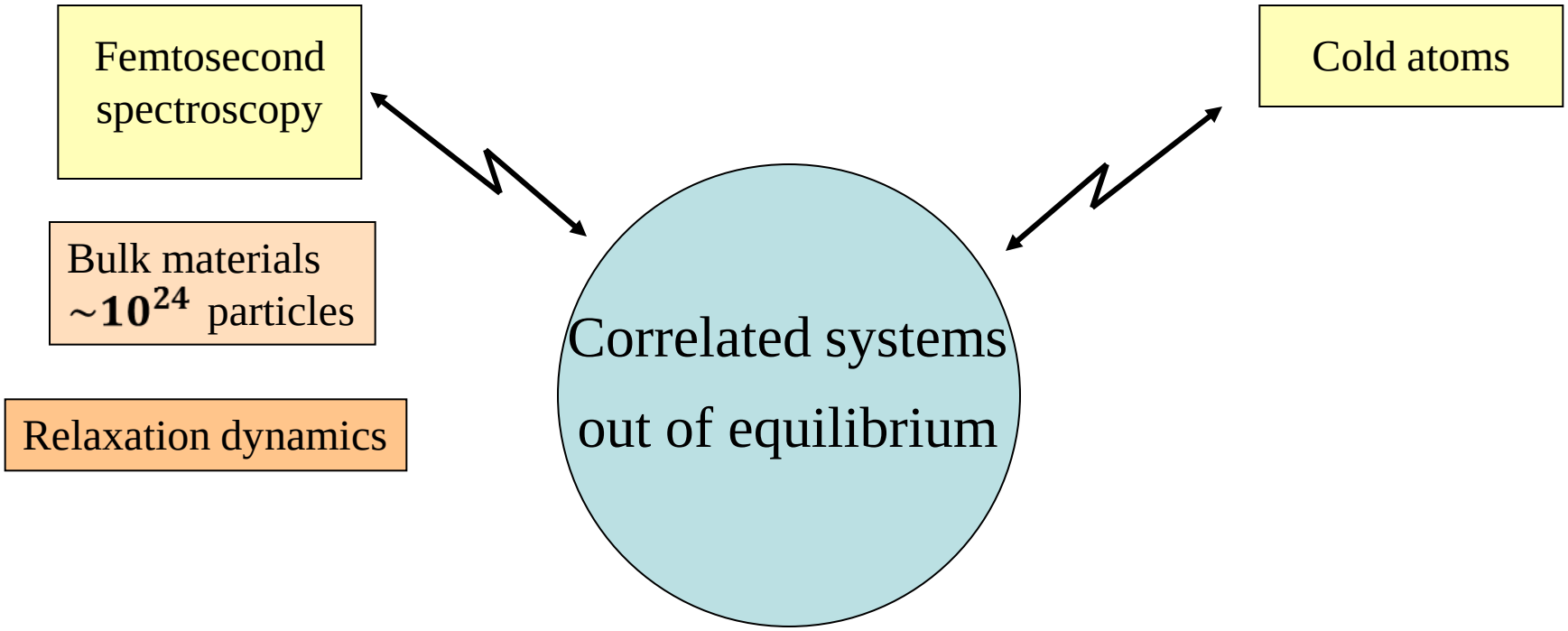
The Hebrew University

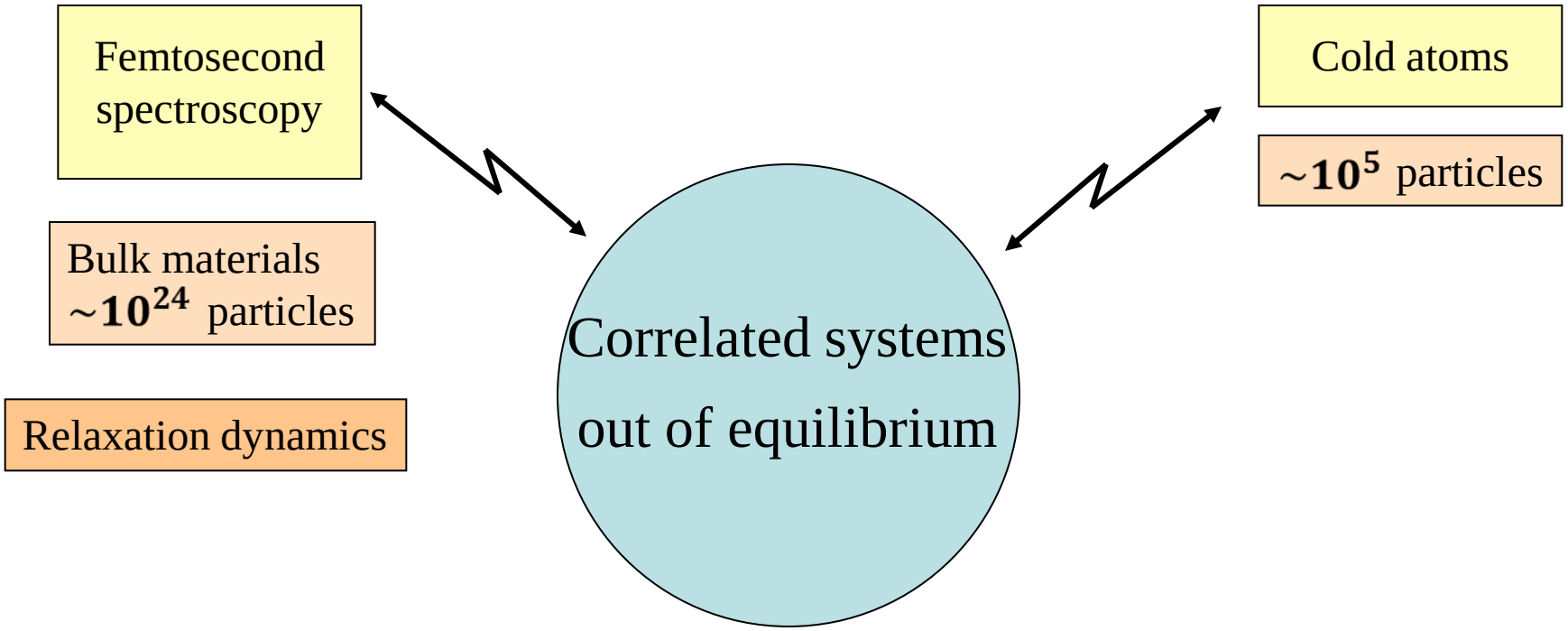

Correlated systems
out of equilibrium

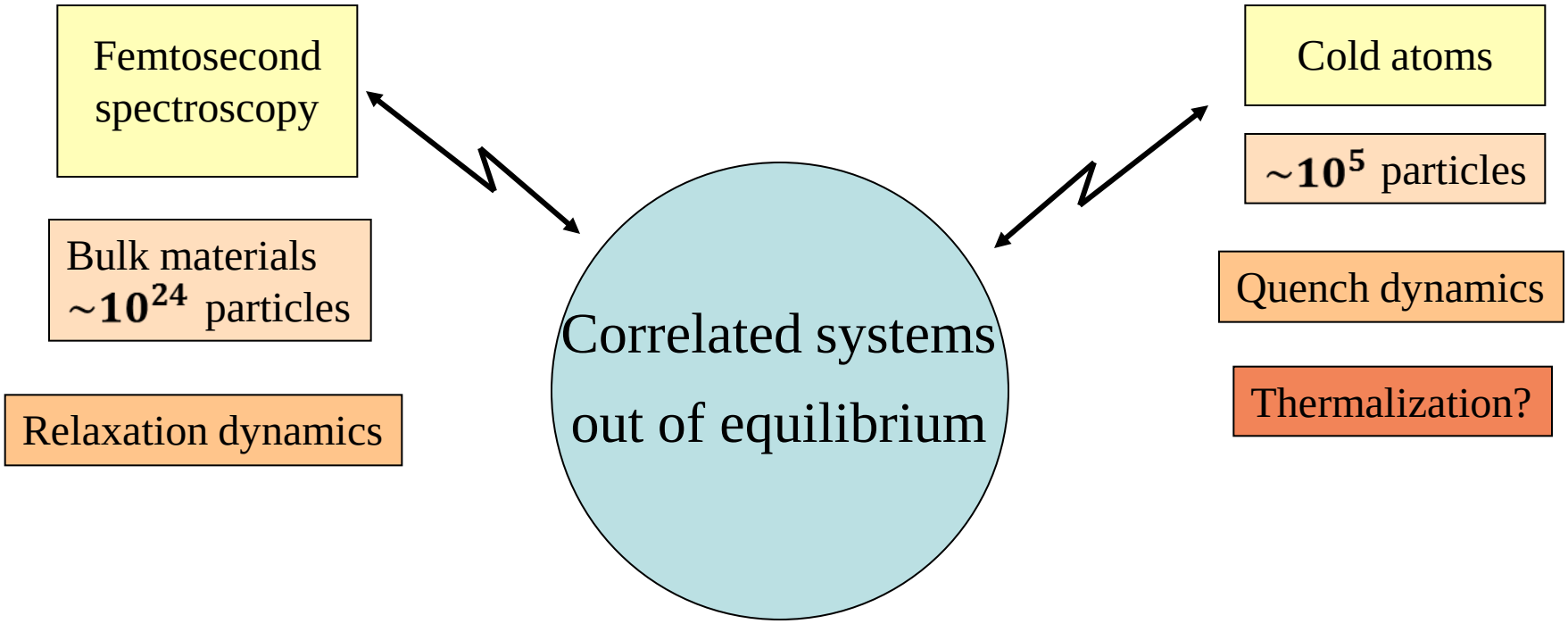

Femtosecond
spectroscopy
Correlated systems
out of equilibrium

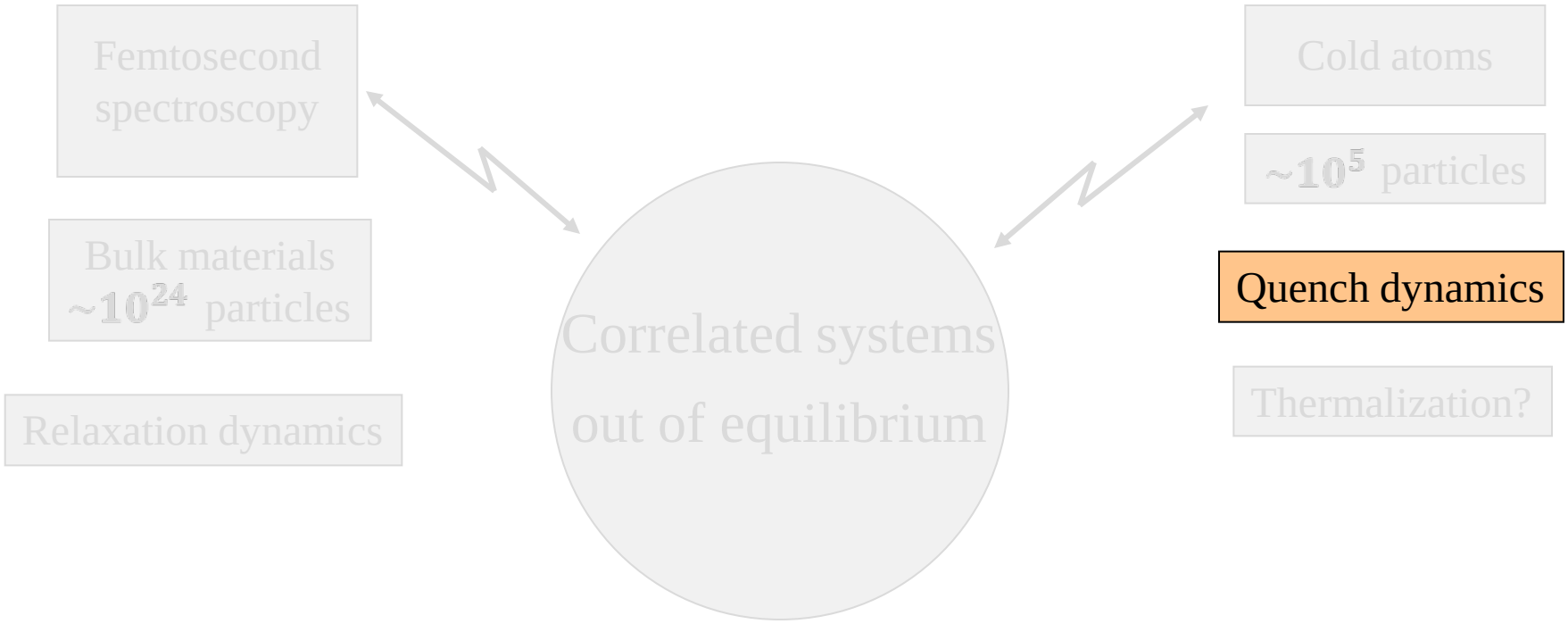

Femtosecond spectroscopy
Bulk materials $\sim 10^{24}$ particles
Correlated systems out of equilibrium


Femtosecond spectroscopy
Bulk materials $\sim 10^{24}$ particles
Relaxation dynamics
Correlated systems out of equilibrium

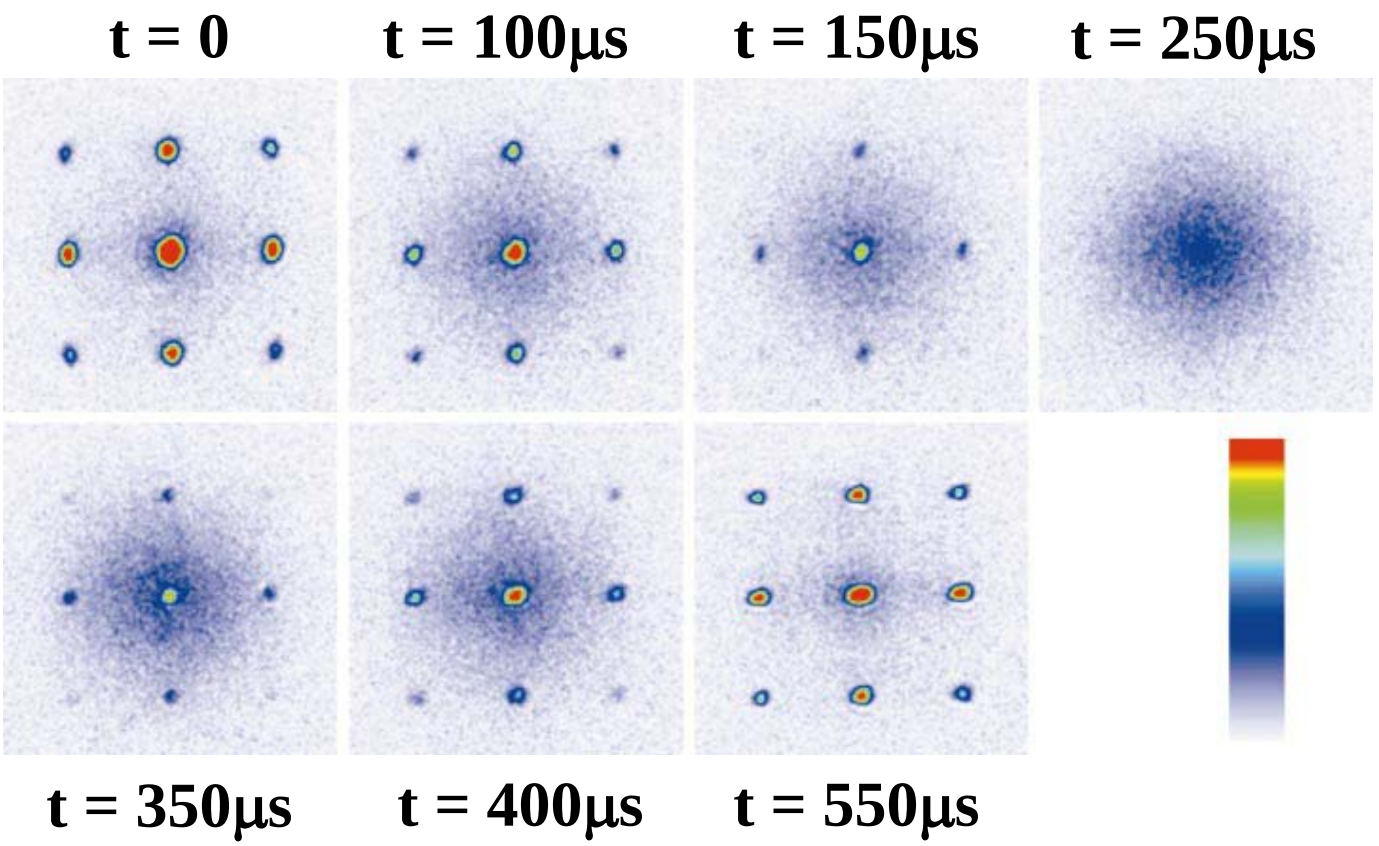

Femtosecond spectroscopy
Cold atoms
Bulk materials $\sim 10^{24}$ particles
Correlated systems out of equilibrium
Relaxation dynamics


Femtosecond spectroscopy
Bulk materials $\sim 10^{24}$ particles
Relaxation dynamics
Correlated systems out of equilibrium
Cold atoms
$\sim 10^{5}$ particles

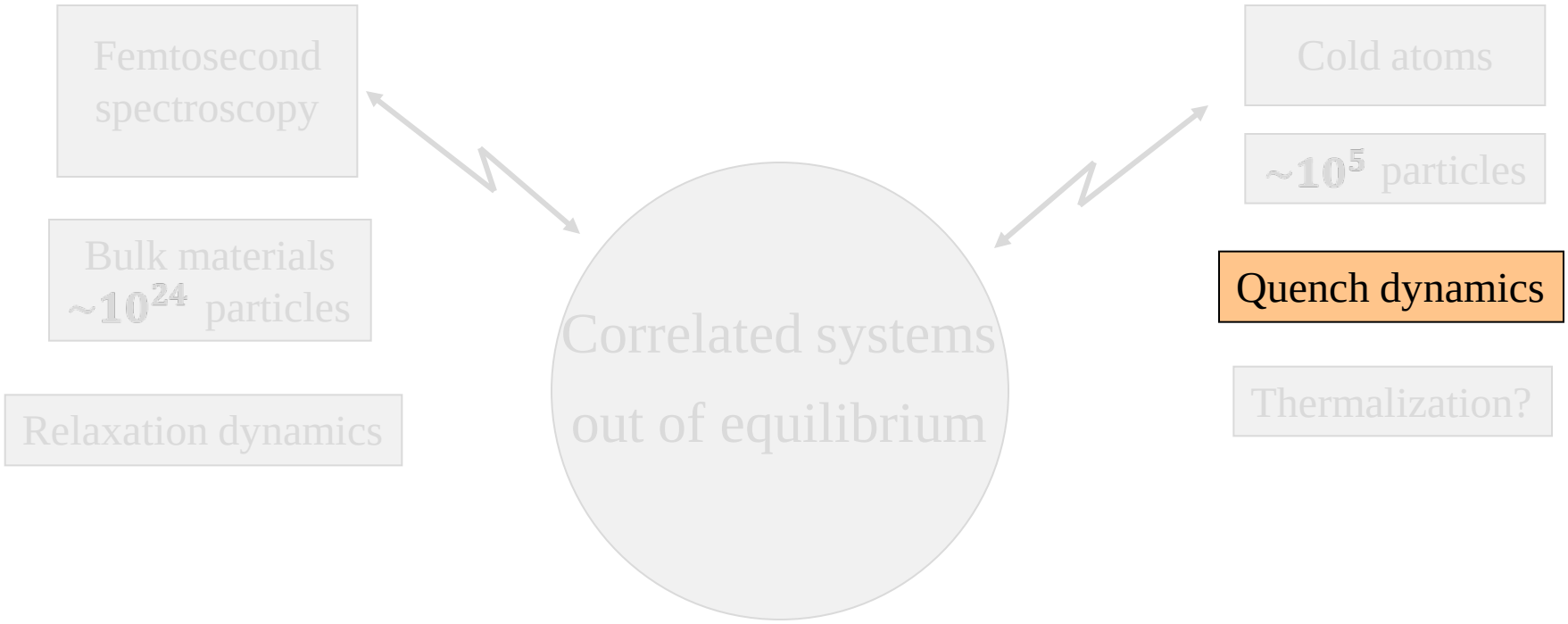

Femtosecond spectroscopy
Bulk materials $\sim 10^{24}$ particles
Relaxation dynamics
Correlated systems out of equilibrium
Cold atoms
$\sim 10^{5}$ particles
Quench dynamics
Thermalization?

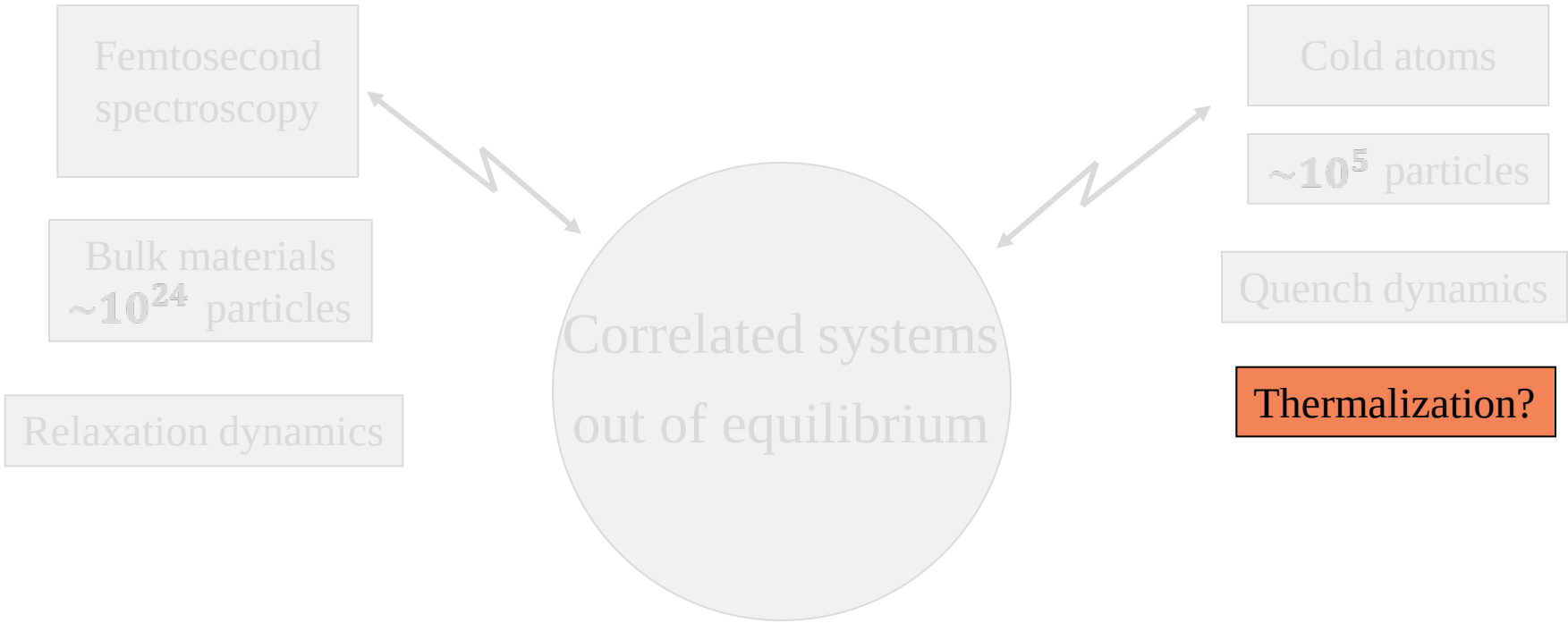

Femtosecond spectroscopy
Bulk materials ~10^24 particles
Relaxation dynamics
Correlated systems out of equilibrium
Cold atoms
~10^5 particles
Quench dynamics
Thermalization?

