Nonequilibrium Physics of Correlated Electron Materials II:

Theory and Computation Concepts and Challenges

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College de France
Sept 29, 2015

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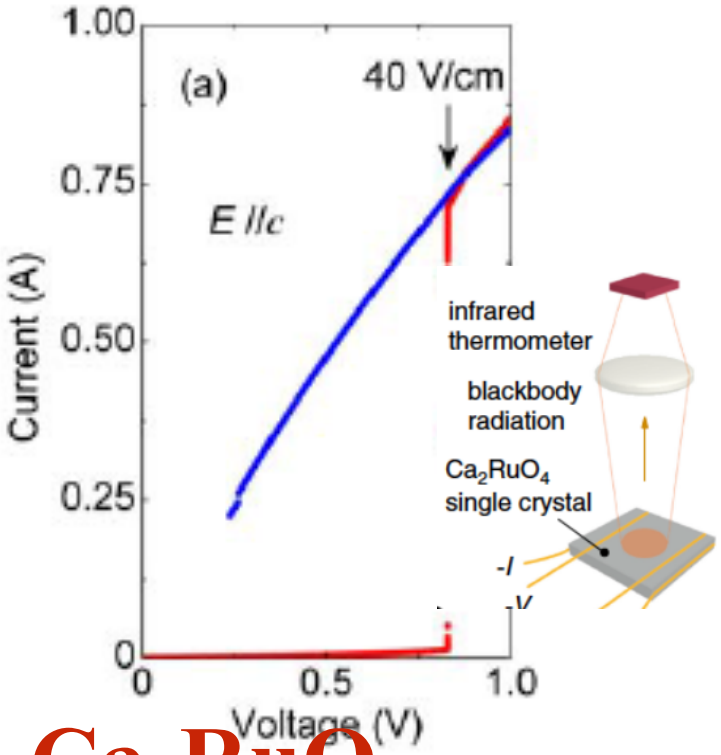
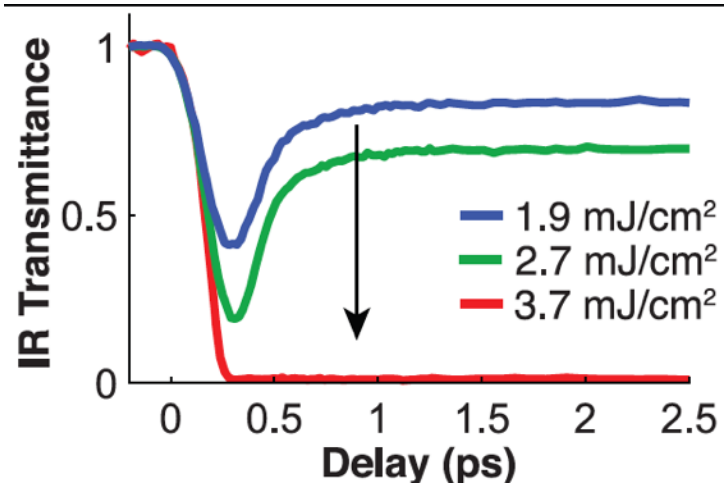
Experiments

Steady-state drive
system in high-T phase
though physical T low



Ca_2RuO_4

Transient perturbation
=>long-duration change of state



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This talk:

- **Quench**
- **Open System: path integral**
- **Numerics**

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``Quench" (change Hamiltonian)

$t<0$, $H=H_0$ $\quad$ $t>0$, $H=H_1$

h

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``Quench" (change Hamiltonian)

t<0, H=H_0 t>0, H=H_1

Example

$$H(h) = -J \sum_{j=1}^{L} \left[\sigma_j^x \sigma_{j+1}^x + h \sigma_j^z \right]$$