Collapse and revival of coherent matter waves

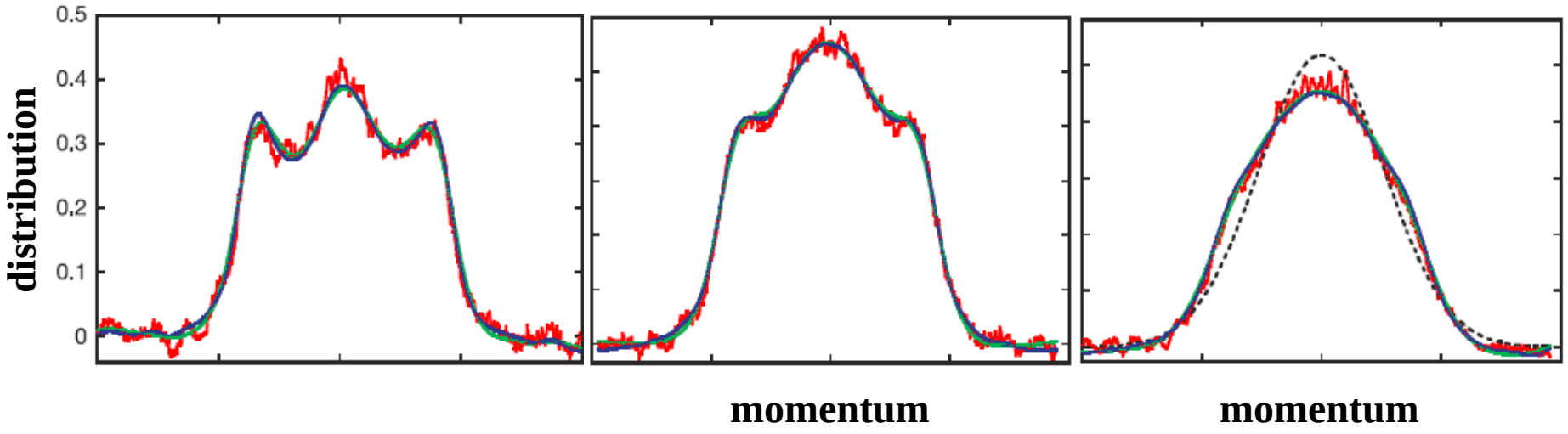


M. Greiner et al., Nature 2002


Femtosecond spectroscopy
Bulk materials ~10^24 particles
Relaxation dynamics
Correlated systems out of equilibrium
Cold atoms
~10^5 particles
Quench dynamics
Thermalization?

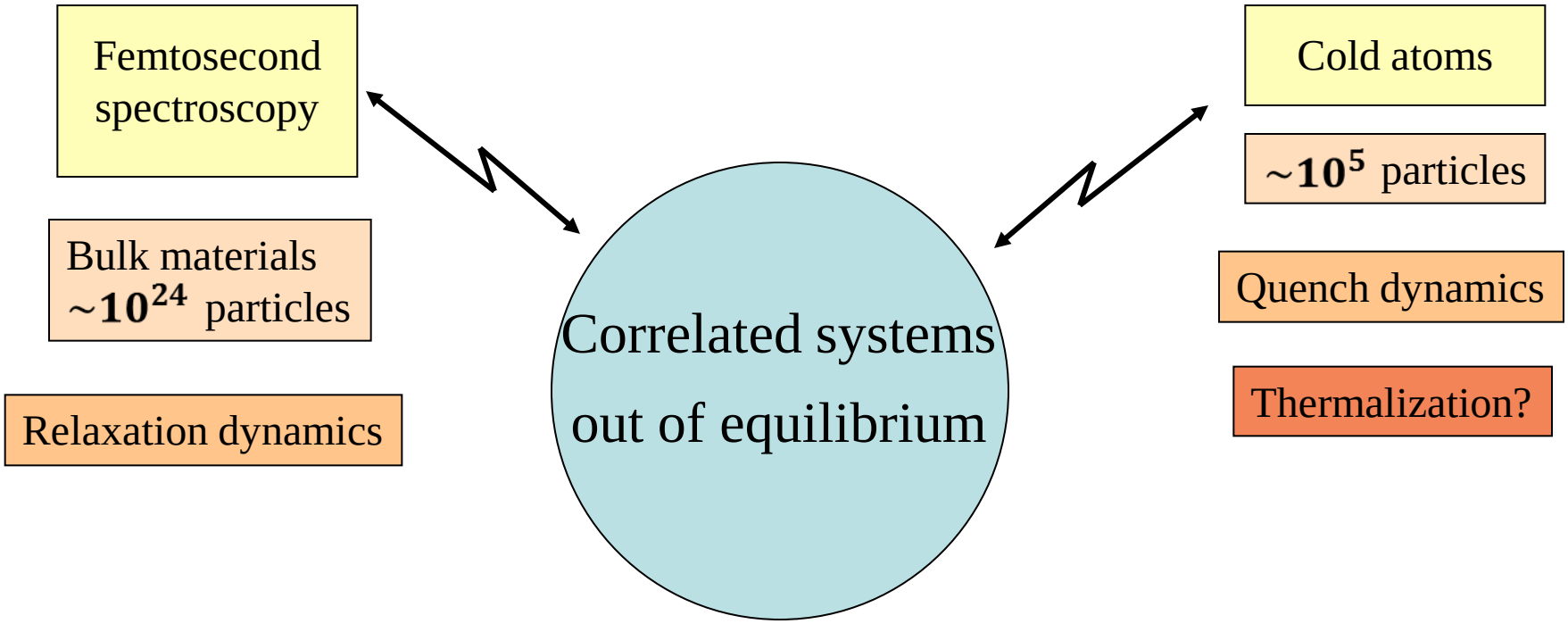

Femtosecond spectroscopy
Bulk materials ~10^24 particles
Relaxation dynamics
Correlated systems out of equilibrium
Cold atoms
~10^5 particles
Quench dynamics
Thermalization?

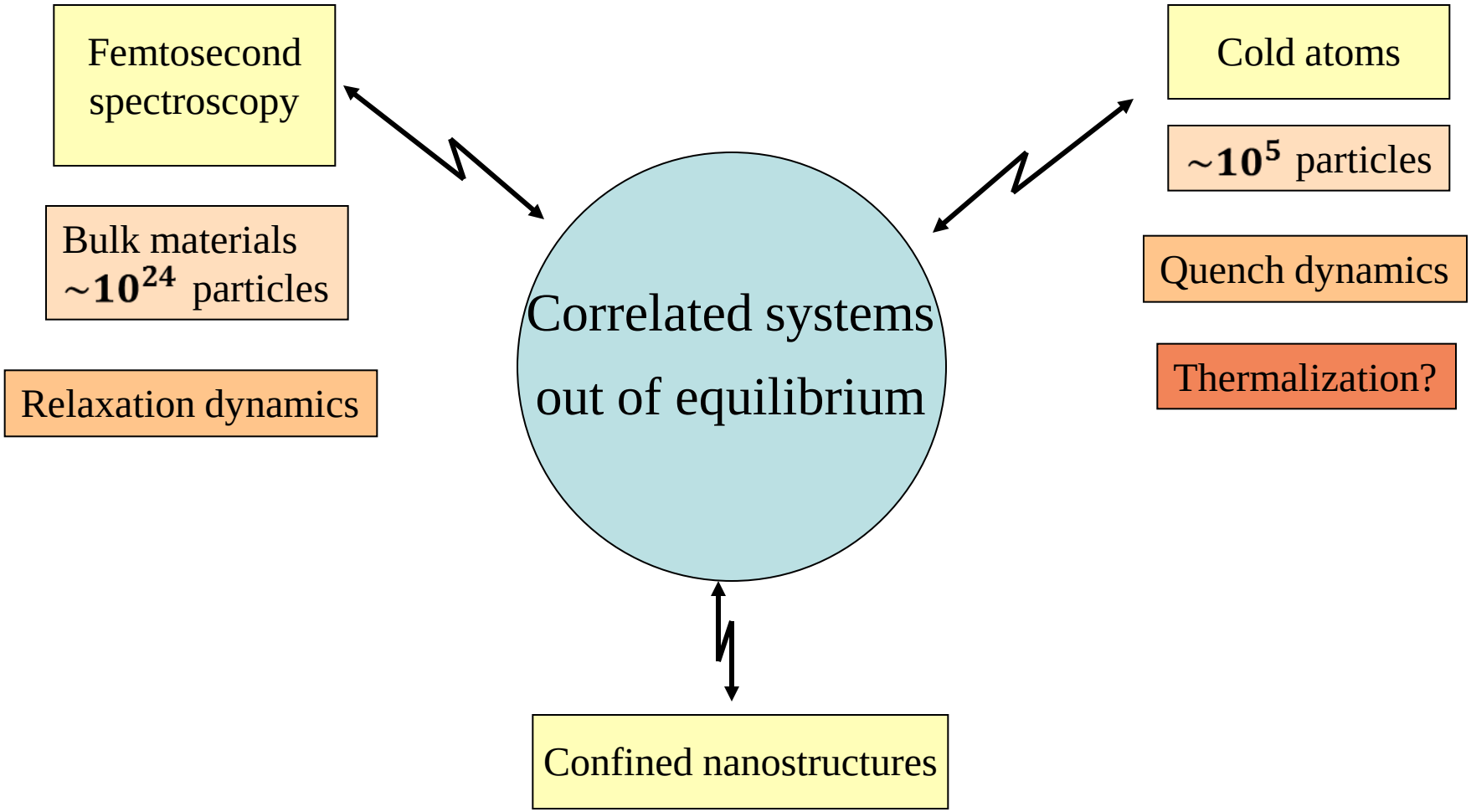
Lack of thermalization in 1D traps

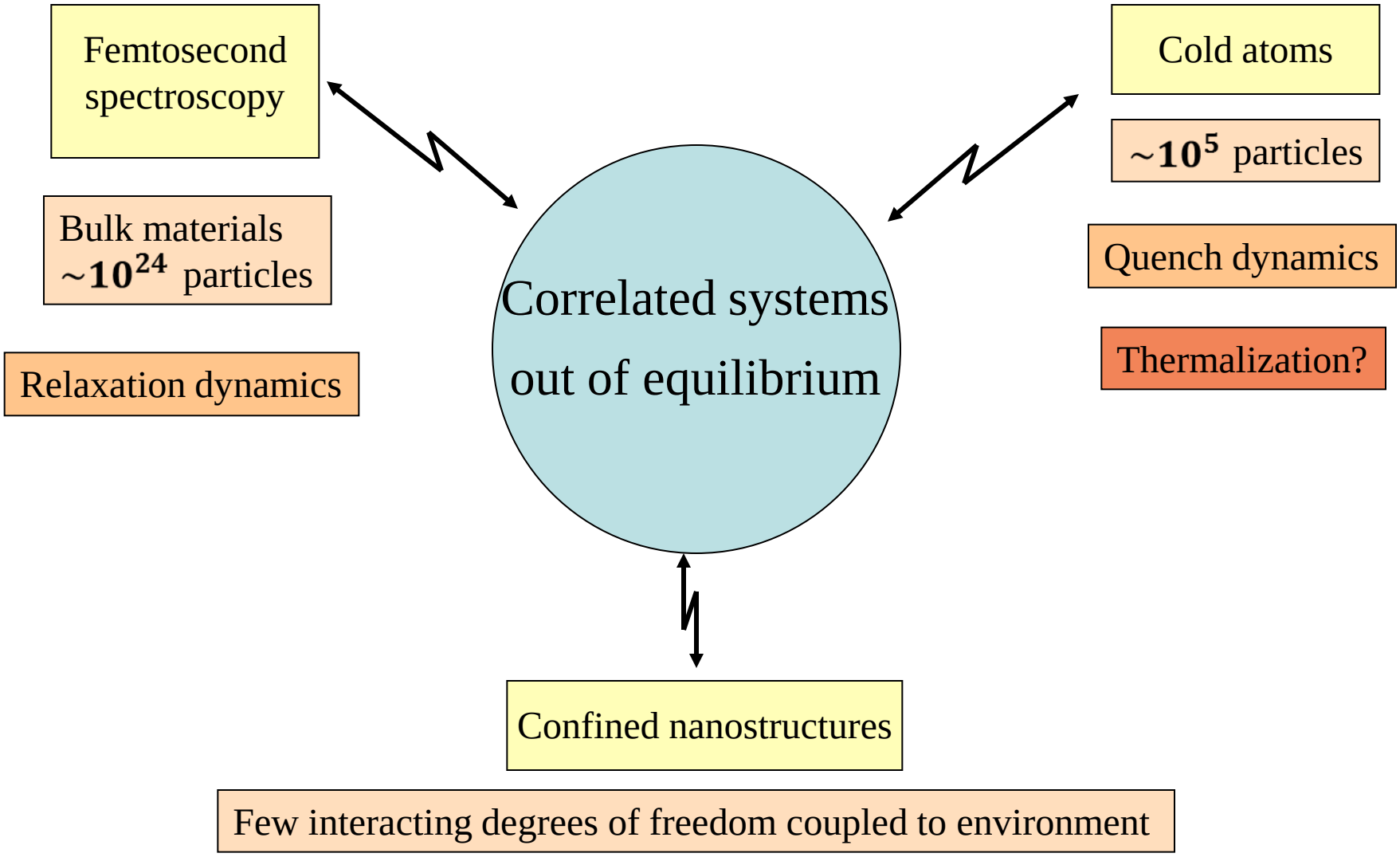


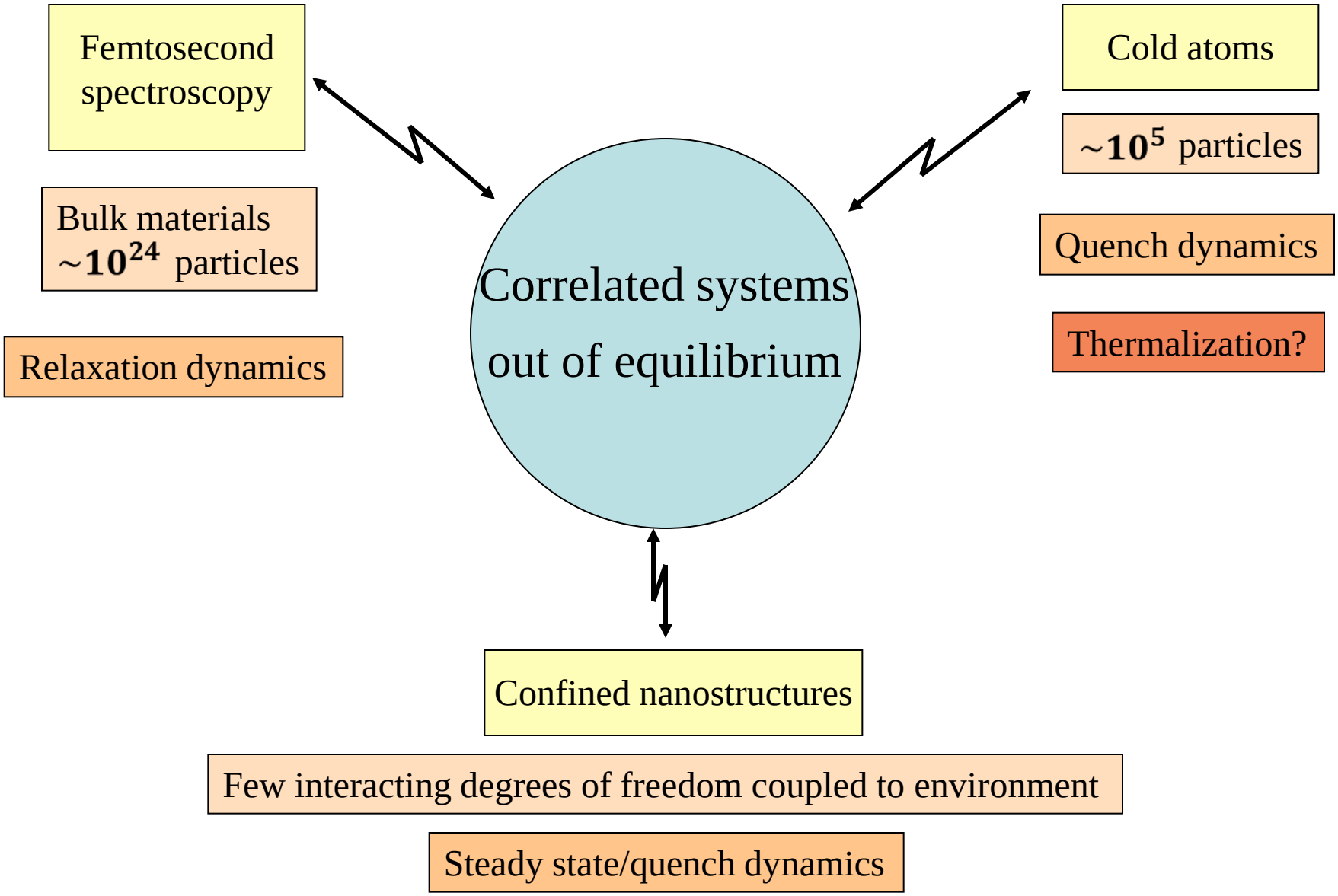
- **Exciting the system and allowing it to evolve in time, the momentum distribution function remains non-Gaussian up to long time scales**
- **Only $\sim 10^2$ atoms per trap**

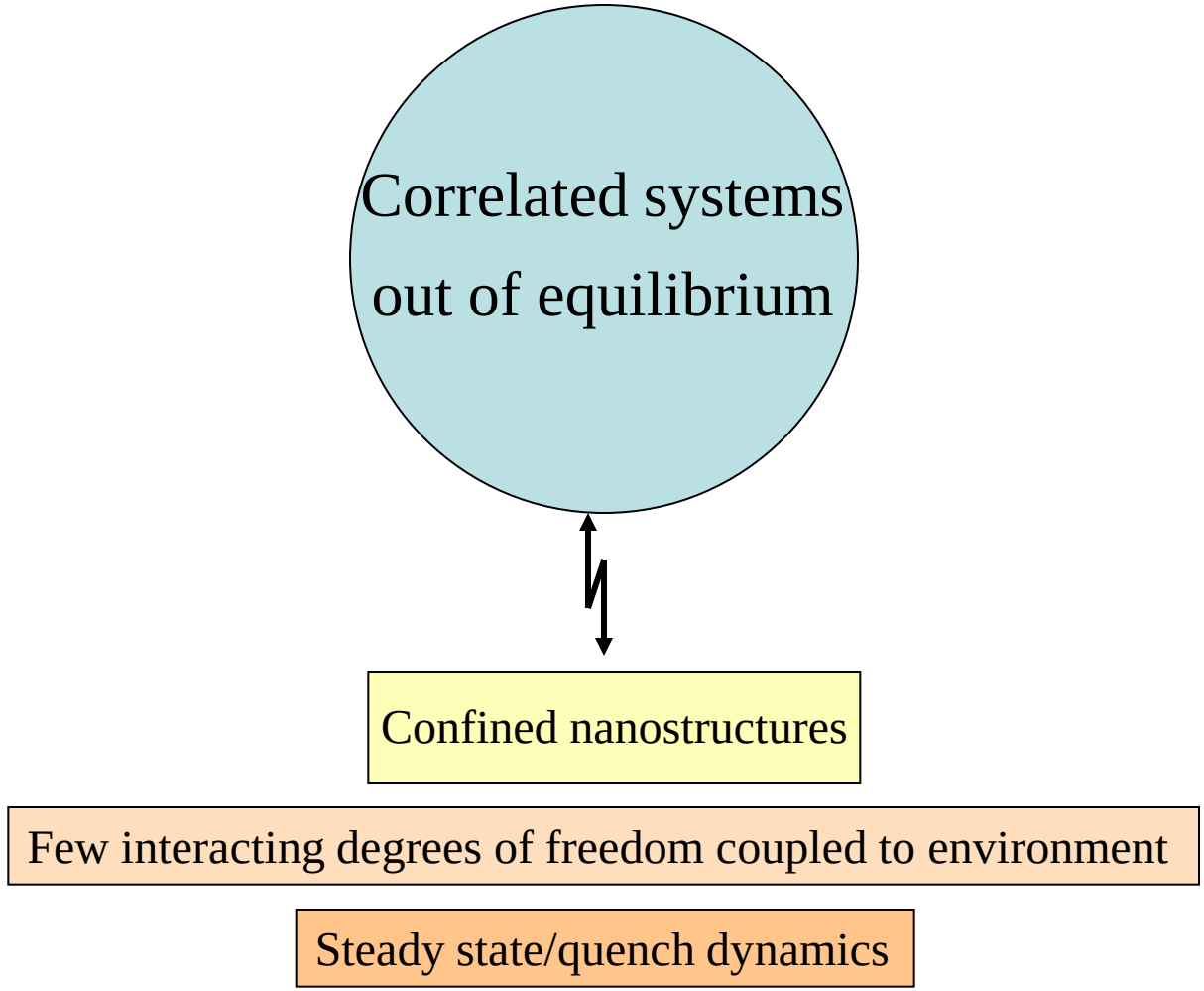
T. Kinoshita et al., Nature 440, 900 (2006).


Femtosecond spectroscopy
Bulk materials $\sim 10^{24}$ particles
Relaxation dynamics
Correlated systems out of equilibrium
Cold atoms
$\sim 10^{5}$ particles
Quench dynamics
Thermalization?