h

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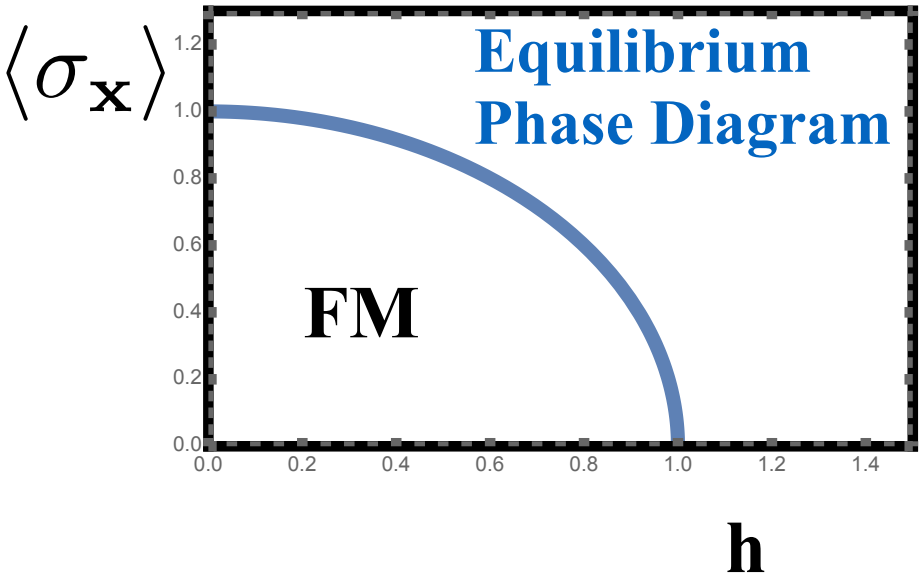

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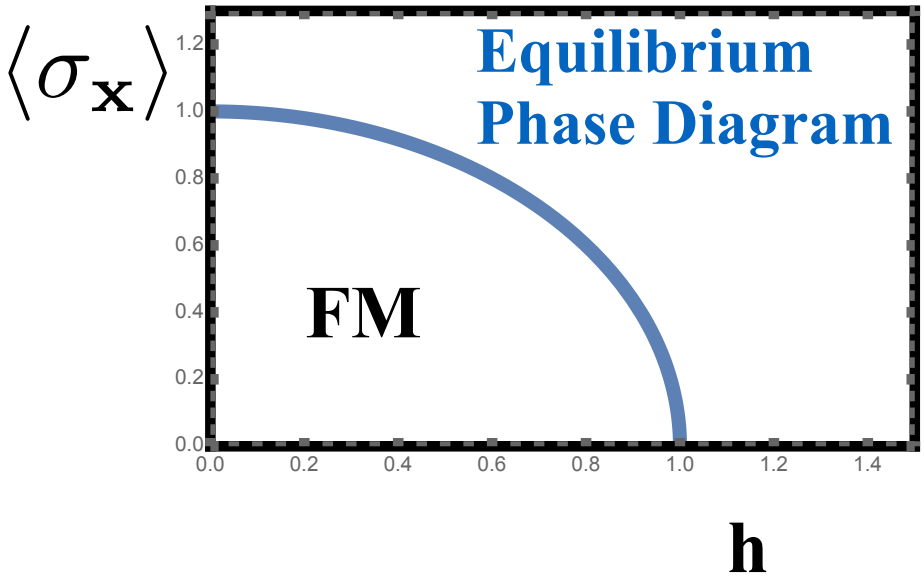

?What happens if suddenly change h?

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How to think about a quench

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How to think about a quench

Non-thermal initial condition: at $t=0^+$ the system is is in a superposition of eigenstates

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How to think about a quench

Non-thermal initial condition: at $t=0^+$ the system is is in a superposition of eigenstates

$$|\psi(\mathbf{t})\rangle = \sum_{\mathbf{n}} \mathbf{e}^{-\mathbf{iE_n t}} |\mathbf{n}\rangle \langle \mathbf{n}|\psi(\mathbf{t}=\mathbf{0}^-)\rangle$$