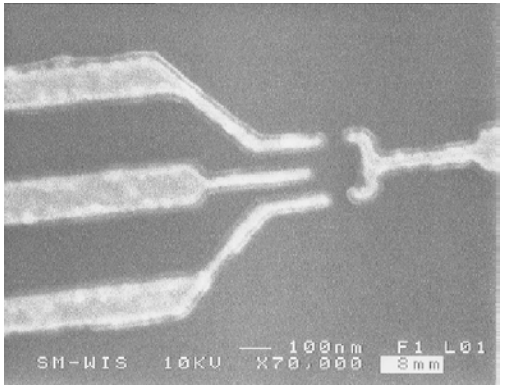

Femtosecond spectroscopy
Bulk materials $\sim 10^{24}$ particles
Relaxation dynamics
Cold atoms
$\sim 10^{5}$ particles
Quench dynamics
Thermalization?
Correlated systems out of equilibrium
Confined nanostructures


Femtosecond spectroscopy
Cold atoms
$\sim 10^5$ particles
Bulk materials $\sim 10^{24}$ particles
Quench dynamics
Correlated systems out of equilibrium
Relaxation dynamics
Thermalization?
Confined nanostructures
Few interacting degrees of freedom coupled to environment

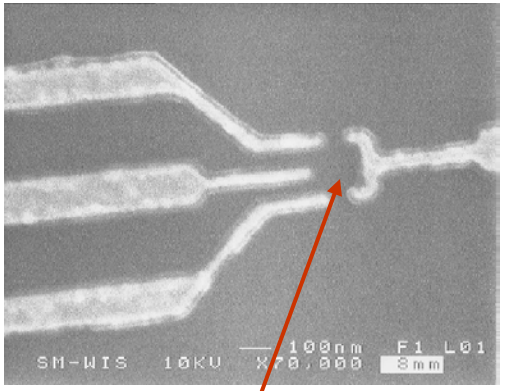

Femtosecond spectroscopy
Bulk materials $\sim 10^{24}$ particles
Relaxation dynamics
Cold atoms
$\sim 10^{5}$ particles
Quench dynamics
Thermalization?
Correlated systems out of equilibrium
Confined nanostructures
Few interacting degrees of freedom coupled to environment
Steady state/quench dynamics


Correlated systems
out of equilibrium
Confined nanostructures
Few interacting degrees of freedom coupled to environment
Steady state/quench dynamics

Kondo effect in ultra-small quantum dots

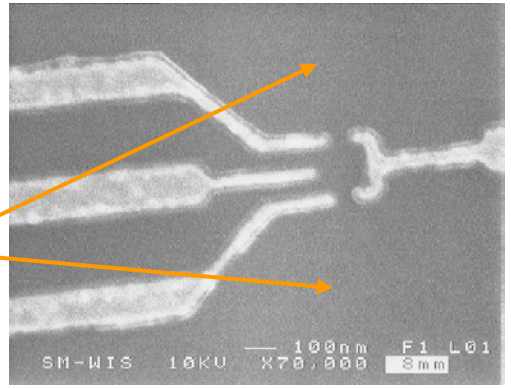


Kondo effect in ultra-small quantum dots

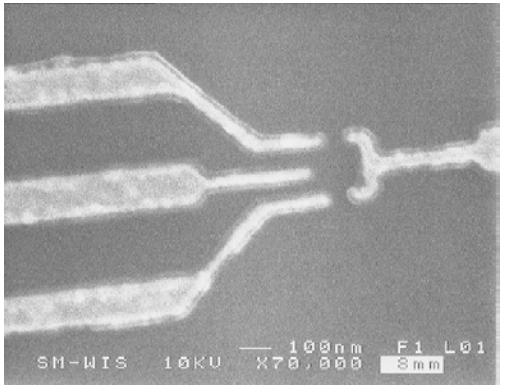


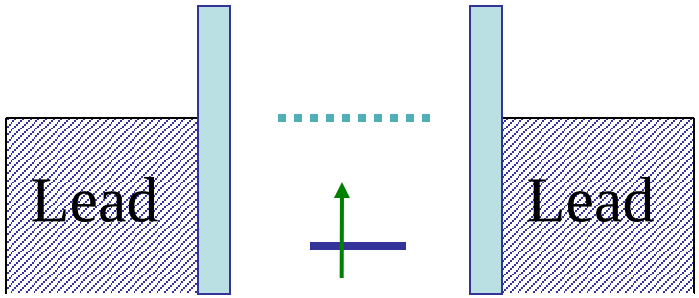
Quantum dot

Kondo effect in ultra-small quantum dots

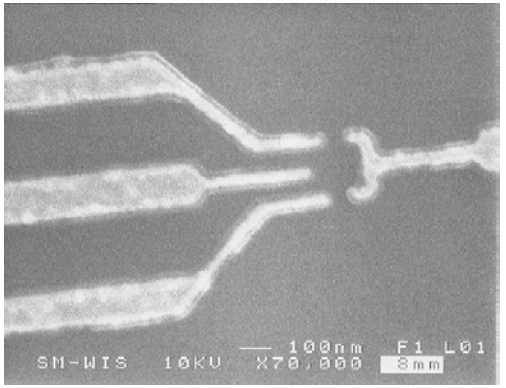


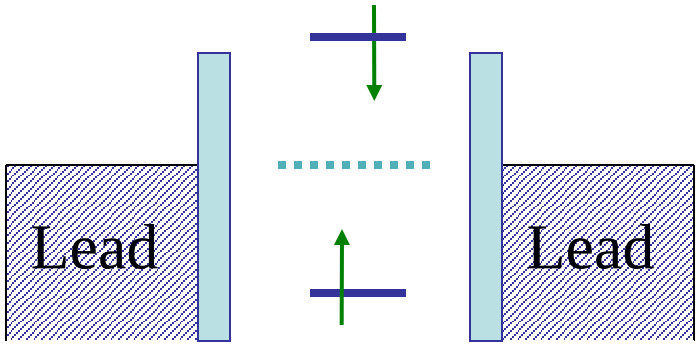
Kondo effect in ultra-small quantum dots



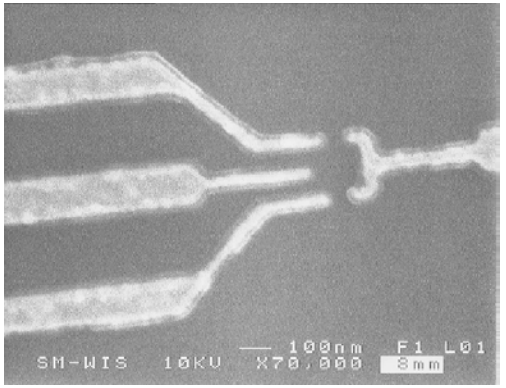


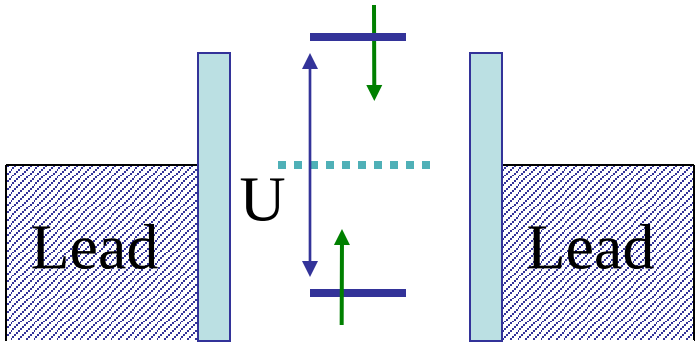
Kondo effect in ultra-small quantum dots





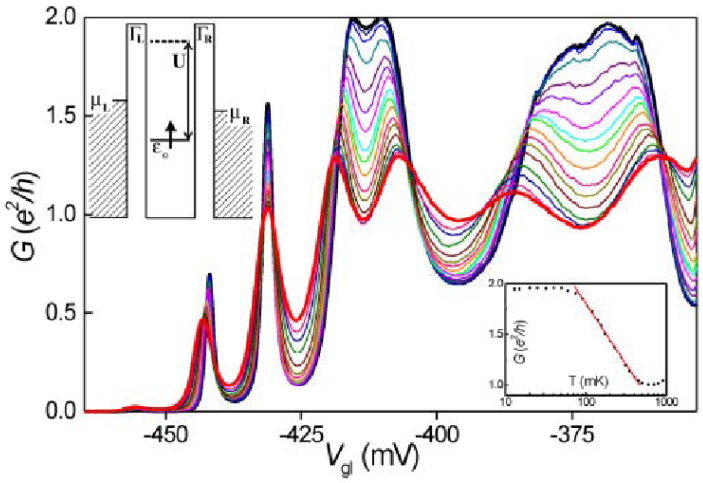
Kondo effect in ultra-small quantum dots

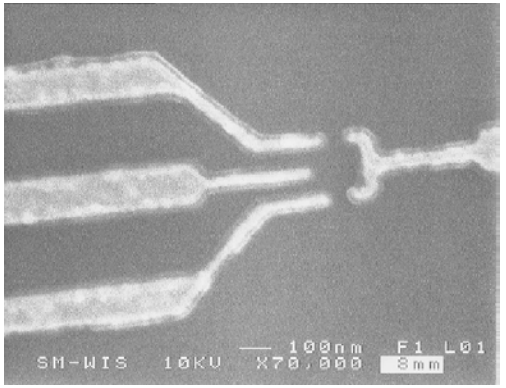


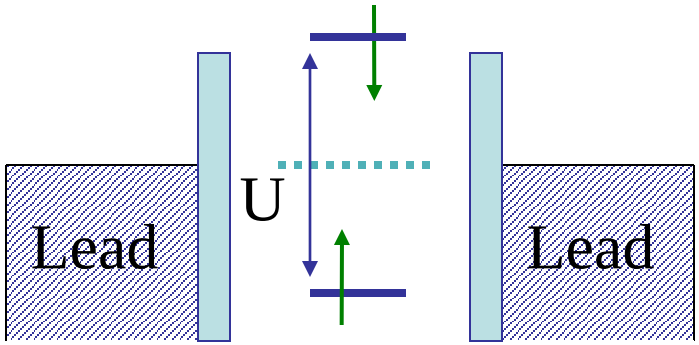


Kondo effect in ultra-small quantum dots

Conductance vs gate voltage

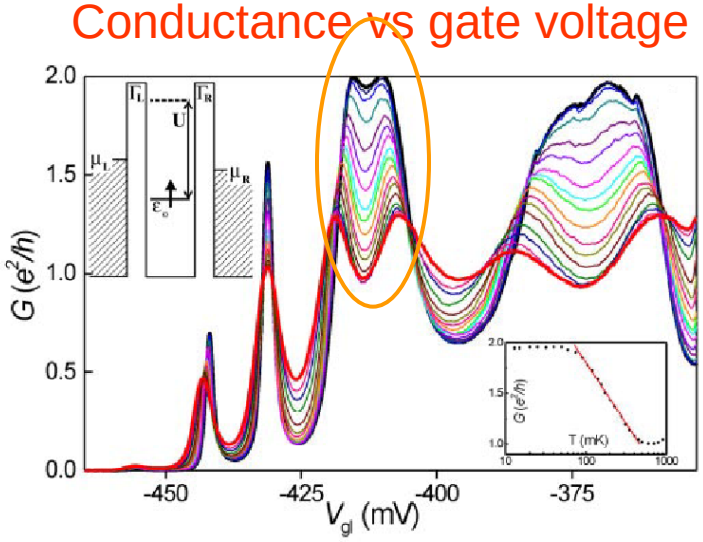


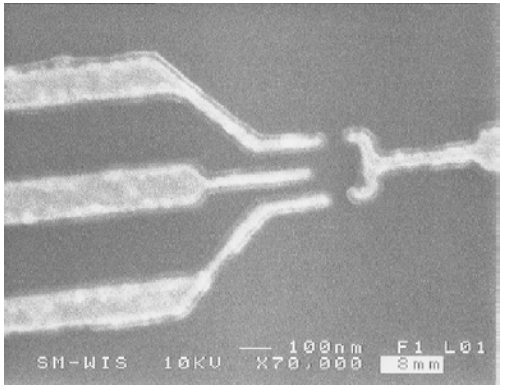


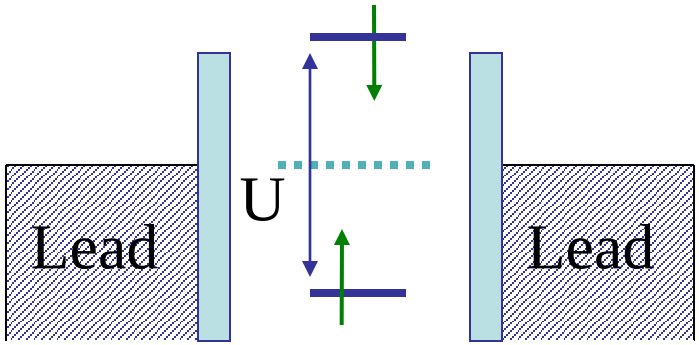


Kondo effect in ultra-small quantum dots

Conductance vs gate voltage

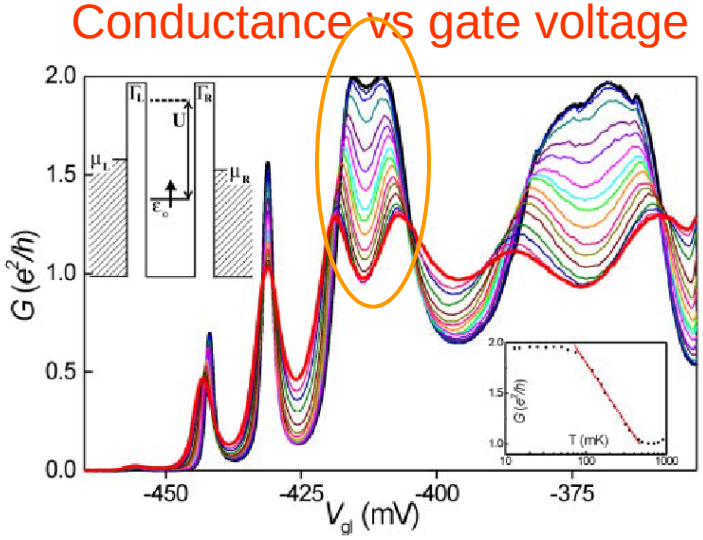


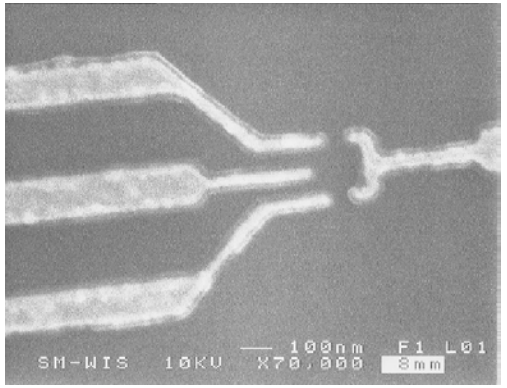


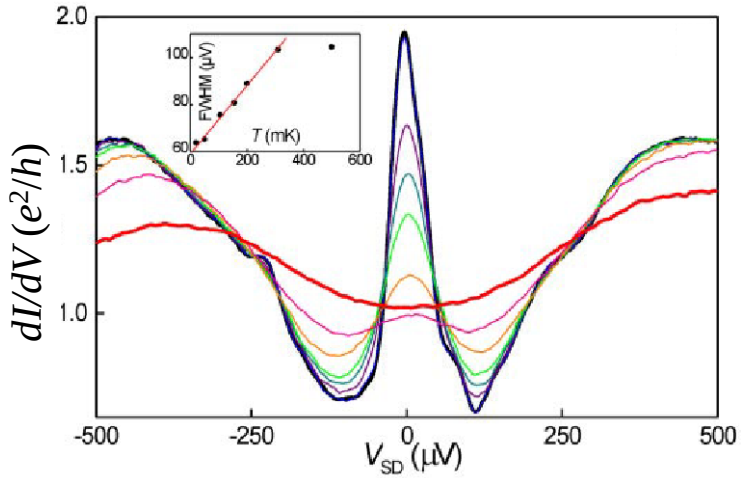


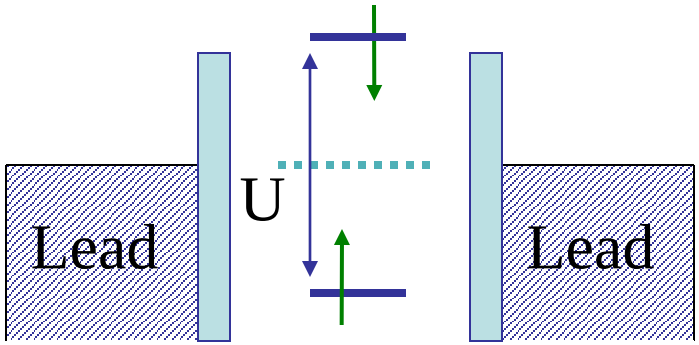
Kondo effect in ultra-small quantum dots

Conductance vs gate voltage





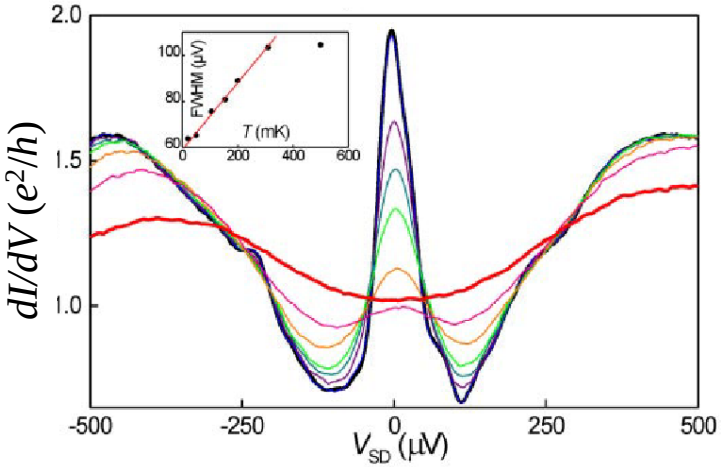




Electronic correlations out of equilibrium

Electronic correlations out of equilibrium

Steady state

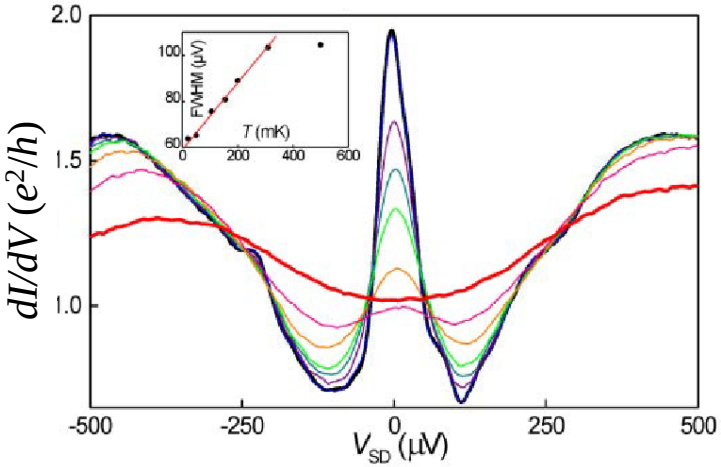


Differential conductance in two-terminal devices

van der Wiel *et al.*,Science 2000

Electronic correlations out of equilibrium

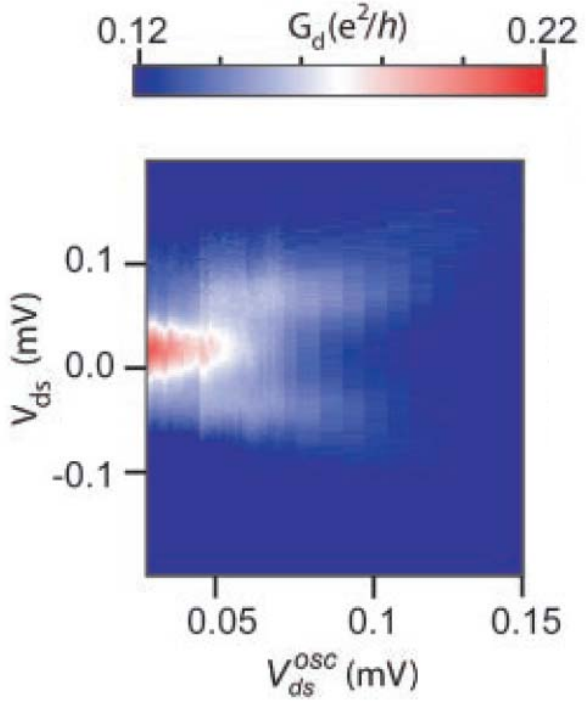
Steady state



Differential conductance in two-terminal devices

van der Wiel *et al.*,Science 2000

ac drive

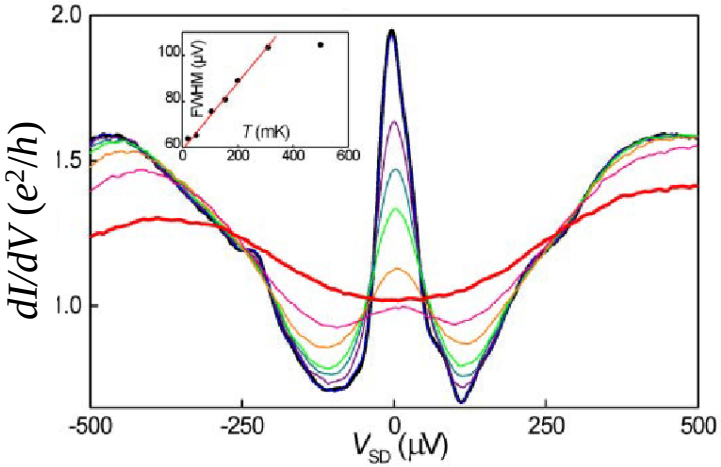


Photon-assisted side peaks

Kogan *et al.*,Science 2004

Electronic correlations out of equilibrium

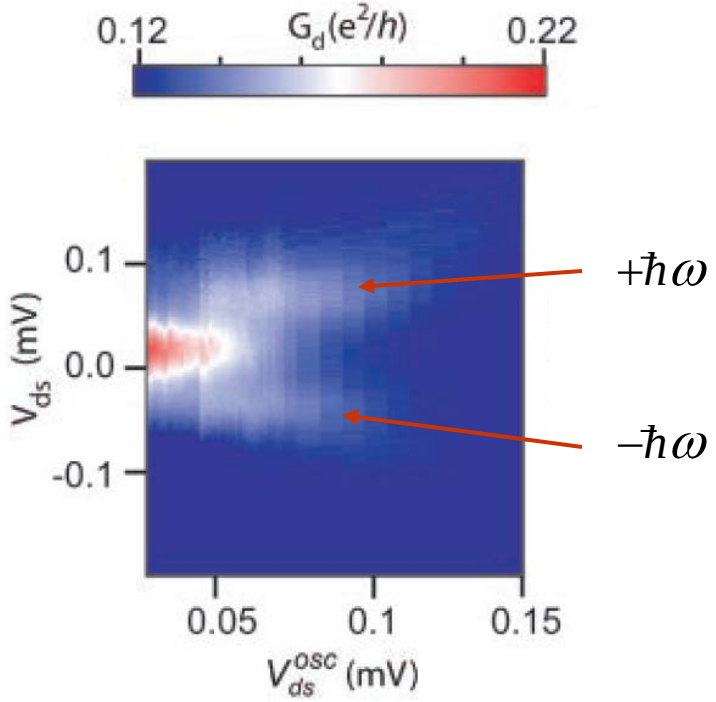
Steady state



Differential conductance in two-terminal devices

van der Wiel *et al.*,Science 2000

ac drive

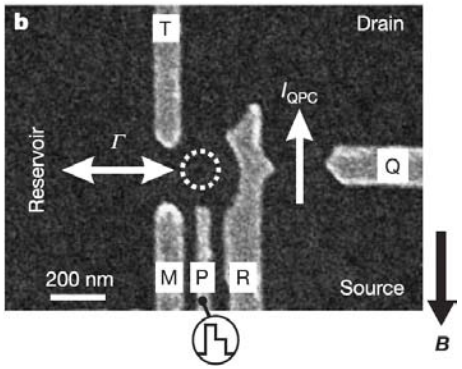


Photon-assisted side peaks

Kogan *et al.*,Science 2004

Electronic correlations out of equilibrium

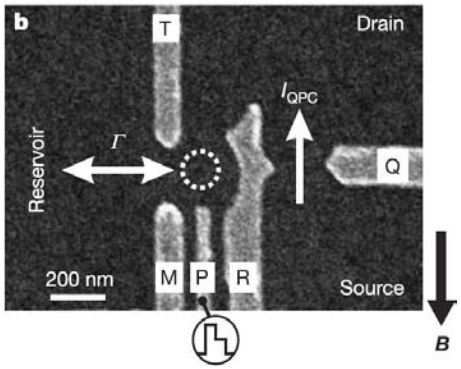
Response to pulsed bias

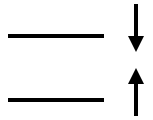


Elzerman *et al*., Nature (2005)

Electronic correlations out of equilibrium

Response to pulsed bias



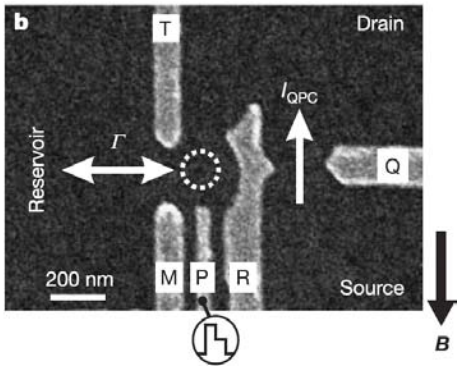


(a)

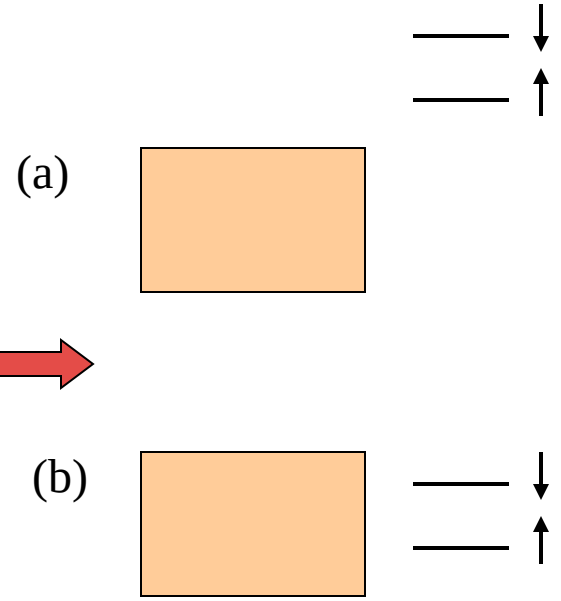
Elzerman *et al*., Nature (2005)