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How to think about a quench

Non-thermal initial condition: at $t=0^+$ the system is is in a superposition of eigenstates

$$|\psi(t)\rangle = \sum_n e^{-iE_n t} |n\rangle \langle n|\psi(t=0^-)\rangle$$

Non-thermal: $$\left|\langle n|\psi(t=0^-)\rangle\right|^2 \neq \frac{e^{-\frac{E_n}{T}}}{Z}$$

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How to think about a quench

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Non-thermal: $$\left|\langle n|\psi(t=0^-)\rangle\right|^2 \neq \frac{e^{-\frac{E_n}{T}}}{Z}$$

Mean energy:

$$\bar{E} \equiv \langle H(t=0^+)\rangle = \sum_n E_n \left|\langle n|\psi(t=0^-)\rangle\right|^2$$

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Dynamics: `simply' evolve t=0 state forward in time

$$|\psi(\mathbf{t})\rangle = \sum_{\mathbf{n}} \mathbf{e}^{-\mathbf{iE_n t}} |\mathbf{n}\rangle \langle \mathbf{n}|\psi(\mathbf{t}=\mathbf{0})\rangle$$

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Dynamics: `simply' evolve t=0 state forward in time

$$|\psi(\mathbf{t})\rangle = \sum_{\mathbf{n}} \mathbf{e}^{-\mathbf{iE_n t}} \, |\mathbf{n}\rangle \, \langle \mathbf{n}|\psi(\mathbf{t}=\mathbf{0})\rangle$$

question: at long times does the system thermalize in the sense that local observables take the values expected from thermal ensemble corresponding to mean energy

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Dynamics: `simply' evolve t=0 state forward in time

$$|\psi(\mathbf{t})\rangle = \sum_{\mathbf{n}} \mathbf{e}^{-\mathbf{iE_n t}} \, |\mathbf{n}\rangle \, \langle \mathbf{n}|\psi(\mathbf{t}=\mathbf{0})\rangle$$

$$\rho(\mathbf{t}) = \sum_{\mathbf{nm}} \mathbf{e}^{-\mathbf{i}(\mathbf{E_n}-\mathbf{E_m})\mathbf{t}} \, |\mathbf{n}\rangle \, \langle \mathbf{m}| \, \langle \mathbf{n}| \, \psi(\mathbf{t}=\mathbf{0}) \, \rangle \langle \, \psi(\mathbf{t}=\mathbf{0}) \, |\mathbf{m}\rangle$$

$$\rightarrow \rho(\mathbf{t}) = \sum_{\mathbf{n}} |\mathbf{n}\rangle \, |\psi_{\mathbf{n}}(\mathbf{t}=\mathbf{0})|^{\mathbf{2}} \, \langle \mathbf{n}|$$

Density matrix becomes diagonal

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eigenstate thermalization hypothesis

For generic (non-integrable) system, belief is that a typical eigenstate of energy E_n gives same local expectation values as thermal state of same mean energy:

$$\langle n|\mathcal{O}|n\rangle = \frac{1}{Z}\sum_m e^{-\frac{E_m}{T}}\langle m|\mathcal{O}|m\rangle$$

if $$E_n = \frac{1}{Z}\sum_m e^{-\frac{E_m}{T}} E_m$$

Fails if system has too many conservation laws.

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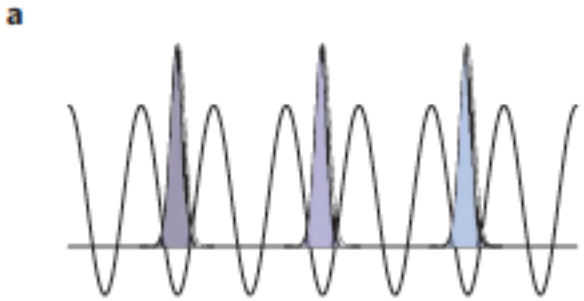
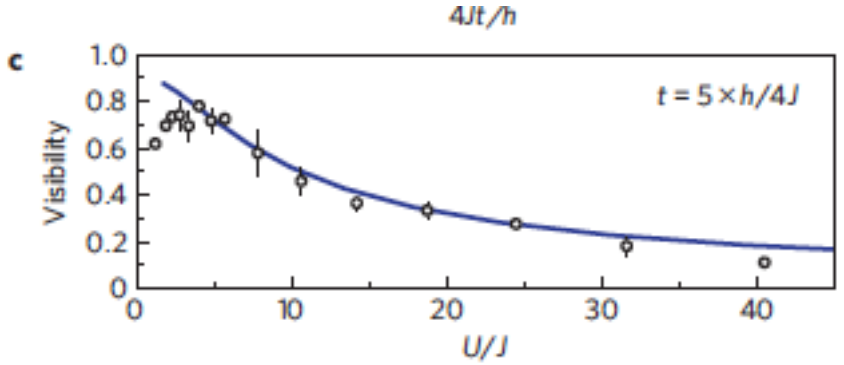
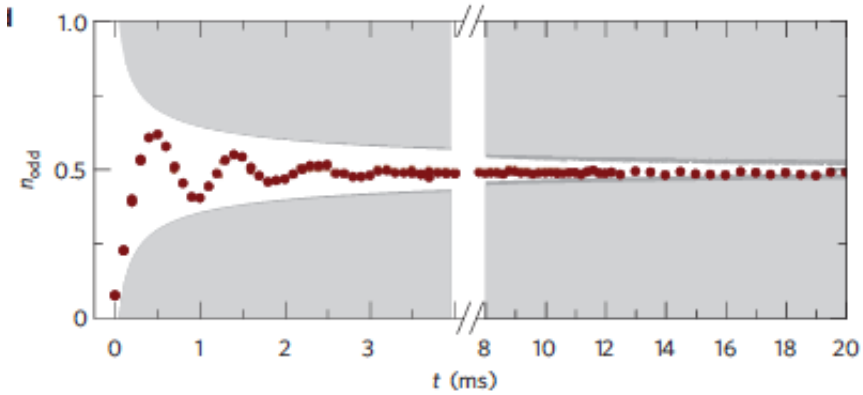
Thermalization sometimes works: experimental quench a one dimensional charge density wave







Nat Phys v 8 p 325

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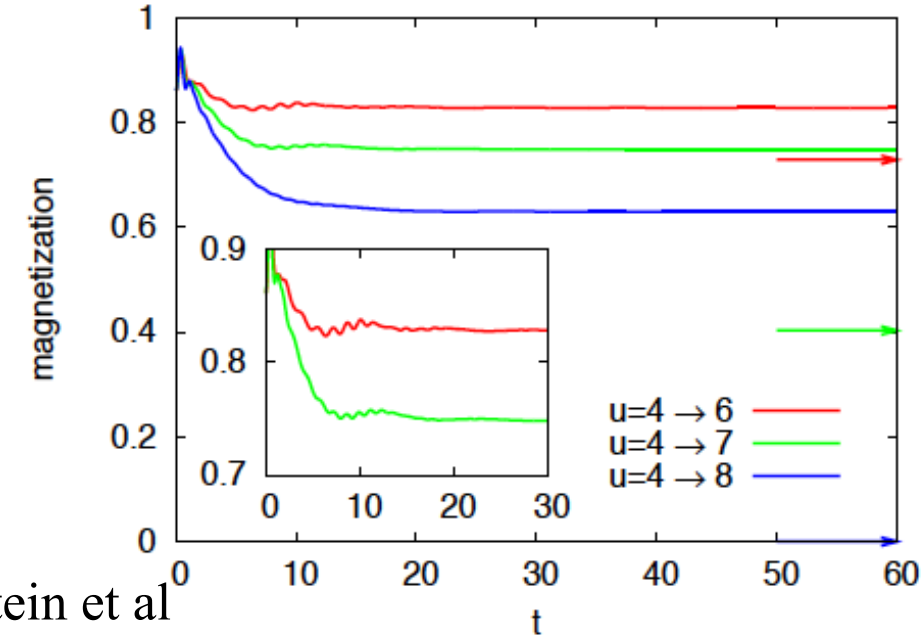
Thermalization sometimes fails