Electronic correlations out of equilibrium

Response to pulsed bias



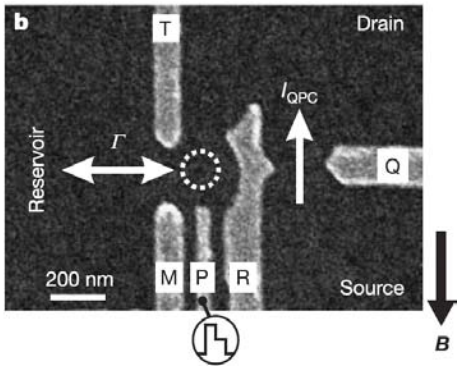
Abrupt change of gate voltage



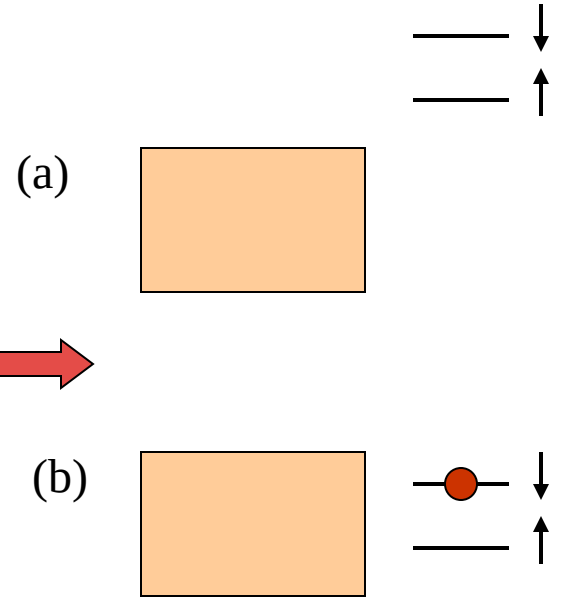
Elzerman *et al*., Nature (2005)

Electronic correlations out of equilibrium

Response to pulsed bias



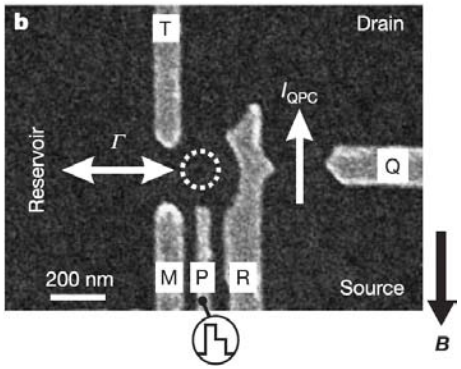
Abrupt change of gate voltage



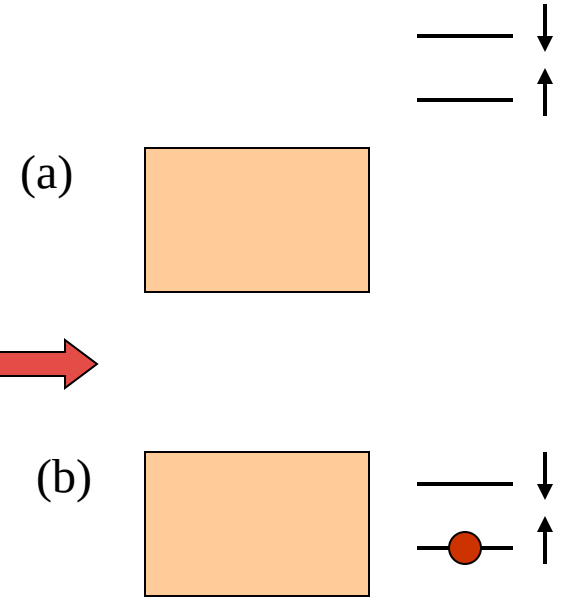
Elzerman *et al*., Nature (2005)

Electronic correlations out of equilibrium

Response to pulsed bias



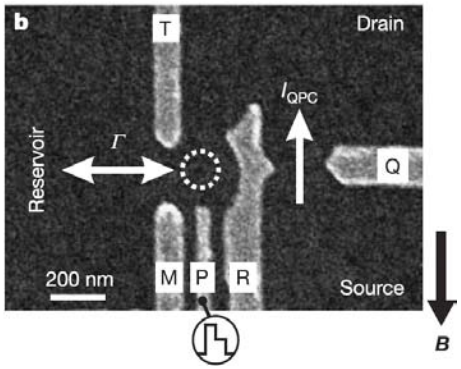
Abrupt change of gate voltage

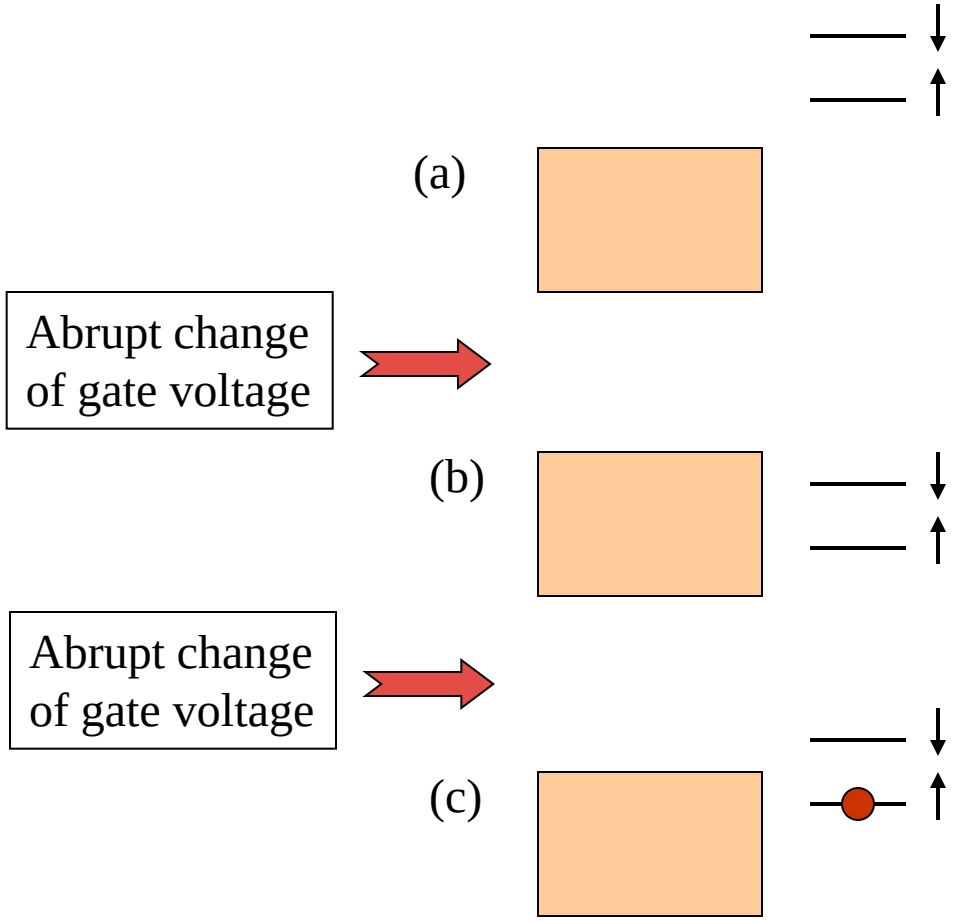


Elzerman *et al*., Nature (2005)

Electronic correlations out of equilibrium

Response to pulsed bias

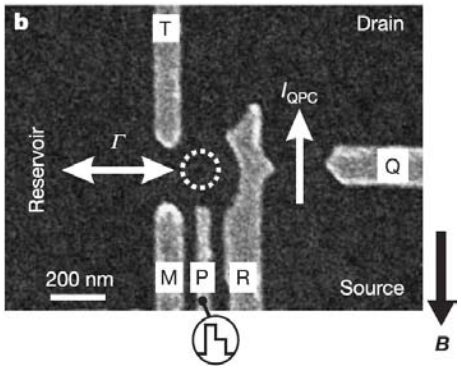




Elzerman *et al*., Nature (2005)

Electronic correlations out of equilibrium

Response to pulsed bias



(a)

Abrupt change of gate voltage

(b)

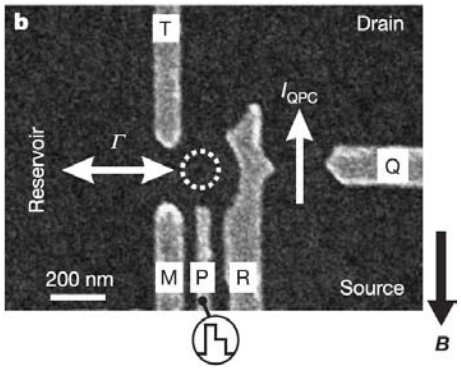
Abrupt change of gate voltage

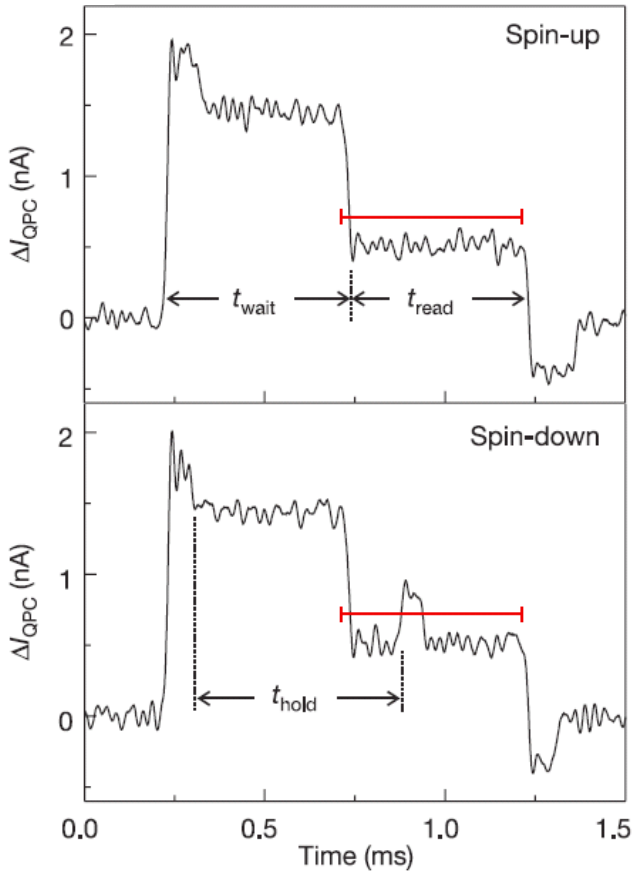
(c)

Elzerman *et al*., Nature (2005)

Electronic correlations out of equilibrium

Response to pulsed bias





Single-shot readout of the spin state of a quantum dot from real-time dynamics

Elzerman *et al.*, Nature (2005)

Nonequilibrium: A theoretical challenge

Nonequilibrium: A theoretical challenge

- **The Goal:** The description of nanostructures at nonzero bias, nonzero driving fields, and/or quench dynamics

Nonequilibrium: A theoretical challenge

- **The Goal:** The description of nanostructures at nonzero bias, nonzero driving fields, and/or quench dynamics

- **Required:** Inherently nonperturbative treatment of nonequilibrium

Nonequilibrium: A theoretical challenge

- **The Goal:** The description of nanostructures at nonzero bias, nonzero driving fields, and/or quench dynamics
- **Required:** Inherently nonperturbative treatment of nonequilibrium
- **Problem:** Unlike equilibrium conditions, density operator is not known in the presence of interactions

Nonequilibrium: A theoretical challenge

- **The Goal:** The description of nanostructures at nonzero bias, nonzero driving fields, and/or quench dynamics
- **Required:** Inherently nonperturbative treatment of nonequilibrium
- **Problem:** Unlike equilibrium conditions, density operator is not known in the presence of interactions

→ Most nonperturbative approaches available in equilibrium are simply inadequate

Nonequilibrium: A theoretical challenge

Two possible strategies to treat steady state

Nonequilibrium: A theoretical challenge

Two possible strategies to treat steady state

Time-independent formulation:

Nonequilibrium: A theoretical challenge

Two possible strategies to treat steady state

Time-independent formulation:

Work directly at steady state by imposing suitable boundary conditions

Nonequilibrium: A theoretical challenge

Two possible strategies to treat steady state

Time-independent formulation:

Work directly at steady state by imposing suitable boundary conditions

e.g., by constructing the many-particle scattering states

Nonequilibrium: A theoretical challenge

Two possible strategies to treat steady state

Time-independent formulation:

Time-dependent formulation

Work directly at steady state by imposing suitable boundary conditions

e.g., by constructing the many-particle scattering states

Nonequilibrium: A theoretical challenge

Two possible strategies to treat steady state

Time-independent formulation:

Work directly at steady state by imposing suitable boundary conditions

e.g., by constructing the many-particle scattering states

Time-dependent formulation

Evolve the system in time to reach steady state

Nonequilibrium: A theoretical challenge

Two possible strategies to treat steady state

Time-independent formulation:

Work directly at steady state by imposing suitable boundary conditions

e.g., by constructing the many-particle scattering states

Time-dependent formulation

Evolve the system in time to reach steady state

Both approaches require an open system!

Brief division of theoretical approaches

Steady state

Brief division of theoretical approaches

Steady state

- Keldysh diagrammatics

Brief division of theoretical approaches

Steady state

- Keldysh diagrammatics

- Scattering Bethe *ansatz*
  (Andrei *et al.*)

Brief division of theoretical approaches

Steady state

- Keldysh diagrammatics

- Scattering Bethe *ansatz*
  (Andrei *et al.*)

- Nonequilibrium variants of perturbative RG
  Poor-man's scaling (Rosch *et al.*)
  Flow equations (Kehrein)
  Real-time diagrammatics (Schoeller *et al.*)
  Functional RG (Meden *et al.*)

Brief division of theoretical approaches

Steady state

- Keldysh diagrammatics

- Scattering Bethe *ansatz*
  (Andrei *et al.*)

- Nonequilibrium variants of perturbative RG
  Poor-man's scaling (Rosch *et al.*)
  Flow equations (Kehrein)
  Real-time diagrammatics (Schoeller *et al.*)
  Functional RG (Meden *et al.*)

- Exactly solvable models:
  Toulouse limit (AS & Hershfield)
  Extension to double dots (Sela & Affleck)

Brief division of theoretical approaches

Evolution in time

Brief division of theoretical approaches

Evolution in time

- Keldysh diagrammatics

Brief division of theoretical approaches

Evolution in time

- Keldysh diagrammatics

- Time-dependent DMRG
  (White, Schollwoeck,…)

Brief division of theoretical approaches

Evolution in time

- Keldysh diagrammatics
- Time-dependent DMRG
  (White, Schollwoeck,…)
- Keldysh Quantum Monte Carlo
  (Werner, Muehlbacher,…)

Brief division of theoretical approaches

Evolution in time

- Keldysh diagrammatics
- Time-dependent DMRG
  (White, Schollwoeck,…)
- Keldysh Quantum Monte Carlo
  (Werner, Muehlbacher,…)
- Nonequilibrium variants of perturbative RG
  Flow equations (Kehrein)
  Real-time diagrammatics (Schoeller *et al.*)

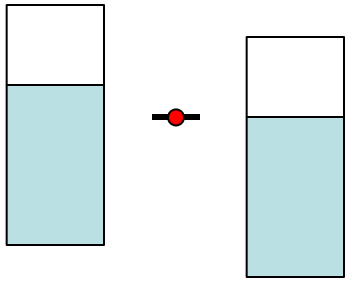
Brief division of theoretical approaches

Evolution in time

- Keldysh diagrammatics
- Time-dependent DMRG
  (White, Schollwoeck,…)
- Keldysh Quantum Monte Carlo
  (Werner, Muehlbacher,…)
- Nonequilibrium variants of perturbative RG
  Flow equations (Kehrein)
  Real-time diagrammatics (Schoeller *et al.*)
- Time-dependent NRG
  (Anders & AS)

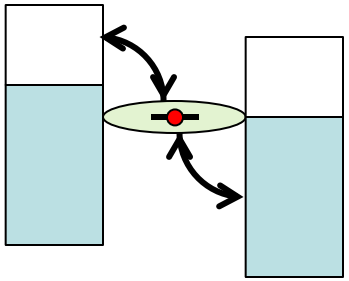
Time-independent formulation: the Lippmann-Schwinger equation

Incoming state: decoupled leads



$$|\phi\rangle = |FS\rangle_L \otimes |FS\rangle_R \otimes |imp\rangle$$

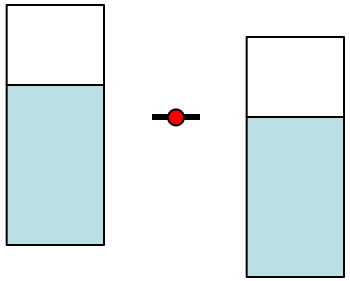
Scattered state: entangled system



$$|\psi\rangle$$

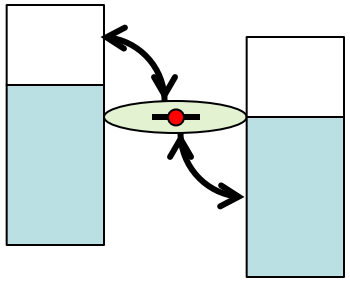
Time-independent formulation: the Lippmann-Schwinger equation

Incoming state: decoupled leads



$$|\phi\rangle = |FS\rangle_L \otimes |FS\rangle_R \otimes |imp\rangle$$

Scattered state: entangled system

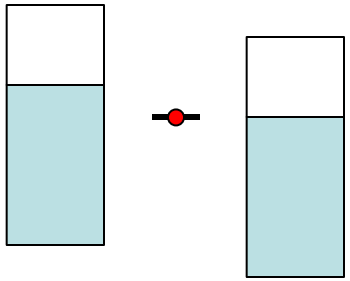


$$|\psi\rangle$$

- Divide H into H_0+H_1, where $H_0|\phi\rangle = E|\phi\rangle$ and H_1 contains all terms that drive the system out of equilibrium.

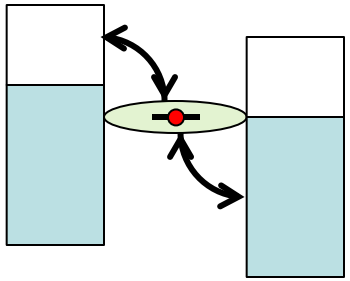
Time-independent formulation: the Lippmann-Schwinger equation

Incoming state: decoupled leads



$$|\phi\rangle = |FS\rangle_L \otimes |FS\rangle_R \otimes |imp\rangle$$

Scattered state: entangled system



$$|\psi\rangle$$

- Divide H into H_0+H_1, where $H_0|\phi\rangle = E|\phi\rangle$ and H_1 contains all terms that drive the system out of equilibrium.

- Assume approach to steady state

Time-independent formulation: the Lippmann-Schwinger equation

Because of the approach to steady state, one can “smear” the initial time:

$$|\psi\rangle = \lim_{\eta\to 0^+} \eta \int_{-\infty}^{0} dt_0 e^{\eta t_0} e^{i(H-E)t_0} |\phi\rangle$$

Gell-Man and Goldberger, 1953

Time-independent formulation: the Lippmann-Schwinger equation

Because of the approach to steady state, one can "smear" the initial time:

$$|\psi\rangle = \lim_{\eta\to 0^+} \eta \int_{-\infty}^{0} dt_0 e^{\eta t_0} e^{i(H-E)t_0} |\phi\rangle$$

$$|\psi\rangle = |\phi\rangle + \frac{1}{E-H+i\eta}(H-E)|\phi\rangle$$

Gell-Man and Goldberger, 1953

Time-independent formulation: the Lippmann-Schwinger equation

Because of the approach to steady state, one can "smear" the initial time:

$$|\psi\rangle = \lim_{\eta\to 0^+} \eta \int_{-\infty}^{0} dt_0 e^{\eta t_0} e^{i(H-E)t_0} |\phi\rangle$$

$$|\psi\rangle = |\phi\rangle + \frac{1}{E-H+i\eta}(H-E)|\phi\rangle$$

Since $(H_0 - E)|\phi\rangle = 0$, we arrive at the Lippmann-Schwinger equation

$$|\psi\rangle = |\phi\rangle + \frac{1}{E-H+i\eta} H_1 |\phi\rangle$$

Gell-Man and Goldberger, 1953

Time-independent formulation: the Lippmann-Schwinger equation

Important points to take note of:

- $|\psi\rangle$ is an eigenstate of H with energy E
- H and H_0 must therefore have continuous overlapping spectra, which implies the limit $L \to \infty$
- There is a well-defined hierarchy of limits:
  $L \to \infty, \quad \eta \to \infty, \text{ but } L\eta \to \infty$

The nonequilibrium steady-state density operator

Starting from $\hat{\rho}_0 = \sum_i p_i \,|\phi_i\rangle\langle\phi_i|$, where p_i are typically equilibrium Boltzmann factors, one formally has that

The nonequilibrium steady-state density operator

Starting from $\hat{\rho}_0 = \sum_i p_i \,|\phi_i\rangle\langle\phi_i|$, where p_i are typically equilibrium Boltzmann factors, one formally has that

$$\hat{\rho}_0 \rightarrow \hat{\rho} = \sum_i p_i \,|\psi_i\rangle\langle\psi_i|$$

with

$$|\psi_i\rangle = |\phi_i\rangle + \frac{1}{E_i - H + i\eta} H_1 \,|\phi_i\rangle$$

The nonequilibrium steady-state density operator

Starting from $\hat{\rho}_0 = \sum_i p_i \,|\phi_i\rangle\langle\phi_i|$, where p_i are typically equilibrium Boltzmann factors, one formally has that

$$\hat{\rho}_0 \rightarrow \hat{\rho} = \sum_i p_i \,|\psi_i\rangle\langle\psi_i|$$

with

$$|\psi_i\rangle = |\phi_i\rangle + \frac{1}{E_i - H + i\eta} H_1 |\phi_i\rangle$$

Assuming the approach to steady state, the form of the nonequilibrium density operator is formally known

Hershfield's mapping onto equilibrium form

Zubarev, 1960's, *Hershfield* 1993, *Doyon* & *Andrei* 2006

Hershfield's mapping onto equilibrium form

In practice, the initial density matrix generically takes the form

$$\hat{\rho}_0 = \frac{e^{-\beta(H_0 - Y_0)}}{\mathrm{Trace}\left\{e^{-\beta(H_0 - Y_0)}\right\}}$$

with $\left[H_0, Y_0\right] = 0$

Zubarev, 1960's, *Hershfield* 1993, *Doyon* & *Andrei* 2006

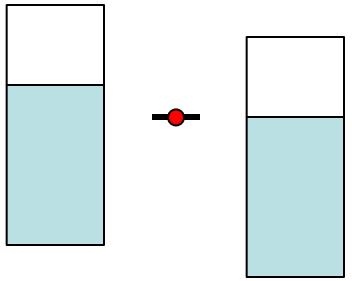
Hershfield's mapping onto equilibrium form

In practice, the initial density matrix generically takes the form

$$\hat{\rho}_0 = \frac{e^{-\beta(H_0 - Y_0)}}{\mathrm{Trace}\left\{e^{-\beta(H_0 - Y_0)}\right\}}$$

with $[H_0, Y_0] = 0$

Indeed, in many cases one takes



$$H_0 = \sum_{\alpha=L,R} \sum_{k,\sigma} (\varepsilon_{\alpha k} + \mu_\alpha) c^+_{\alpha k\sigma} c_{\alpha k\sigma}$$

$$Y_0 = \sum_{\alpha=L,R} \sum_{k,\sigma} \mu_\alpha c^+_{\alpha k\sigma} c_{\alpha k\sigma}$$

Zubarev, 1960's, *Hershfield* 1993, *Doyon* & *Andrei* 2006

Hershfield's mapping onto equilibrium form

In this case $\hat{\rho}$ can be written in the form

$$\hat{\rho} = \frac{e^{-\beta(H-Y)}}{\text{Trace}\left\{e^{-\beta(H-Y)}\right\}}$$

with

$$[Y, H] = i\eta(Y_0 - Y) \rightarrow 0$$

Zubarev, 1960's, *Hershfield* 1993, *Doyon* & *Andrei* 2006

Hershfield's mapping onto equilibrium form

In this case $\hat{\rho}$ can be written in the form

$$\hat{\rho} = \frac{e^{-\beta(H-Y)}}{\text{Trace}\left\{e^{-\beta(H-Y)}\right\}}$$

with

$$\left[Y, H\right] = i\eta(Y_0 - Y) \;\rightarrow\; 0$$

The steady-state density operator takes an equilibrium-like form!