``Quantum quench" in infinite-d Hubbard model

DMFT study of Hubbard model with instantaneous change of interaction

$$H(t) = \sum_{ij,\sigma} V_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U(t) \sum_{i} \left(n_{i\uparrow} - \tfrac{1}{2}\right)\left(n_{i\downarrow} - \tfrac{1}{2}\right)$$



Eckstein et al
arXiv:1208:0743

Long-time state is not thermal one

Lack of equilibration attributed to conservation of `doublons'

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Dynamical Mean Field Theory

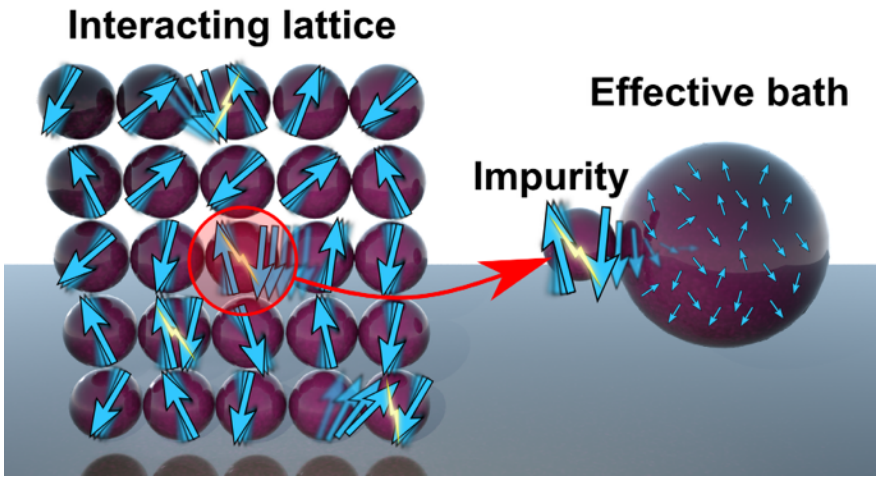

Figure: G. Cohen after A. Georges

Approximation to electron self energy of real problem from solution of:

- **``impurity problem": a few sites coupled to non-interacting bath**
- **self-consistency condition**

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Nonequilibrium DMFT

Original formulation:

- Schmidt and Monien, arXiv:cond-mat/0202046
- Freericks, Turkowski, and Zlatic, PRL 97, 266408

Nice description of modern understandng

Aoki, Tsuji, Eckstein, Kollar, Oka, Werner, (1310.5329 (RMP 2014)

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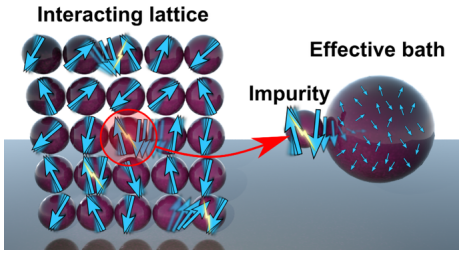
Computational task: solve impurity model

Impurity model action: local (on impurity) terms plus bath

$$\mathbf{S} = -\mathbf{i}\int_{\mathcal{C}} dt H_{imp}(t) - \mathbf{i}\int_{\mathcal{C}} dt_1 dt_2 \psi^\dagger(t_1)\Delta(t_1,t_2)\psi(t_2)$$

$\psi^\dagger$ creates state on impurity

Δ parametrizes hopping onto and off of bath



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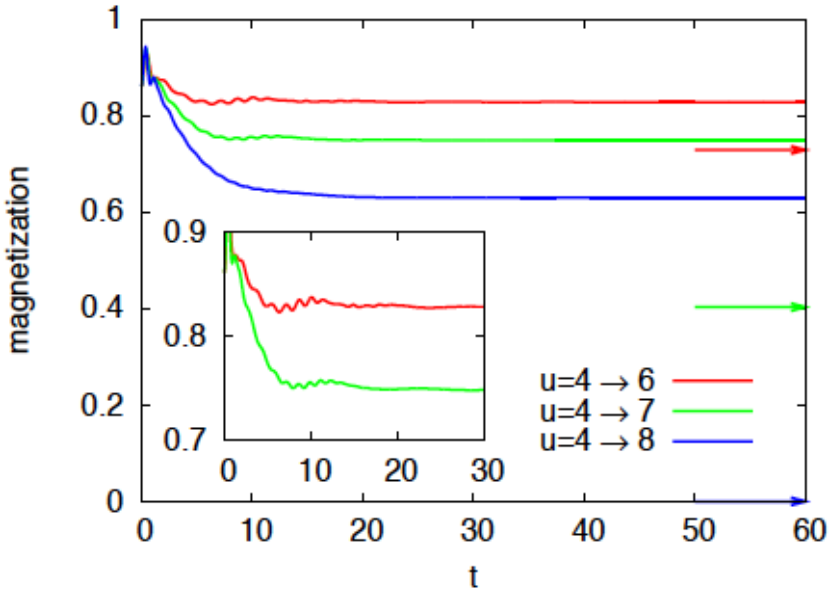
Key concept: prethermalization



Very often, system approaches state which is thermal given that some quantity (here, double occupancy) is approximately conserved. Long time scale associated with decay of approximately conserved quantity

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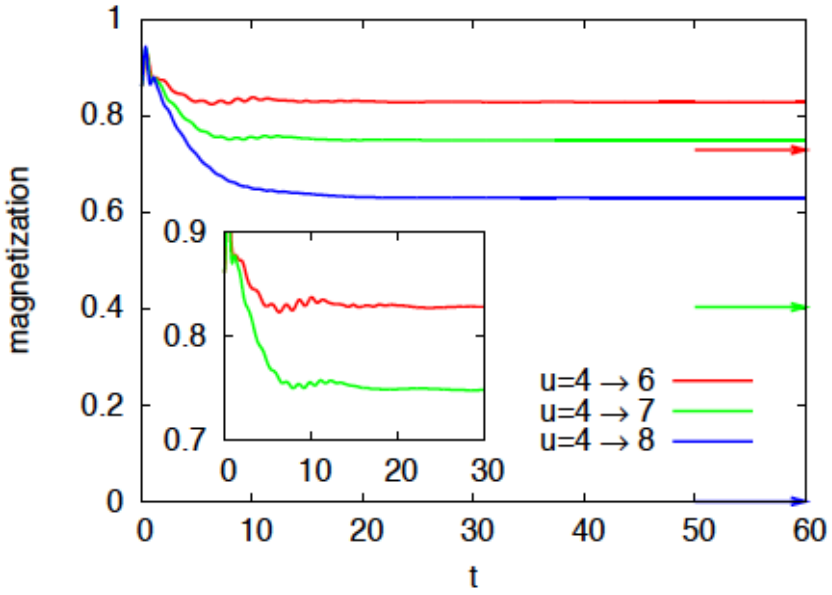
Key concept: prethermalization



Very often, system approaches state which is thermal given that some quantity (here, double occupancy) is approximately conserved. Long time scale associated with decay of approximately conserved quantity or with metastability of ordered state