Zubarev, 1960's, *Hershfield* 1993, *Doyon* & *Andrei* 2006

Generalized fermionic scattering states

The steady-state density operator can be represented in terms of generalized fermionic scattering states:

$$H - Y = \sum_{\alpha=L,R} \sum_{k,\sigma} \varepsilon_{\alpha k} \psi^{+}_{\alpha k \sigma} \psi_{\alpha k \sigma}$$

with

$$\left[\psi^{+}_{\alpha k \sigma}, H\right] = -\varepsilon_{\alpha k} \psi^{+}_{\alpha k \sigma} + i\eta (c^{+}_{\alpha k \sigma} - \psi^{+}_{\alpha k \sigma})$$

Hershfield 1993, *Han* 2007

Generalized fermionic scattering states

The steady-state density operator can be represented in terms of generalized fermionic scattering states:

$$H - Y = \sum_{\alpha=L,R} \sum_{k,\sigma} \varepsilon_{\alpha k} \psi^{+}_{\alpha k \sigma} \psi_{\alpha k \sigma}$$

with

$$\left[\psi^{+}_{\alpha k \sigma}, H \right] = -\varepsilon_{\alpha k} \psi^{+}_{\alpha k \sigma} + i\eta (c^{+}_{\alpha k \sigma} - \psi^{+}_{\alpha k \sigma})$$

In general $\psi^{+}_{\alpha k \sigma}$ is a complicated many-body operator:

$$\psi^{+}_{\alpha k \sigma} = c^{+}_{\alpha k \sigma} + \sum_{i} A^{\alpha k}_{i} c^{+}_{i} + \sum_{i,j,k} B^{\alpha k}_{ijl} c^{+}_{i} c^{+}_{j} c_{l} + \ldots$$

Hershfield 1993, *Han* 2007

Generalized fermionic scattering states

In the absence of interactions $\psi_{\alpha k\sigma}$ reduce to the familiar single-particle scattering states

$$\psi^{+}_{\alpha k\sigma} = c^{+}_{\alpha k\sigma} + \sum_{i} A_i^{\alpha k} c_i^{+}$$

and one recovers the Landauer-Buttiker formulation

Hershfield 1993

Time-dependent formulation

Time-dependent formulation

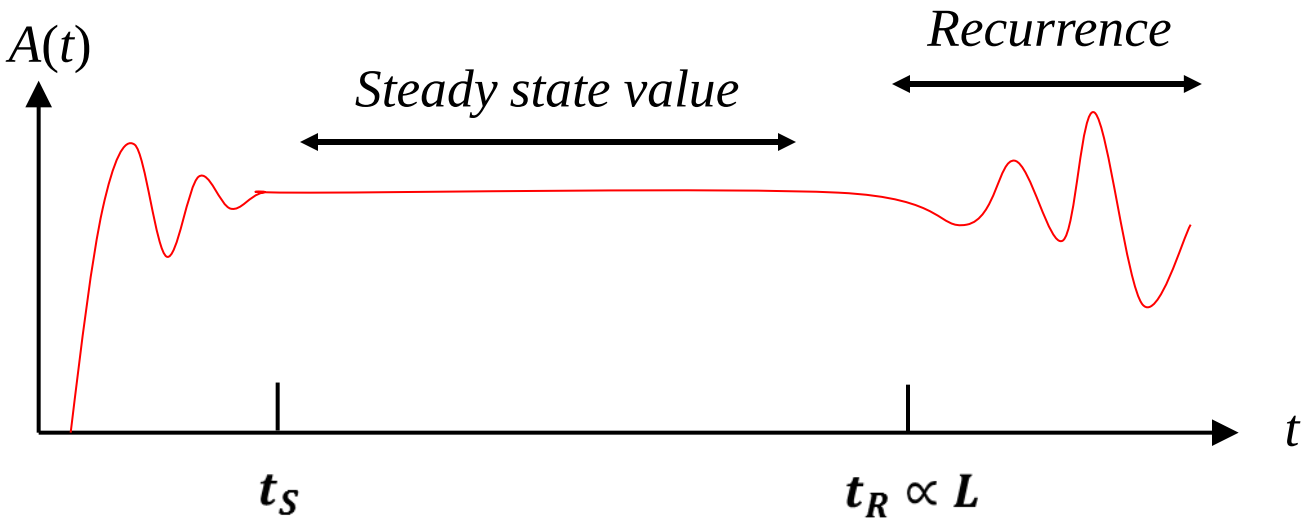
Starting from $\hat{\rho}_0 = \sum_i p_i \,|\phi_i\rangle\langle\phi_i|$ at time t_0, expectation values are explicitly propagated in time:

$$\left\langle \hat{A}(t) \right\rangle = \mathrm{Trace}\left\{ \hat{\rho}_0 U^{+}(t,t_0)\hat{A}U(t,t_0) \right\}$$

Time-dependent formulation

Starting from $\hat{\rho}_0 = \sum_i p_i \,|\phi_i\rangle\langle\phi_i|$ at time t_0, expectation values are explicitly propagated in time:

$$\left\langle \hat{A}(t) \right\rangle = \mathrm{Trace}\left\{ \hat{\rho}_0 U^{+}(t,t_0)\hat{A}U(t,t_0) \right\}$$



Time-dependent formulation

True steady state is reached only for $L \to \infty$

Time-dependent formulation

→ True steady state is reached only for $L \to \infty$

→ To gain reliable information about nonequilibrium steady state from the study of finite systems, L must large enough such that

$$t_S \ll t_R$$

Time-dependent formulation

→ True steady state is reached only for $L \to \infty$

→ To gain reliable information about nonequilibrium steady state from the study of finite systems, L must large enough such that

$$t_S \ll t_R$$

A challenge when the system features small energy Scales such as the Kondo temperature!

Selected review of theoretical approaches

- Scattering Bethe *ansatz*
- Nonequilbrium variants of perturbative RG
- Time-dependent NRG

Selected review of theoretical approaches

- Scattering Bethe *ansatz*
- Nonequilbrium variants of perturbative RG
- Time-dependent NRG

Will not addressed:

- Keldysh-based approaches (Hans Kroha's talk)
- Theories based on Fermi-liquid theory (weak nonequilibrium)
- Keldysh Quantum Monte Carlo
- Time-dependent DMRG

Scattering Bethe *ansatz*

- One uses the Bethe *ansatz* approach, adjusted to open boundary conditions, to explicitly construct the many-particle scattering states

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

- One uses the Bethe *ansatz* approach, adjusted to open boundary conditions, to explicitly construct the many-particle scattering states

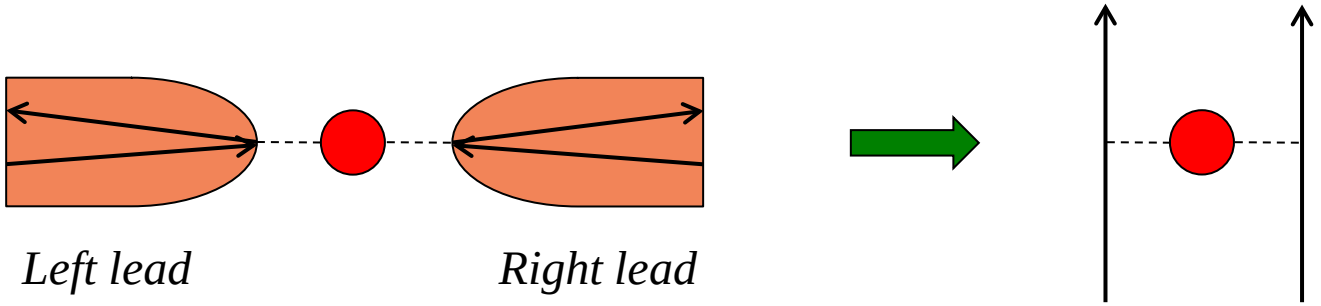
Step 1: Conversion to continuum-limit Hamiltonian

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

- One uses the Bethe *ansatz* approach, adjusted to open boundary conditions, to explicitly construct the many-particle scattering states

Step 1: Conversion to continuum-limit Hamiltonian

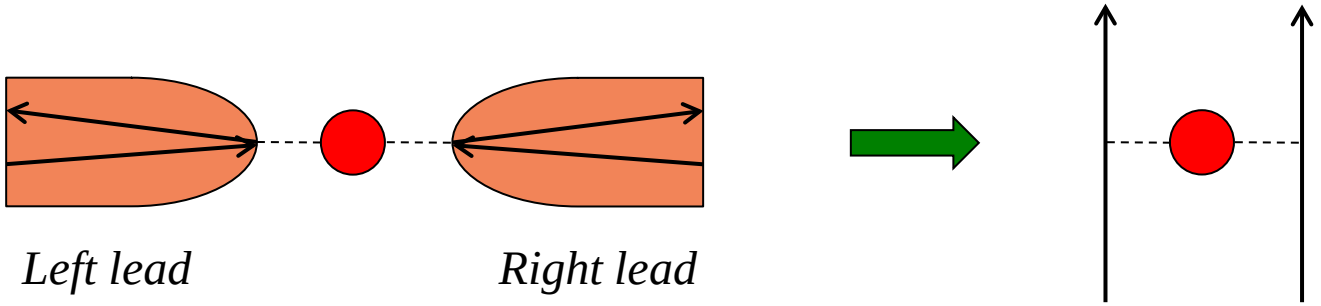


Mehta & Andrei, 2005

Scattering Bethe *ansatz*

- One uses the Bethe *ansatz* approach, adjusted to open boundary conditions, to explicitly construct the many-particle scattering states

Step 1: Conversion to continuum-limit Hamiltonian



$$\boldsymbol{H = -iv_F \int \psi_\alpha^+(x)\partial_x\psi_\alpha(x)dx \;+\; t\{[\psi_L^+(0)+\psi_R^+(0)]d + H.c.\} + \;\ldots}$$

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

General form of *N*-electron wave function:

$$|\psi\rangle = \sum_a \int dx_1 \dots dx_N \, F_a(x_1, \dots, x_N) \psi^+(x_1) \dots \psi^+(x_N) |a\rangle$$

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

General form of *N*-electron wave function:

$$|\psi\rangle = \sum_a \int dx_1 \dots dx_N \, F_a(x_1, \dots, x_N) \psi^+(x_1) \dots \psi^+(x_N) |a\rangle$$

Impurity states

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

General form of *N*-electron wave function:

$$|\psi\rangle = \sum_a \int dx_1 \dots dx_N \, F_a(x_1, \dots, x_N) \psi^+(x_1) \dots \psi^+(x_N) |a\rangle$$

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

General form of *N*-electron wave function:

$$|\psi\rangle = \sum_a \int dx_1 \dots dx_N \, F_a(x_1, \dots, x_N) \psi^+(x_1) \dots \psi^+(x_N) |a\rangle$$

where *F* obeys the Schroedinger-type equation

$$-iv_F(\partial_1 + \cdots + \partial_N) F_a(x_1, \dots, x_N) + t \sum_j \delta(x_j) \dots = E F_a(x_1, \dots, x_N)$$

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

General form of *N*-electron wave function:

$$|\psi\rangle = \sum_a \int dx_1 \dots dx_N \, F_a(x_1, \dots, x_N) \psi^+(x_1) \dots \psi^+(x_N) |a\rangle$$

where *F* obeys the Schroedinger-type equation

$$-iv_F(\partial_1 + \cdots + \partial_N) F_a(x_1, \dots, x_N) + t \sum_j \delta(x_j) \dots = E F_a(x_1, \dots, x_N)$$

Within each sector where $x_1, \dots, x_N$, and $x_0 = 0$ obey some fixed ordering, *F* has solutions in terms of plane waves

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The Bethe *ansatz* then seeks solutions of the form

$$F_a(x_1, \ldots, x_N) = \sum_{P \in S_{N+1}} \theta(X_P) A^P e^{i(k_1 x_1 + \cdots + k_N x_N)}$$

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The Bethe *ansatz* then seeks solutions of the form

$$F_a(x_1, \ldots, x_N) = \sum_{P \in S_{N+1}} \theta(X_P) A^P e^{i(k_1 x_1 + \cdots + k_N x_N)}$$

Projection onto the ordering affiliated with P

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The Bethe *ansatz* then seeks solutions of the form

$$F_a(x_1, \ldots, x_N) = \sum_{P \in S_{N+1}} \theta(X_P) A^P e^{i(k_1 x_1 + \cdots + k_N x_N)}$$

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The Bethe *ansatz* then seeks solutions of the form

$$F_a(x_1, \ldots, x_N) = \sum_{P \in S_{N+1}} \theta(X_P) A^P e^{i(k_1 x_1 + \cdots + k_N x_N)}$$

- The existence of such solutions is highly nontrivial, and requires special conditions known as the Yang-Baxter equations

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The Bethe *ansatz* then seeks solutions of the form

$$F_a(x_1, \ldots, x_N) = \sum_{P \in S_{N+1}} \theta(X_P) A^P e^{i(k_1 x_1 + \cdots + k_N x_N)}$$

- The existence of such solutions is highly nontrivial, and requires special conditions known as the Yang-Baxter equations

- In the Scattering Bethe *ansatz* one further wishes to impose the boundary condition that $F_a(x_1, \ldots, x_N)$ corresponds for $x_1, \ldots, x_N \to \infty$ to free Fermi seas, each filled up to its own chemical potential

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The main sources of difficulty:

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The main sources of difficulty:

- Free filled Fermi seas can only be properly recovered in the Limit of infinite bandwidth, $D \rightarrow \infty$

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The main sources of difficulty:

- Free filled Fermi seas can only be properly recovered in the Limit of infinite bandwidth, $D \rightarrow \infty$
- Expectation values of the current operators are extremely difficult to evaluate with respect to the Bethe *ansatz* wave function

Mehta & Andrei, 2005

Scattering Bethe *ansatz*

The main sources of difficulty:

- Free filled Fermi seas can only be properly recovered in the Limit of infinite bandwidth, $D \rightarrow \infty$
- Expectation values of the current operators are extremely difficult to evaluate with respect to the Bethe *ansatz* wave function

Remarkably

Mehta and Andrei succeeded in obtaining an exact solution for the interacting resonant-level model, though even there the limit was not worked out analytically

Mehta & Andrei, 2005

Nonequilibrium variants of perturbative RG

Nonequilibrium variants of perturbative RG

- Perturbative RG has become one of the key concepts in analyzing correlated electron systems in thermal equilibrium
- The basic idea is to systematically reduce the energy scale by integrating high-energy excitations, thus generating a sequence of Hamiltonians for each energy scale
- Interactions correspond to irreducible vertices, whose evolution one tracks

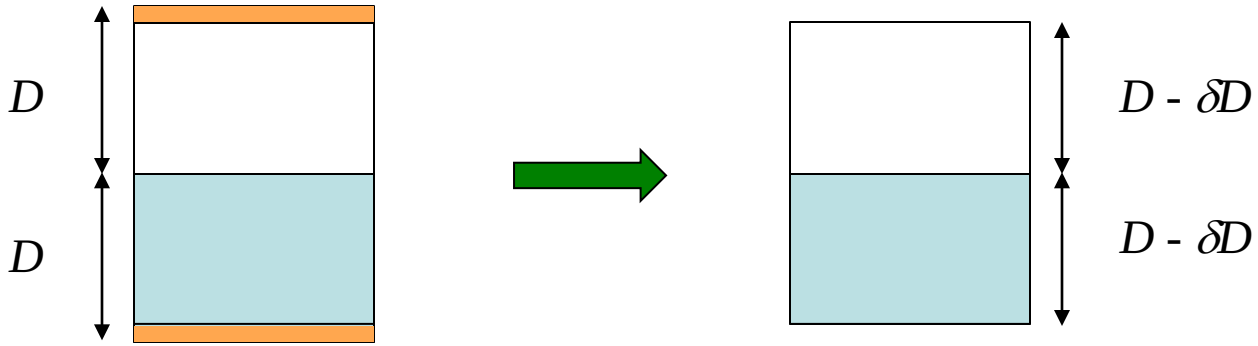
Nonequilibrium variants of perturbative RG

- Perturbative RG has become one of the key concepts in analyzing correlated electron systems in thermal equilibrium

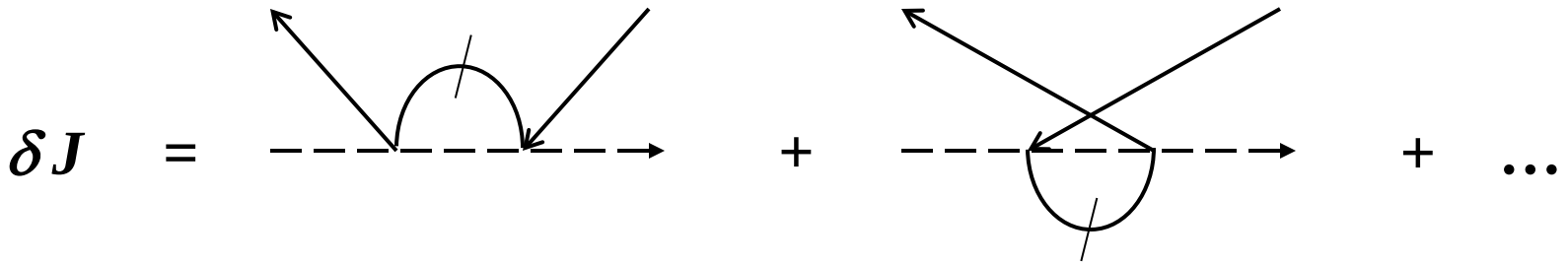
- The basic idea is to systematically reduce the energy scale by integrating high-energy excitations, thus generating a sequence of Hamiltonians for each energy scale

- Interactions correspond to irreducible vertices, whose evolution one tracks

Generic example in equilibrium – the Kondo model

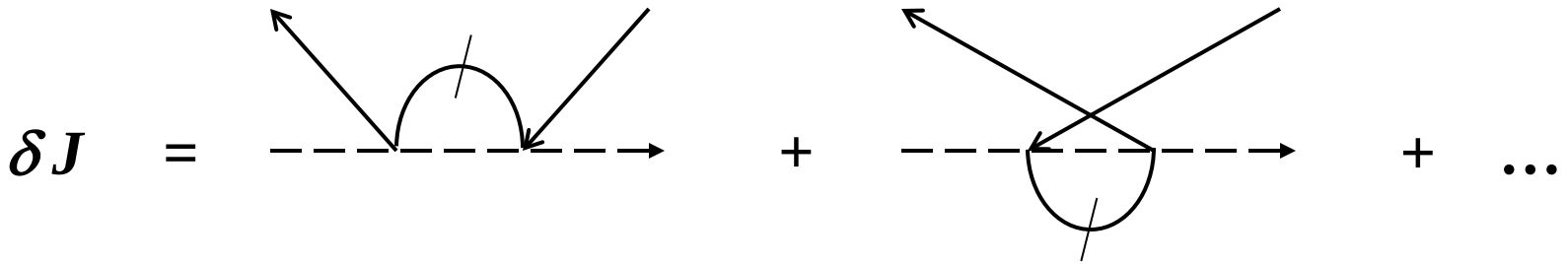


Nonequilibrium variants of perturbative RG



$$\Rightarrow \quad \frac{d\tilde{J}}{dl} = \tilde{J}^2 \qquad \text{with} \qquad l = \ln(D_0/D) \qquad \text{and} \qquad \tilde{J} = \rho J$$

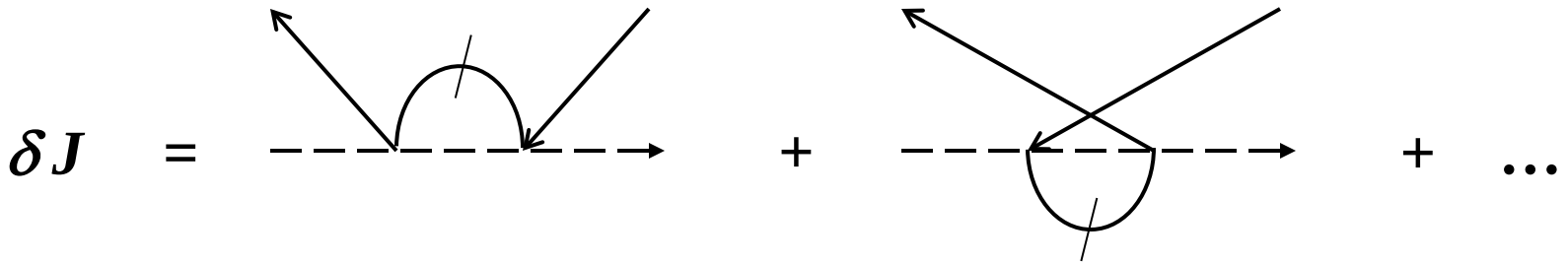
Nonequilibrium variants of perturbative RG



$$\Rightarrow \quad \frac{d\tilde{J}}{dl} = \tilde{J}^2 \qquad \text{with} \qquad l = \ln(D_0/D) \qquad \text{and} \qquad \tilde{J} = \rho J$$

- In equilibrium only $J(\omega = 0)$ is important for thermodynamics

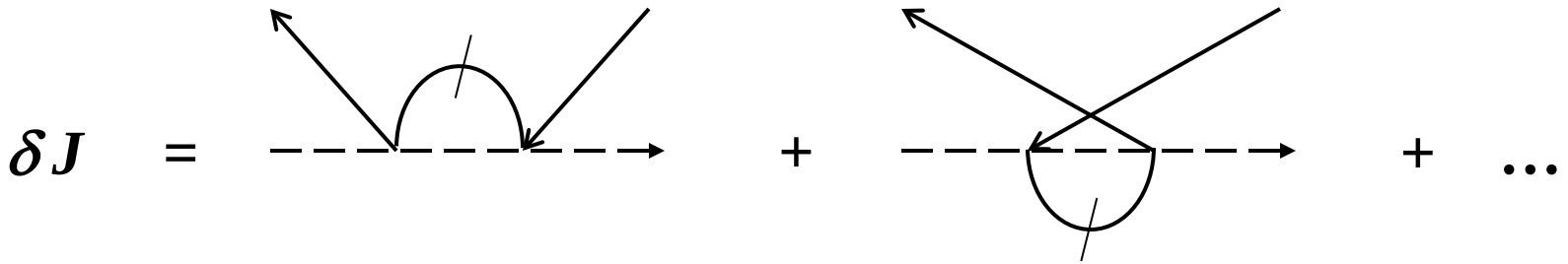
Nonequilibrium variants of perturbative RG



$$\Rightarrow \quad \frac{d\tilde{J}}{dl} = \tilde{J}^2 \qquad \text{with} \qquad l = \ln(D_0/D) \qquad \text{and} \qquad \tilde{J} = \rho J$$

- In equilibrium only $J(\omega = 0)$ is important for thermodynamics
- Out of equilibrium one needs to keep track of $J(\omega)$, as transport properties are determined by a window of energies