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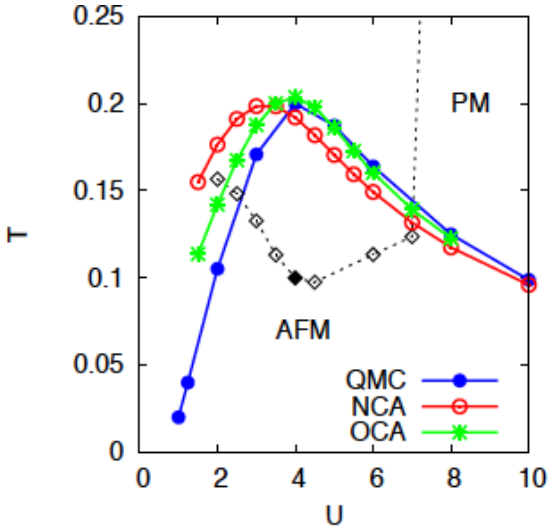
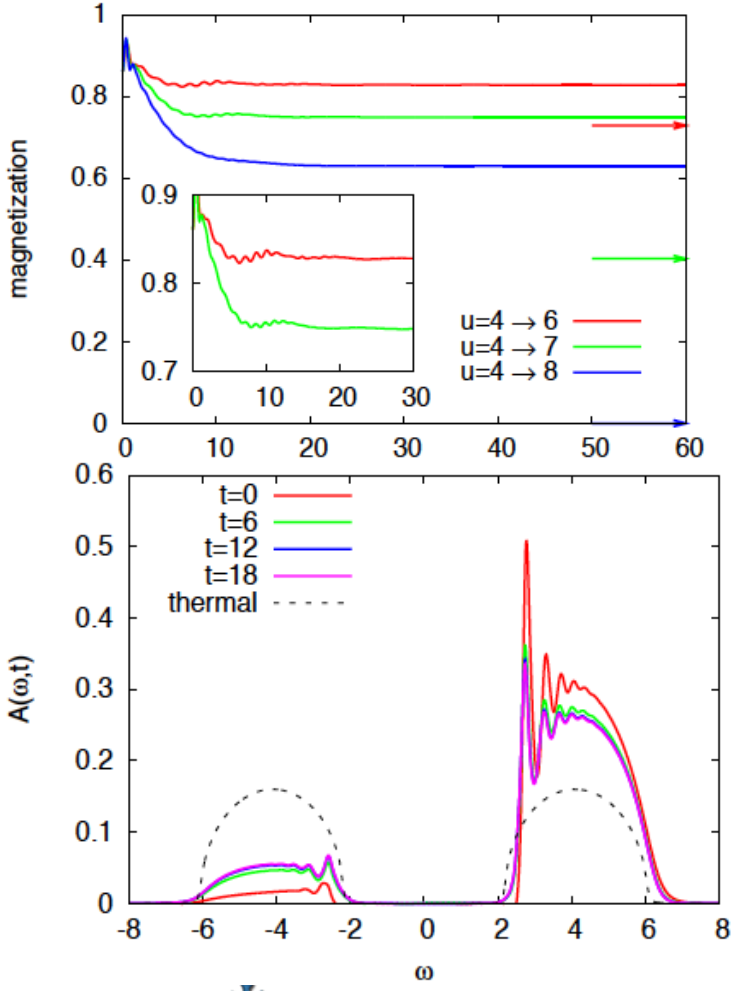
Thermalization can fail (or be very slow) due to metastability of long ranged order