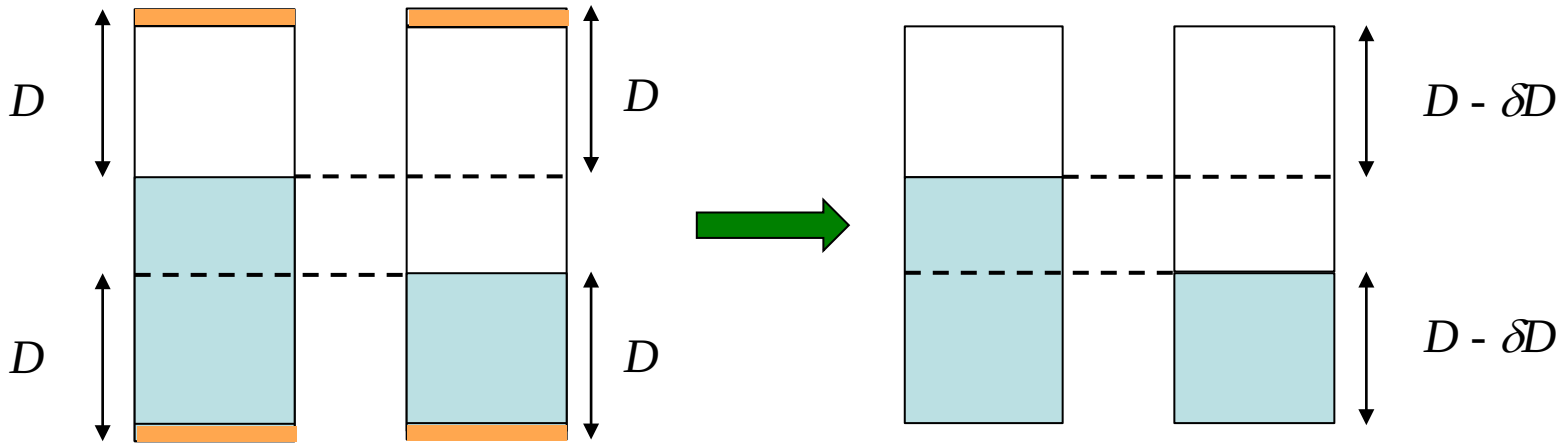
Nonequilibrium variants of perturbative RG



$$\Rightarrow \quad \frac{d\tilde{J}}{dl} = \tilde{J}^2 \qquad \text{with} \quad l = \ln(D_0/D) \qquad \text{and} \quad \tilde{J} = \rho J$$

- In equilibrium only $J(\omega = 0)$ is important for thermodynamics
- Out of equilibrium one needs to keep track of $J(\omega)$, as transport properties are determined by a window of energies
- Different strategies have been put forward to implement these RG ideas out of equilibrium

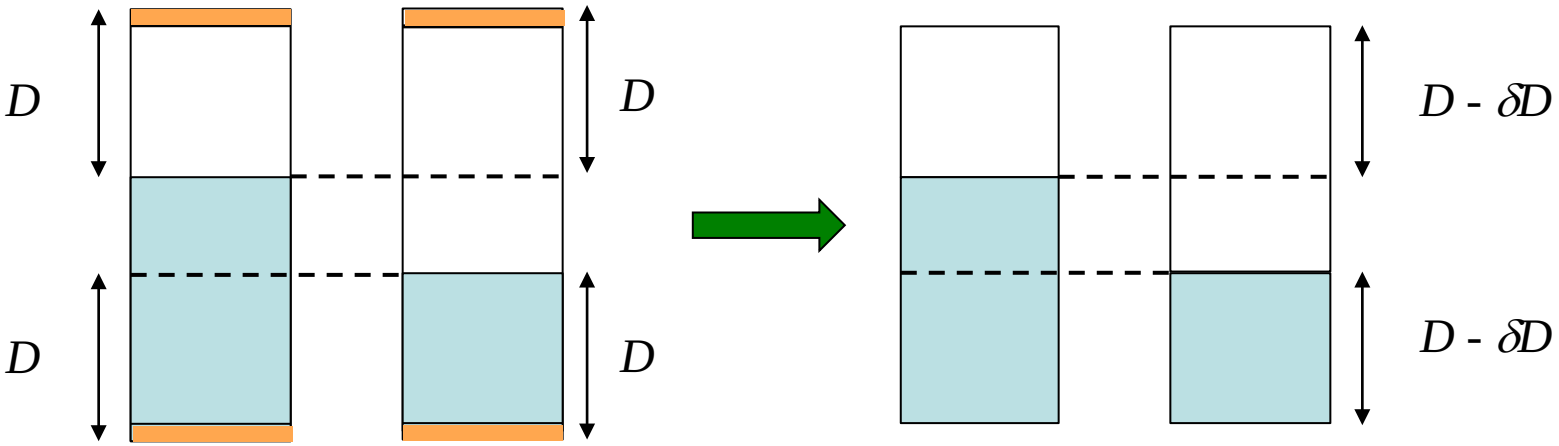
Nonequilibrium variants of perturbative RG



Yields and RG-type differential equation for $J(\omega = 0)$

Rosch et al., 2003

Nonequilibrium variants of perturbative RG



Yields and RG-type differential equation for $J(\omega = 0)$

The logarithmic singularities at μ_L and μ_R are cut off by the effective spin-flip rate, which is inserted by hand

Rosch et al., 2003

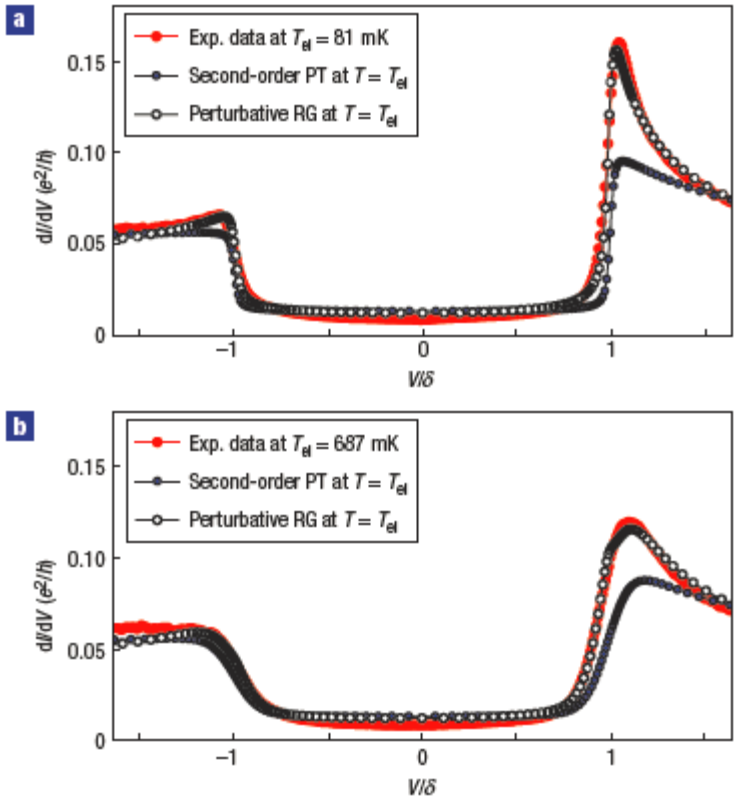
Nonequilibrium variants of perturbative RG

Example: The singlet-triplet transition in carbon nanotube quantum dots

Paaske et al., 2006

Nonequilibrium variants of perturbative RG

Example: The singlet-triplet transition in carbon nanotube quantum dots



Paaske et al., 2006

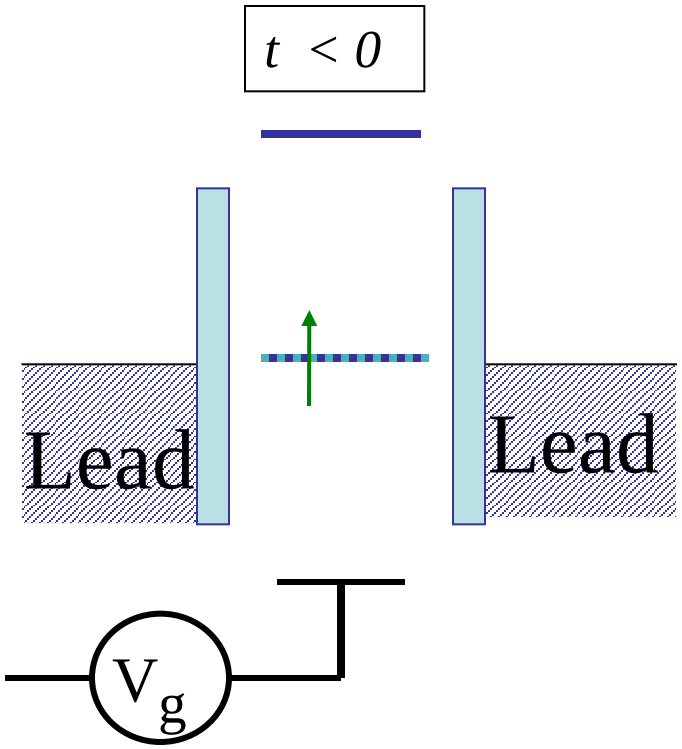
Time-dependent numerical RG

Time-dependent numerical RG

- Consider a quantum impurity (e.g., quantum dot) in equilibrium, to which a sudden perturbation is applied at time $t = 0$

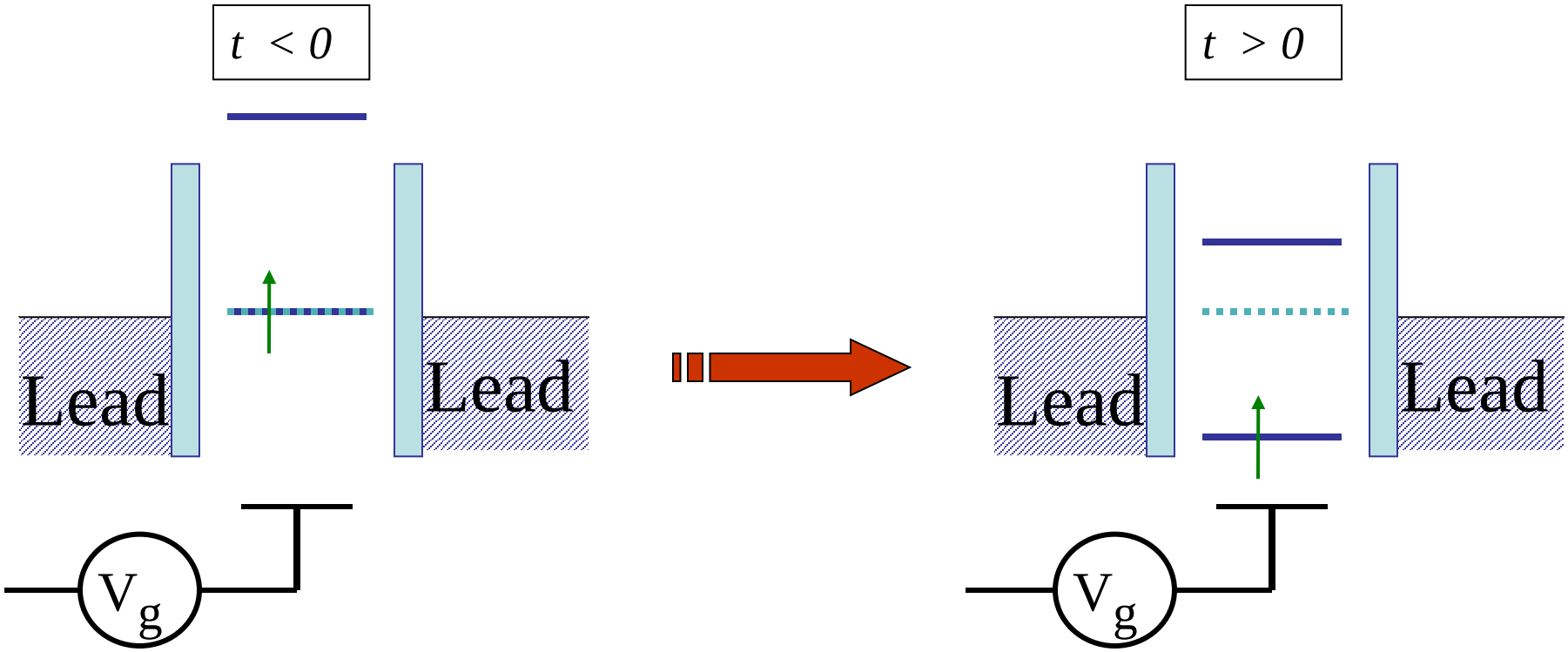
Time-dependent numerical RG

- Consider a quantum impurity (e.g., quantum dot) in equilibrium, to which a sudden perturbation is applied at time $t = 0$



Time-dependent numerical RG

- Consider a quantum impurity (e.g., quantum dot) in equilibrium, to which a sudden perturbation is applied at time $t = 0$



Time-dependent numerical RG

- Consider a quantum impurity (e.g., quantum dot) in equilibrium, to which a sudden perturbation is applied at time $t = 0$

Time-dependent numerical RG

- Consider a quantum impurity (e.g., quantum dot) in equilibrium, to which a sudden perturbation is applied at time $t = 0$

Initial density operator

$$\left\langle \hat{O} \right\rangle_{t>0} = \text{Trace}\left\{ \hat{\rho}(t)\hat{O} \right\} = \text{Trace}\left\{ e^{-iHt}\,\hat{\rho}_0 e^{iHt}\hat{O} \right\}$$

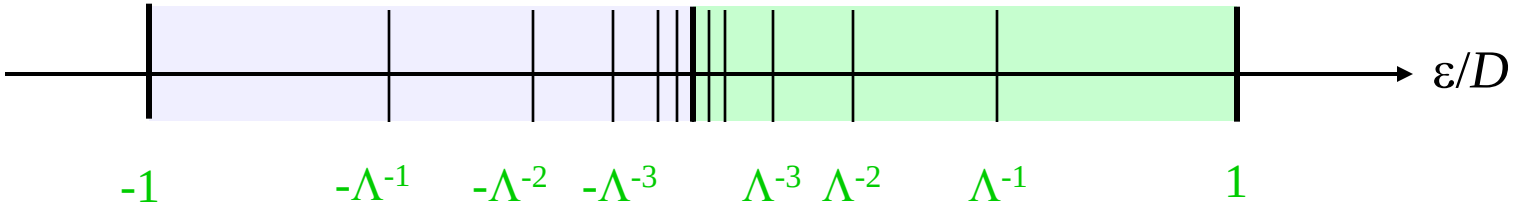
Perturbed Hamiltonian

Wilson's numerical RG

Wilson's numerical RG

- Logarithmic discretization of band:

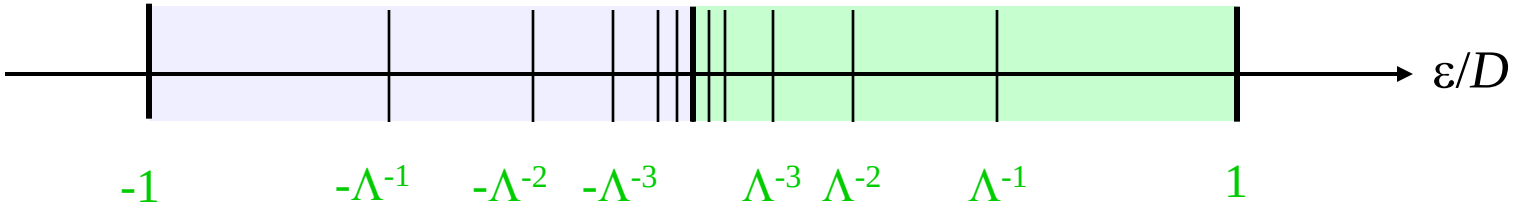
$$\Lambda > 1$$



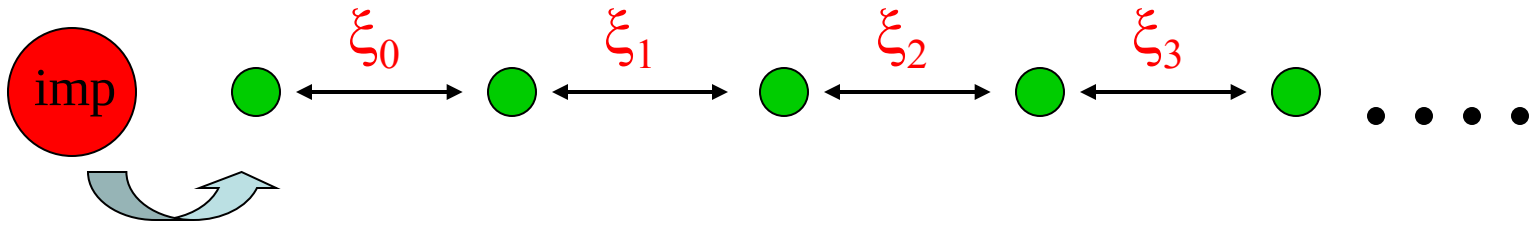
Wilson's numerical RG

- Logarithmic discretization of band:

$$\Lambda > 1$$



- After a unitary transformation the bath is represented by a semi-infinite chain



Wilson's numerical RG

Why logarithmic discretization?

Wilson's numerical RG

Why logarithmic discretization?

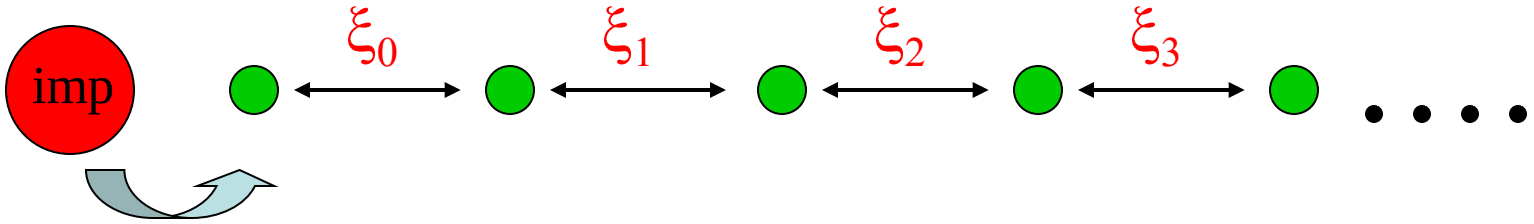
- To properly account for the logarithmic infra-red divergences

Wilson's numerical RG

Why logarithmic discretization?

- To properly account for the logarithmic infra-red divergences
- Hopping decays exponentially along the chain:

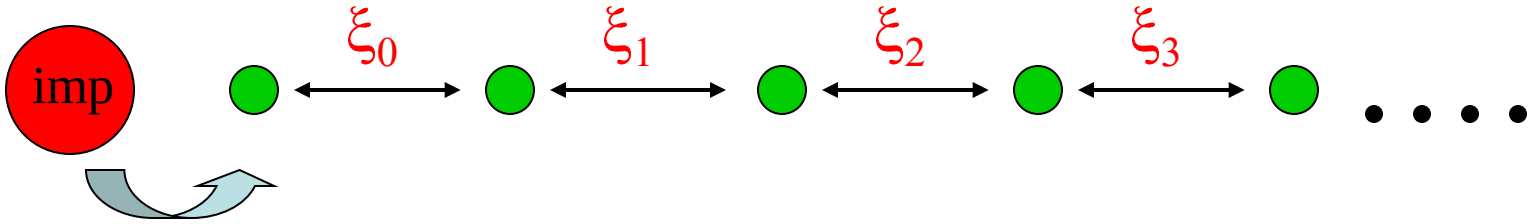
$$\xi_n \propto \Lambda^{-n/2}, \quad \Lambda > 1$$



Wilson's numerical RG

Why logarithmic discretization?

- To properly account for the logarithmic infra-red divergences
- Hopping decays exponentially along the chain: $\xi_n \propto \Lambda^{-n/2}, \quad \Lambda > 1$

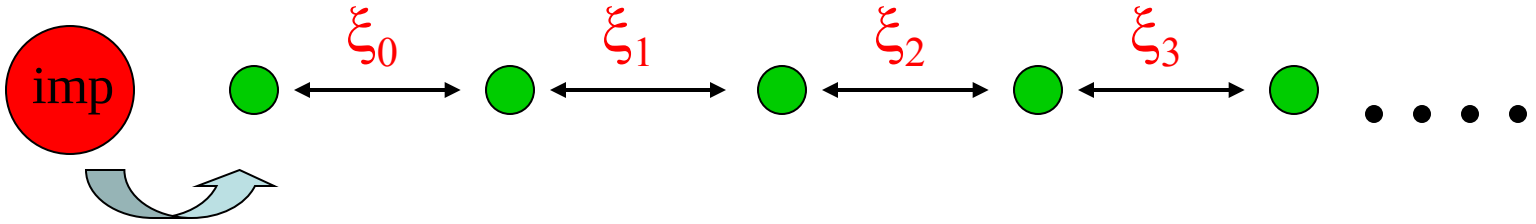


⇒ Separation of energy scales along the chain

Wilson's numerical RG

Why logarithmic discretization?

- To properly account for the logarithmic infra-red divergences
- Hopping decays exponentially along the chain: $\xi_n \propto \Lambda^{-n/2}, \quad \Lambda > 1$



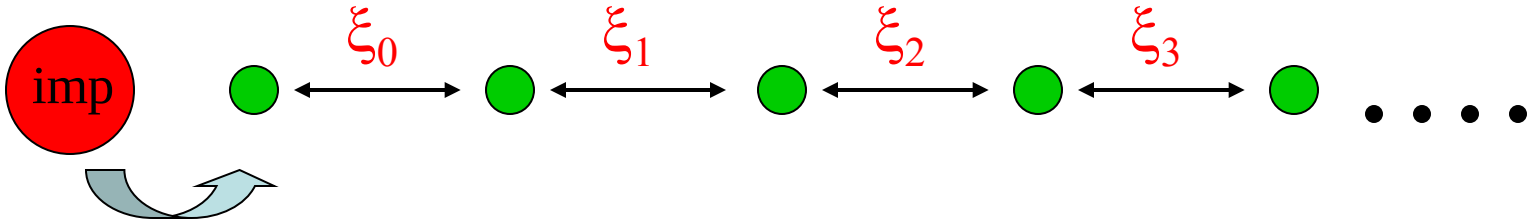
Separation of energy scales along the chain

Exponentially small energy scales can be accessed, limited by T only

Wilson's numerical RG

Why logarithmic discretization?

- To properly account for the logarithmic infra-red divergences
- Hopping decays exponentially along the chain: $\xi_n \propto \Lambda^{-n/2}, \quad \Lambda > 1$



⇒ Separation of energy scales along the chain

Exponentially small energy scales can be accessed, limited by T only

- Iterative solution, starting from a core cluster and enlarging the chain by one site at a time. High-energy states are discarded at each step, refining the resolution as energy is decreased.

Wilson's numerical RG

Equilibrium NRG:

- Geared towards fine energy resolution at low energies
- Discards high-energy states

Wilson's numerical RG

Equilibrium NRG:

- Geared towards fine energy resolution at low energies
- Discards high-energy states

Problem: Real-time dynamics involves all energy scales

Wilson's numerical RG

Equilibrium NRG:

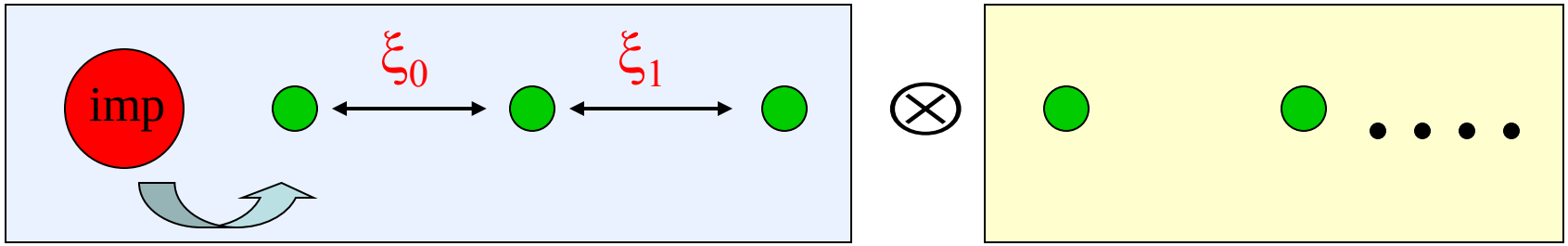
- Geared towards fine energy resolution at low energies
- Discards high-energy states

Problem: Real-time dynamics involves all energy scales

Resolution: Combine information from all NRG iterations

Time-dependent NRG

(Anders & AS, PRL'05, PRB'06)



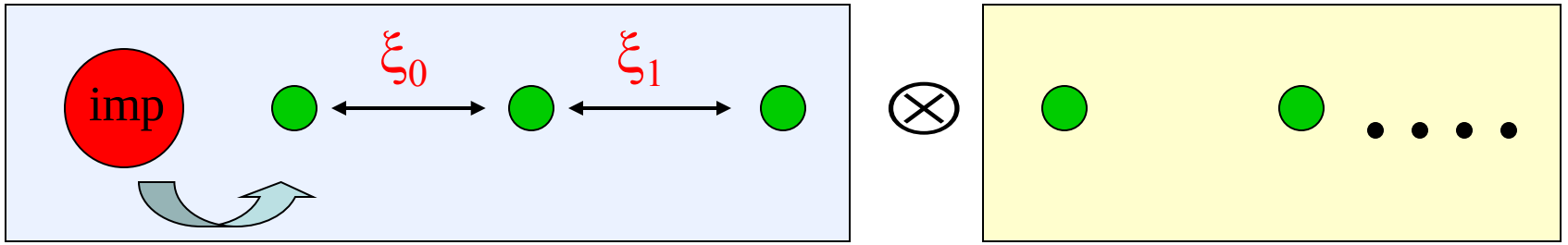
$|r\rangle$ $|e\rangle$

NRG eigenstate of relevant iteration

Basis set for the "environment" states

Time-dependent NRG

(Anders & AS, PRL'05, PRB'06)



$$|r\rangle \qquad |e\rangle$$

NRG eigenstate of relevant iteration

Basis set for the "environment" states

For each NRG iteration, we trace over its "environment"

Time-dependent NRG

Sum over all chain lengths (all energy scales)

$$\langle O(t)\rangle = \sum_{m=1}^{N}\sum_{s,r}^{trun} O^{m}_{s,r}\rho^{\mathrm{red}}_{r,s}(m)e^{i(E^{m}_{s}-E^{m}_{r})t}$$

Sum over discarded NRG states of chain of length m

Matrix element of O on the m-site chain

Reduced density matrix for the m-site chain

$$\rho^{\mathrm{red}}_{r,s}(m) = \sum_{e}\langle r,e;m|\rho_0|s,e;m\rangle$$

Trace over the environment, i.e., sites not included in chain of length m

(Hostetter, PRL 2000)

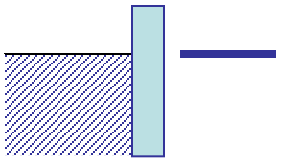
Fermionic benchmark: Resonant-level model

$$H = \sum_k \varepsilon_k c_k^+ c_k + E_d(t) d^+ d + V \sum_k (c_k^+ d + d^+ c_k)$$

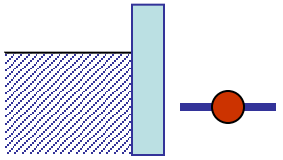
Fermionic benchmark: Resonant-level model

$$H = \sum_k \varepsilon_k c_k^+ c_k + E_d(t) d^+ d + V \sum_k (c_k^+ d + d^+ c_k)$$

$$E_d(t<0) = 0$$



$$E_d(t>0) = E_d^1 < 0$$

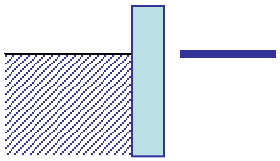


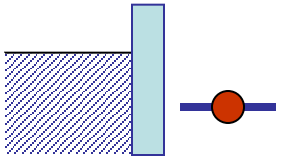
Fermionic benchmark: Resonant-level model

$$H = \sum_k \varepsilon_k c_k^+ c_k + E_d(t) d^+ d + V \sum_k (c_k^+ d + d^+ c_k)$$

$$E_d(t<0) = 0$$

$$E_d(t>0) = E_d^1 < 0$$



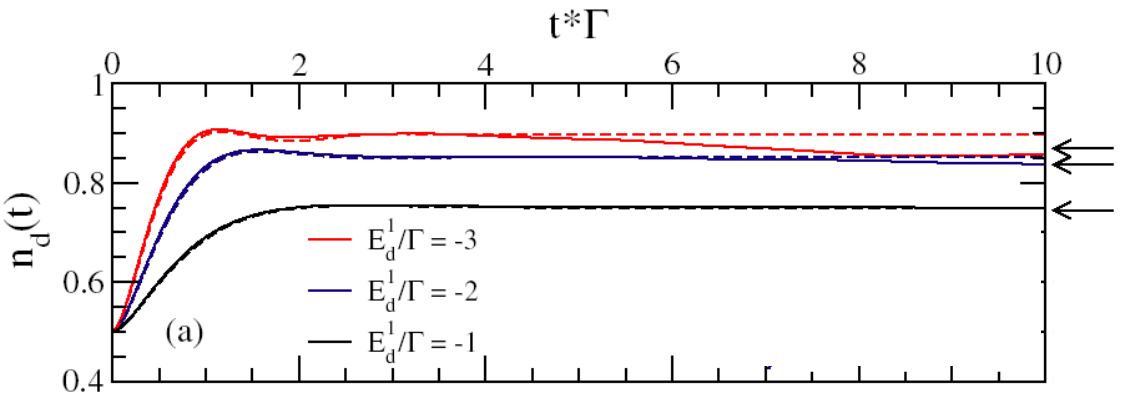


- We focus on $n_d(t) = \langle d^+ d \rangle(t)$ and compare the TD-NRG to exact analytic solution in the wide-band limit (i.e., for an infinite system)

- Basic energy scale: $\Gamma = \pi \rho V^2$

Fermionic benchmark: Resonant-level model

$T = 0$

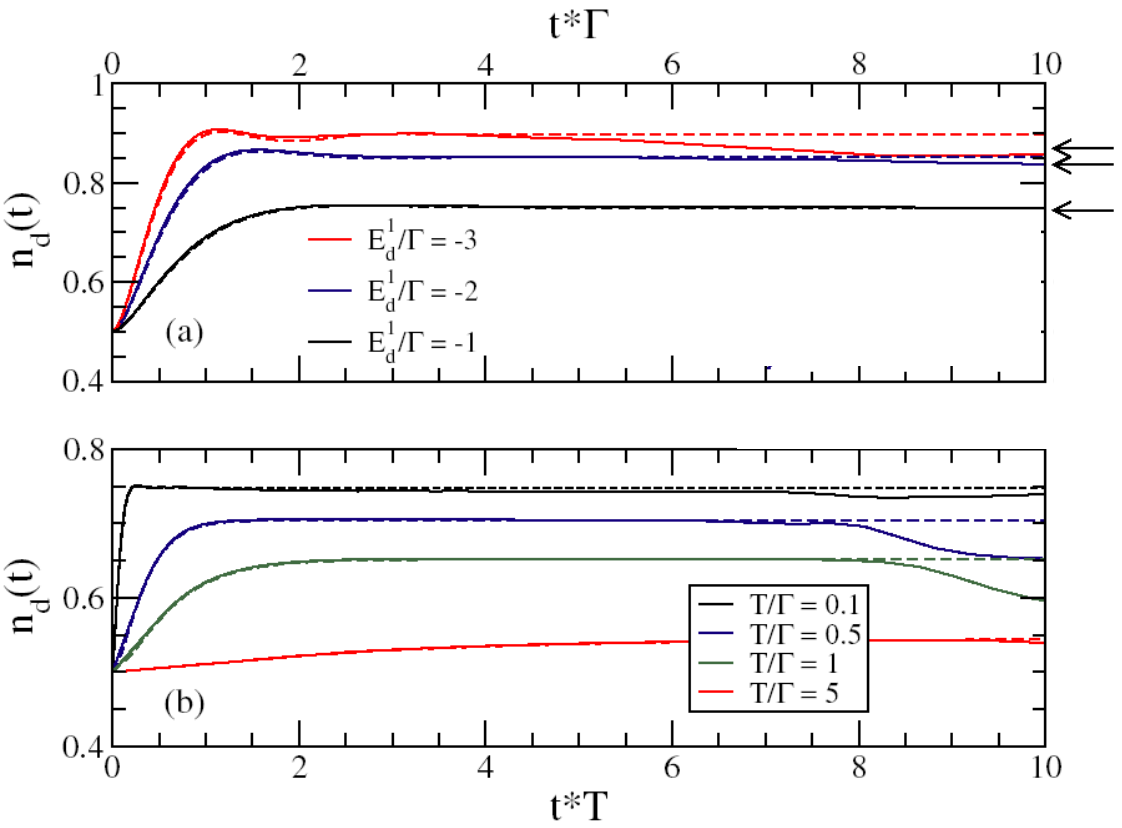


Relaxed values (no runaway!)

Fermionic benchmark: Resonant-level model

$T = 0$

$T > 0$

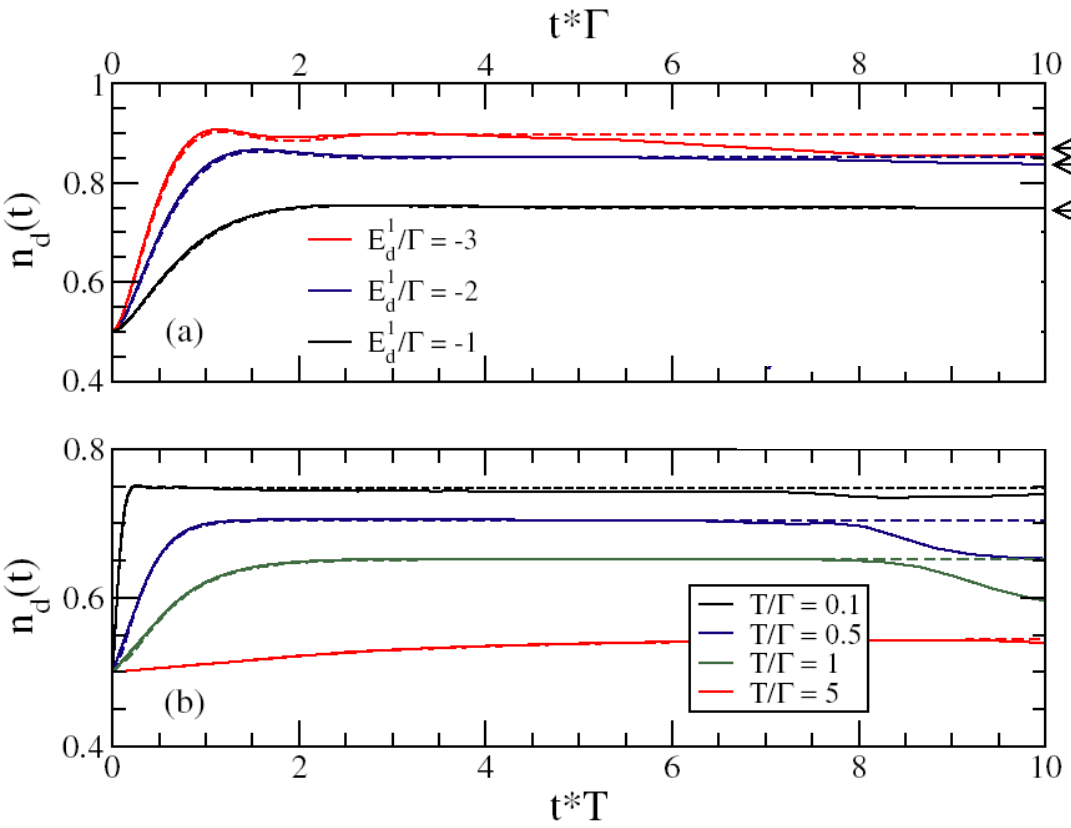


Relaxed values (no runaway!)

Fermionic benchmark: Resonant-level model

$T = 0$

$T > 0$



Relaxed values (no runaway!)

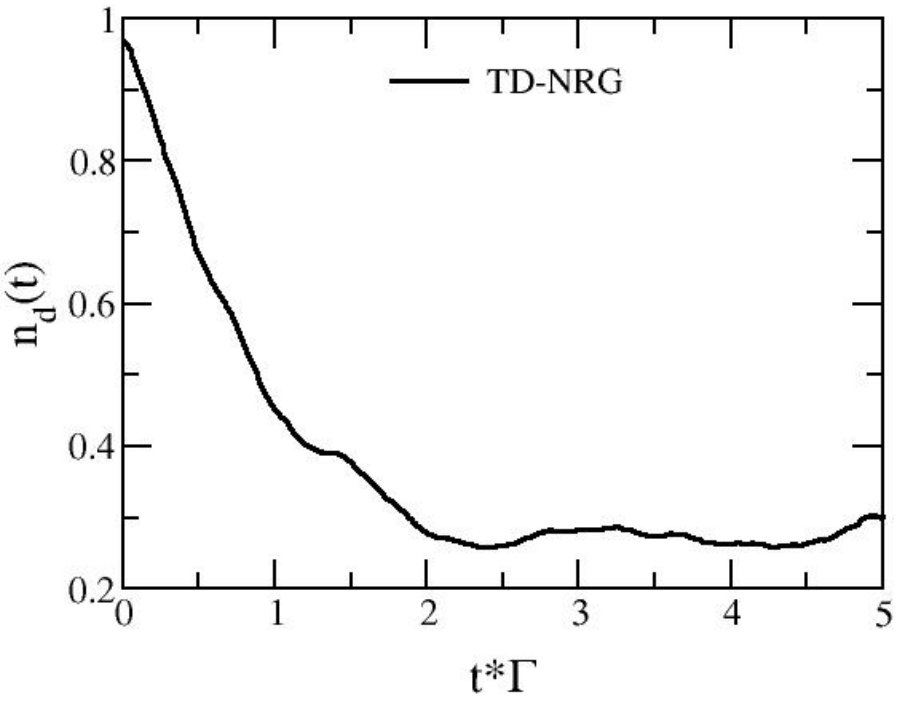
- For $T > 0$, the TD-NRG works well up to $t \approx 1/T$
- The deviation of the relaxed T=0 value from the new thermodynamic value is a measure for the accuracy of the TD-NRG on all time scales

Source of inaccuracies

$T = 0$

$E_d(t < 0) = -10\Gamma \qquad E_d(t > 0) = \Gamma$

$\Lambda = 2$

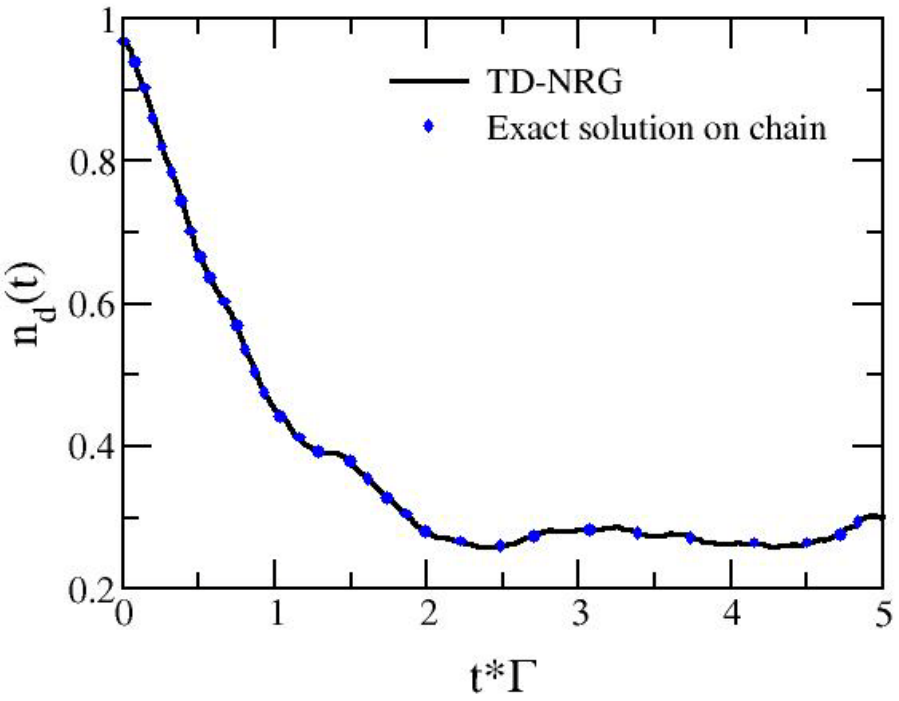


Source of inaccuracies

$T = 0$

$E_d(t < 0) = -10\Gamma \qquad E_d(t > 0) = \Gamma$

$\Lambda = 2$

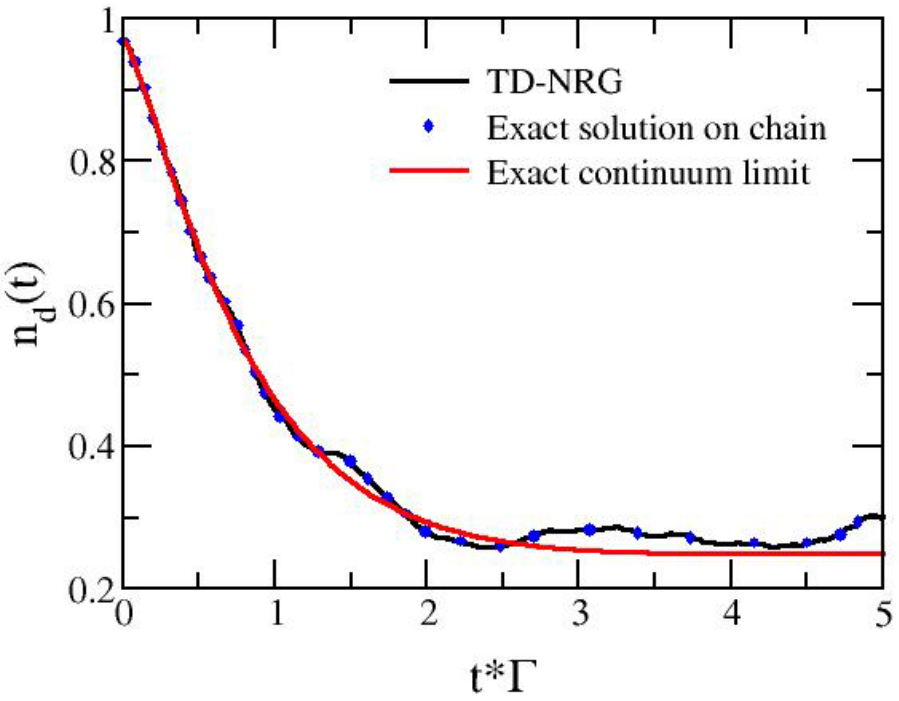


Source of inaccuracies

$T = 0$

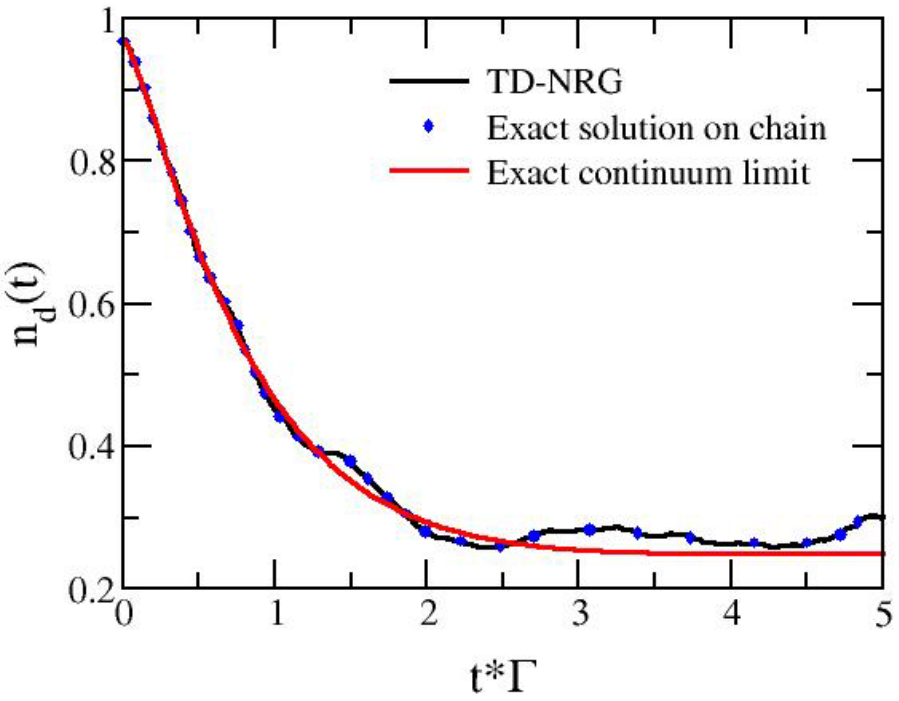
$E_d(t < 0) = -10\Gamma \qquad E_d(t > 0) = \Gamma$

$\Lambda = 2$



Source of inaccuracies

$T = 0$ $\quad E_d(t < 0) = -10\Gamma \quad E_d(t > 0) = \Gamma$ $\quad \Lambda = 2$



- TD-NRG is essentially exact on the Wilson chain
- Main source of inaccuracies is due to discretization

Bosonic benchmark: Spin-boson model

$$H = \sum_i \omega_i b_i^+ b_i - \frac{\Delta}{2}\sigma_x + \frac{\sigma_z}{2}\sum_i \lambda_i (b_i^+ + b_i)$$

$$J(\omega < \omega_c) = \pi \sum_i \lambda_i^2 \delta(\omega - \omega_i) = 2\pi\alpha\omega_c^{s-1}\omega^s$$

Bosonic benchmark: Spin-boson model

$$H = \sum_i \omega_i b_i^+ b_i - \frac{\Delta}{2}\sigma_x + \frac{\sigma_z}{2}\sum_i \lambda_i (b_i^+ + b_i)$$

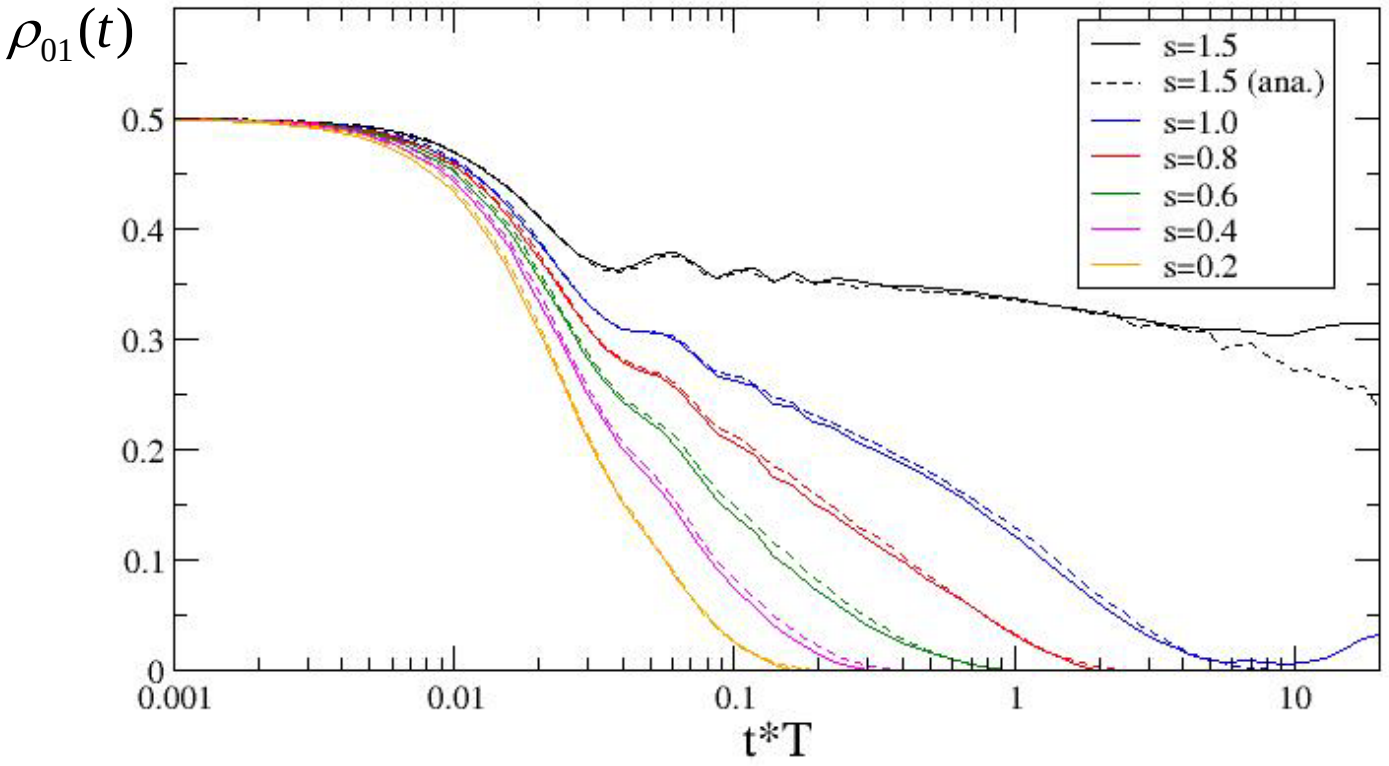
$$J(\omega < \omega_c) = \pi \sum_i \lambda_i^2 \delta(\omega - \omega_i) = 2\pi\alpha\omega_c^{s-1}\omega^s$$

- Setting Δ=0, we start from the pure spin state

$$\hat{\rho}(t=0) = \left|\sigma_x = 1\right\rangle\left\langle\sigma_x = 1\right| \otimes \hat{\rho}_{Thermal-Bath}$$

and compute $$\rho_{01}(t) = \left\langle \sigma_z = 1 \left| Tr_{Bath}\left\{\hat{\rho}(t)\right\} \right| \sigma_z = -1 \right\rangle$$

Bosonic benchmark: Spin-boson model



- Excellent agreement between TD-NRG (full lines) and the exact analytic solution (dashed lines) up to $t \approx 1/T$

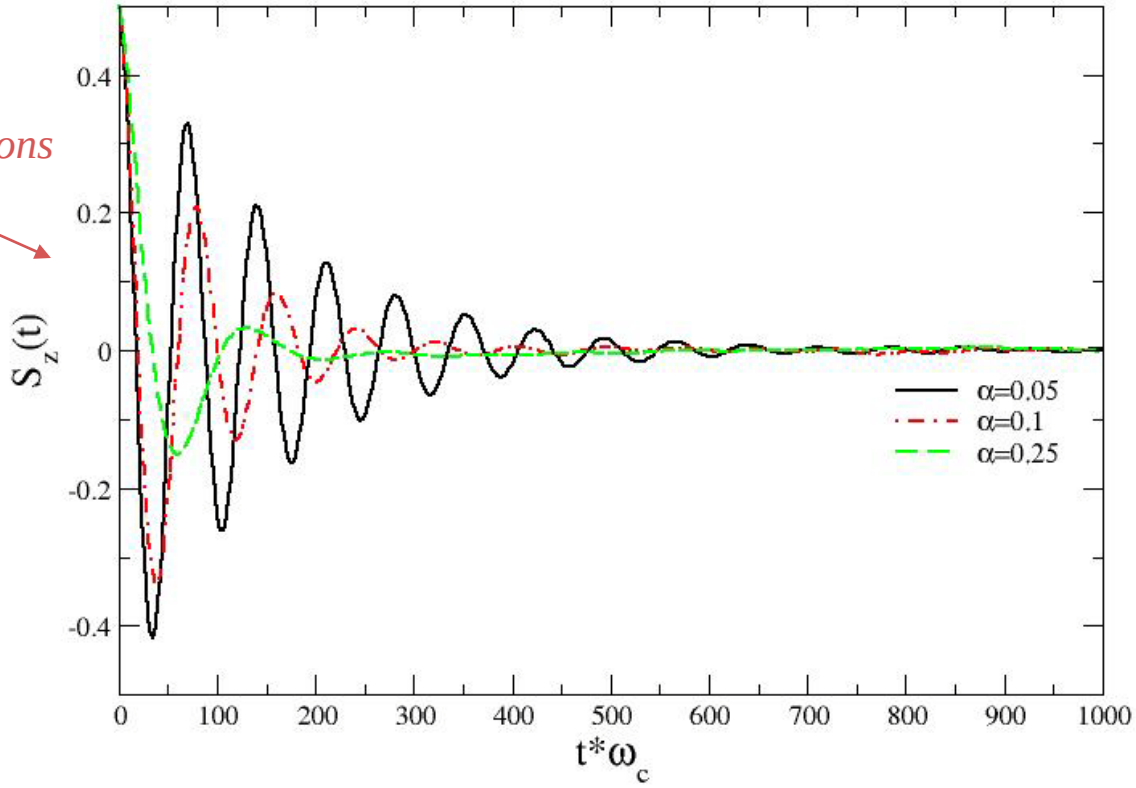
Bosonic benchmark: Spin-boson model

- For nonzero Δ and $s = 1$ (Ohmic bath), we prepare the system such that the spin is initially fully polarized ($S_z = 1/2$)

Bosonic benchmark: Spin-boson model

- For nonzero Δ and $s = 1$ (Ohmic bath), we prepare the system such that the spin is initially fully polarized ($S_z = 1/2$)

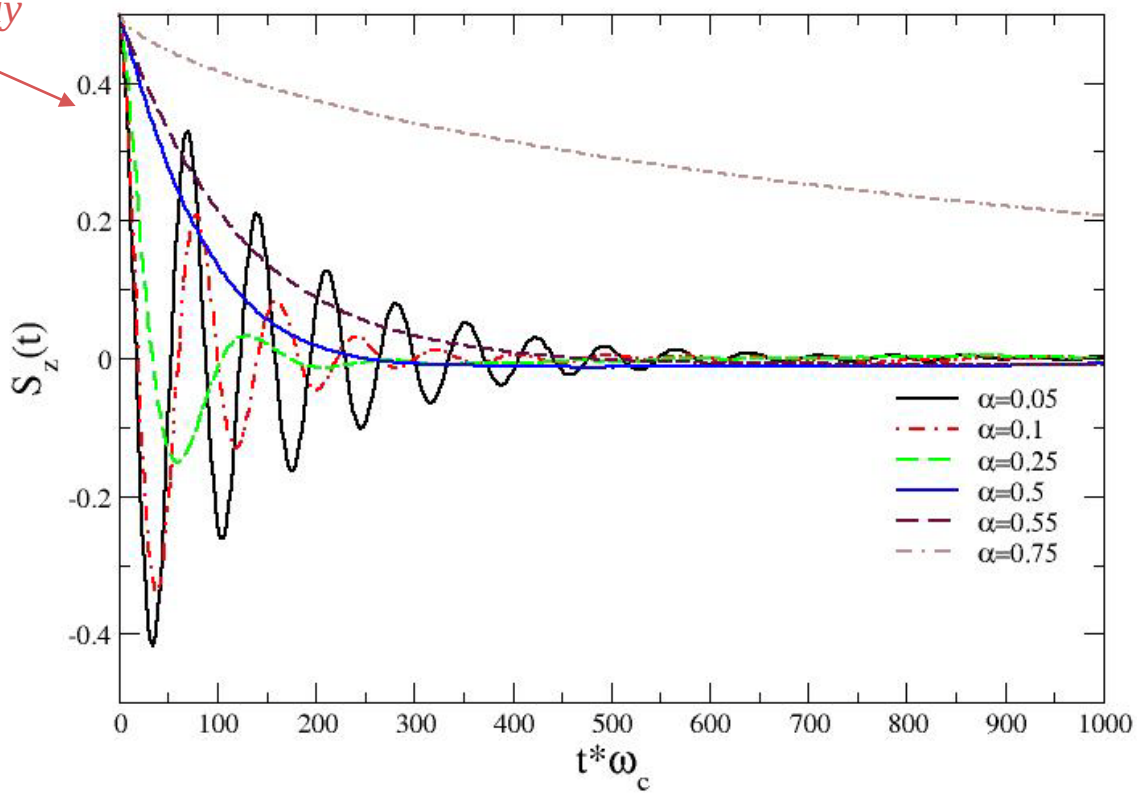
Damped oscillations



Bosonic benchmark: Spin-boson model

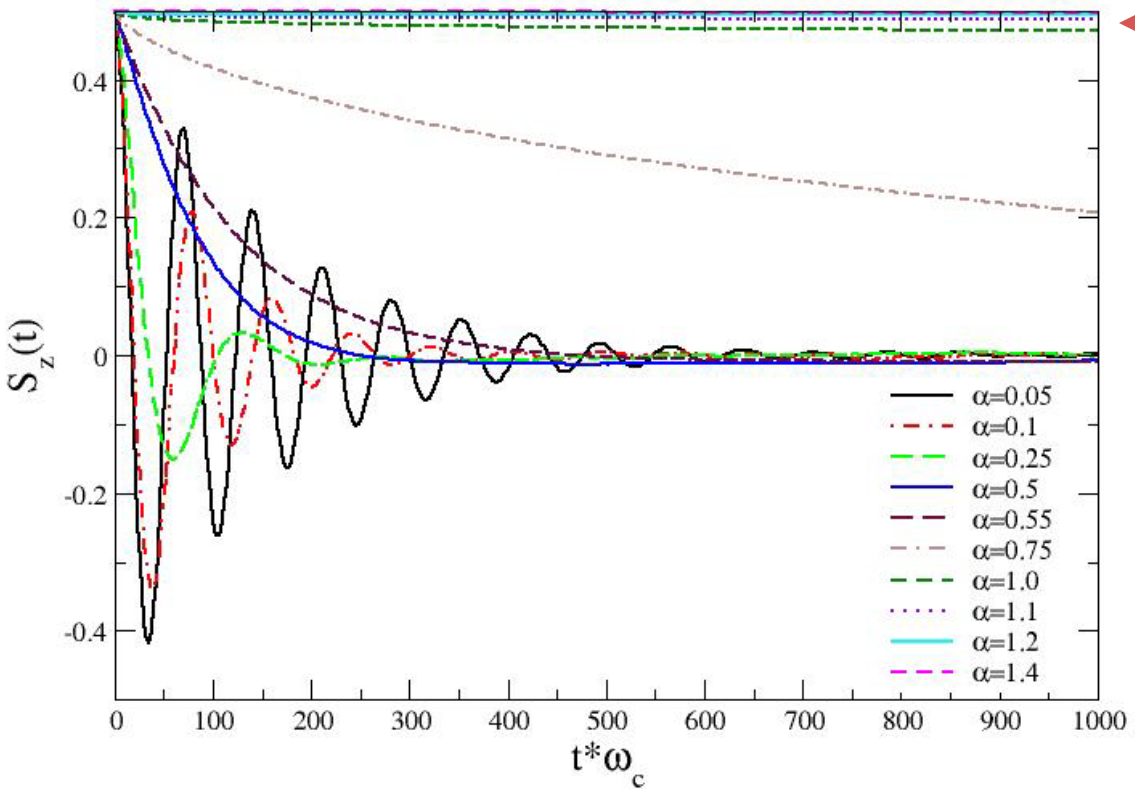
- For nonzero Δ and $s = 1$ (Ohmic bath), we prepare the system such that the spin is initially fully polarized ($S_z = 1/2$)

Monotonic decay



Bosonic benchmark: Spin-boson model

- For nonzero Δ and $s = 1$ (Ohmic bath), we prepare the system such that the spin is initially fully polarized ($S_z = 1/2$)



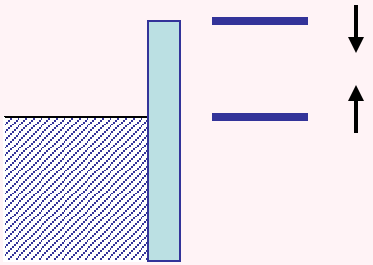
Localized phase

Anderson impurity model

$$H=\sum_{k,\sigma}\varepsilon_k c^{+}_{k\sigma}c_{k\sigma}+\sum_{\sigma}\left[E_d(t)-\frac{\sigma}{2}H(t)\right]d^{+}_{\sigma}d_{\sigma}$$

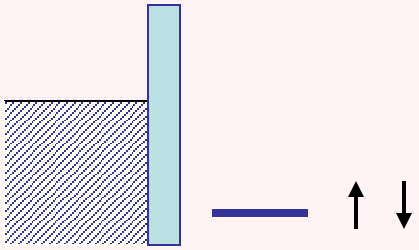
$$+V(t)\sum_{k,\sigma}(c^{+}_{k\sigma}d_{\sigma}+d^{+}_{\sigma}c_{k\sigma})+Ud^{+}_{\uparrow}d_{\uparrow}d^{+}_{\downarrow}d_{\downarrow}$$

$t < 0$



$$\pi\rho V^2=\Gamma_0$$

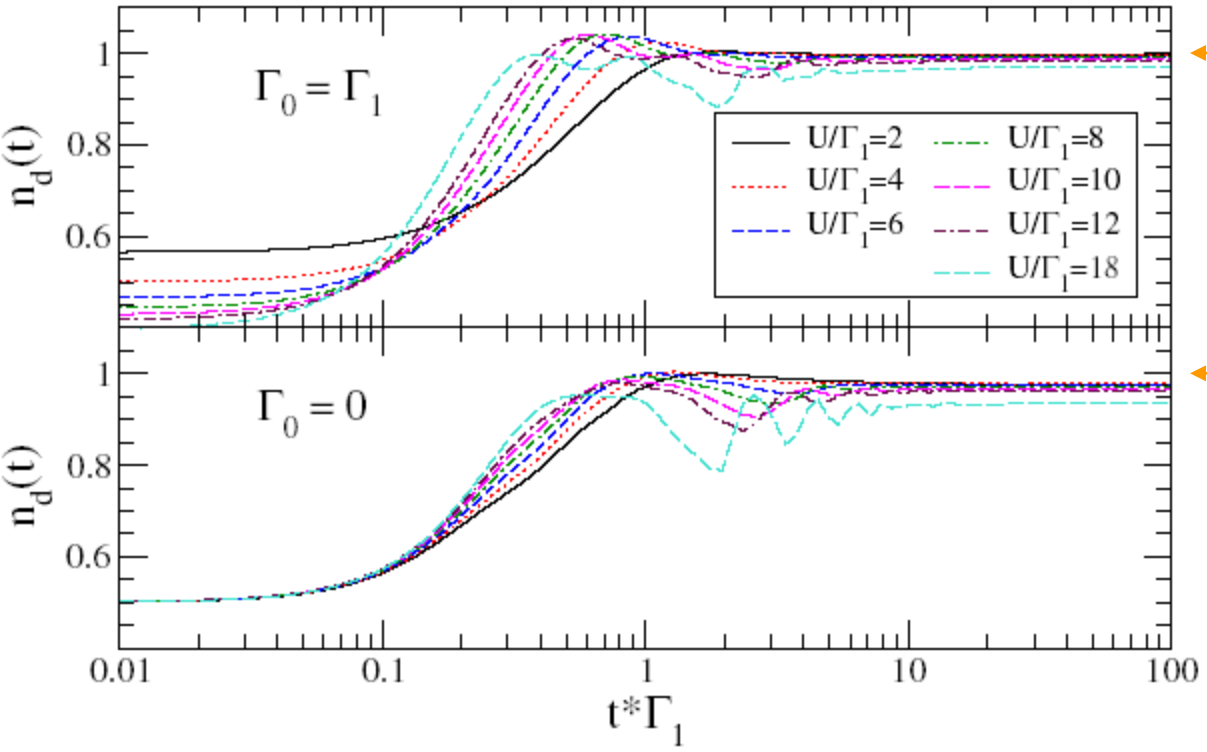
$t > 0$



$$E_d=-U/2$$

$$\pi\rho V^2=\Gamma_1$$

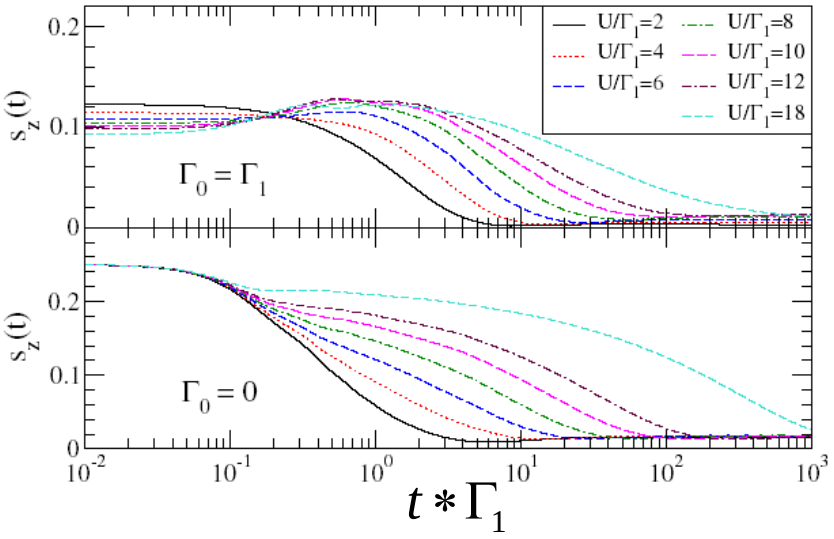
Anderson impurity model: Charge relaxation



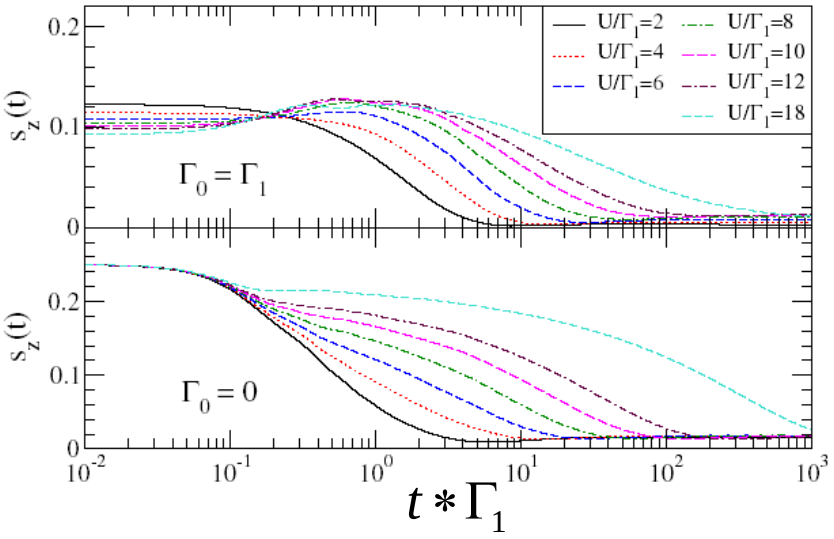
Exact new Equilibrium values

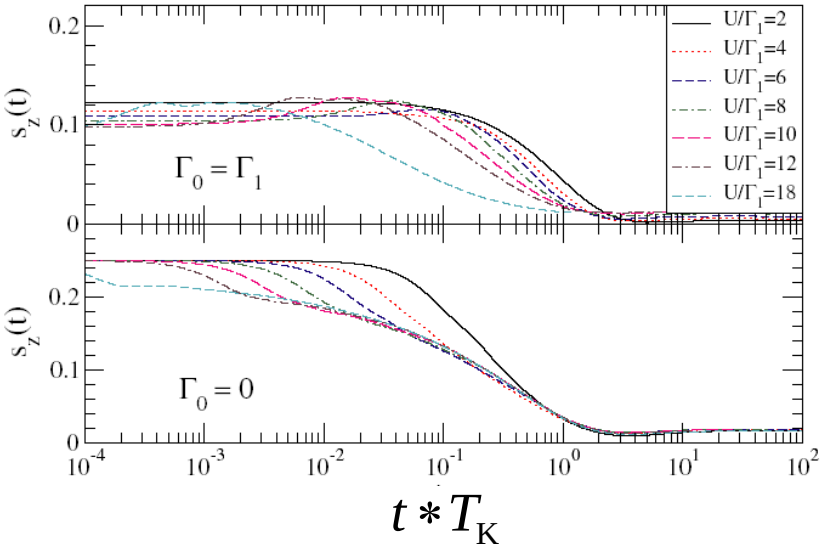
- Charge relaxation is governed by $t_{ch}=1/\Gamma_1$
- TD-NRG works better for interacting case!

Anderson impurity model: Spin relaxation

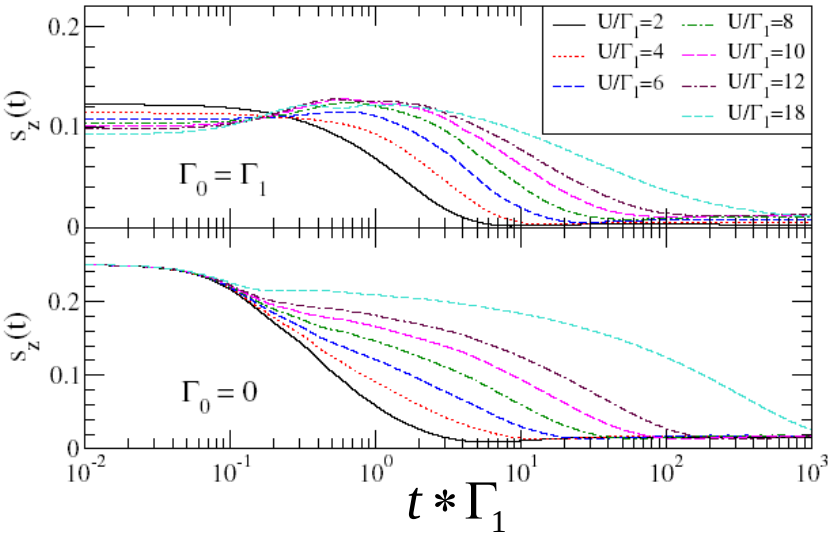


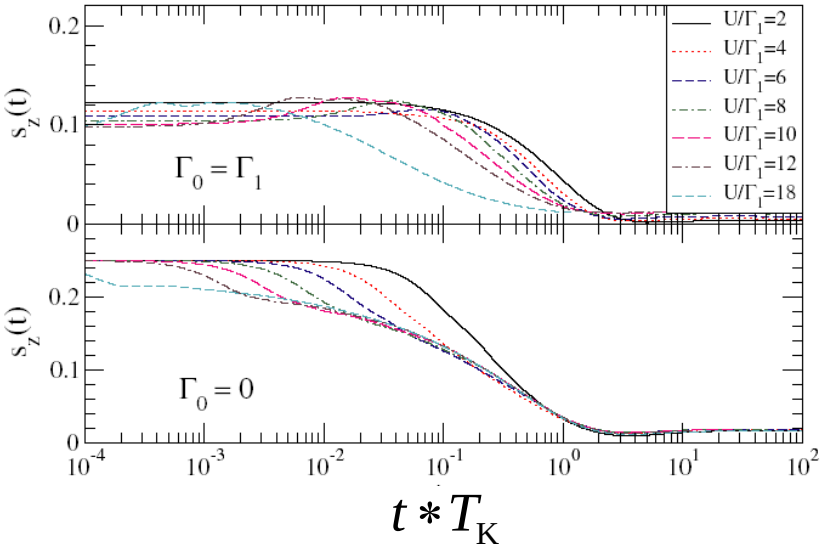
Anderson impurity model: Spin relaxation





Anderson impurity model: Spin relaxation





- Spin relaxes on a much longer time scale $t_{sp} >> t_{ch}$
- Spin relaxation is sensitive to initial conditions!
- Starting from a decoupled impurity, spin relaxation approaches a universal function of t/t_{sp} with $t_{sp}=1/T_K$

On-going projects:

- Eliminating discretization errors
- Extending approach to multiple switching events

New hybrid approach