$U_{init}=4$ $T_{init}=0.1$
$t_{final}=0.11, 0.12, 0.7$





Werner et al, arXiv:1208.0743

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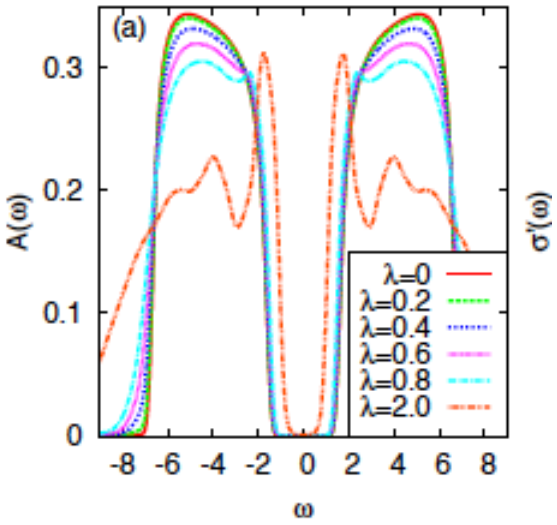
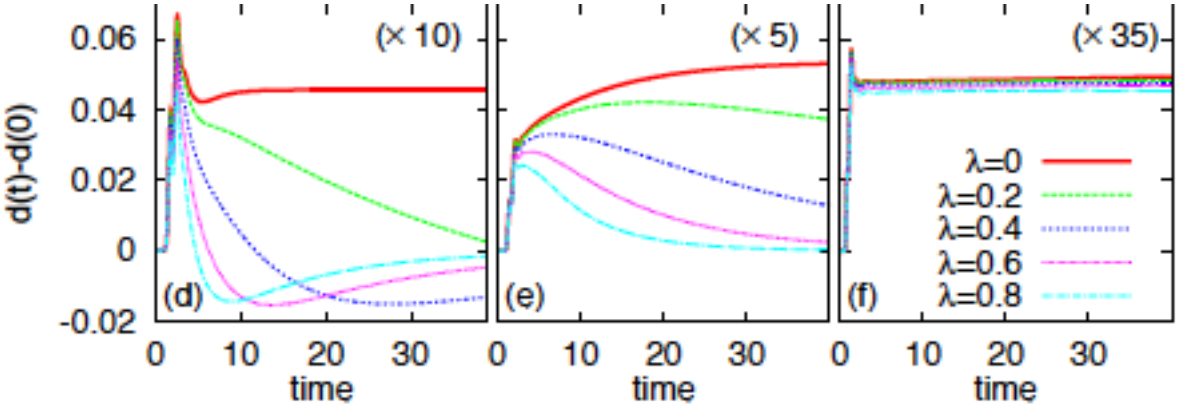
Theory: Werner and Eckstein

Hubbard model coupled to phonons (frequency 1)

Small number (1%) of excited particle-hole pairs





If gap large relative to phonon frequency, then no relaxation

arXiv:1207.0402

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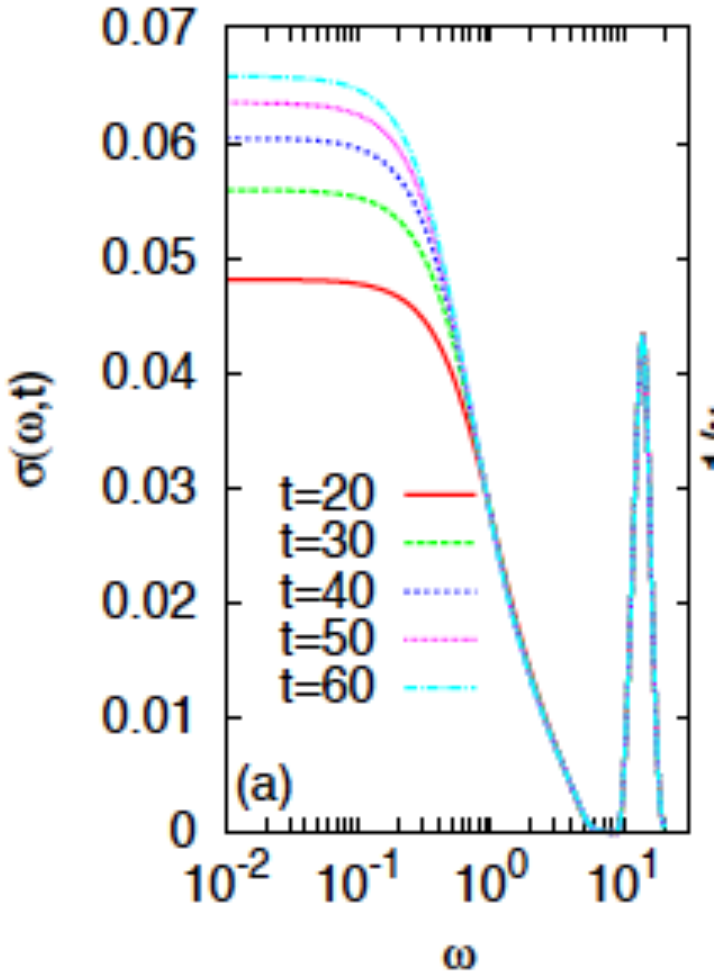
Theory: Werner and Eckstein



Result: long-lived metallic state. Particle number increases slowly (Auger up-scattering) but coherence properties are not time dependent

arXiv:1207.0402

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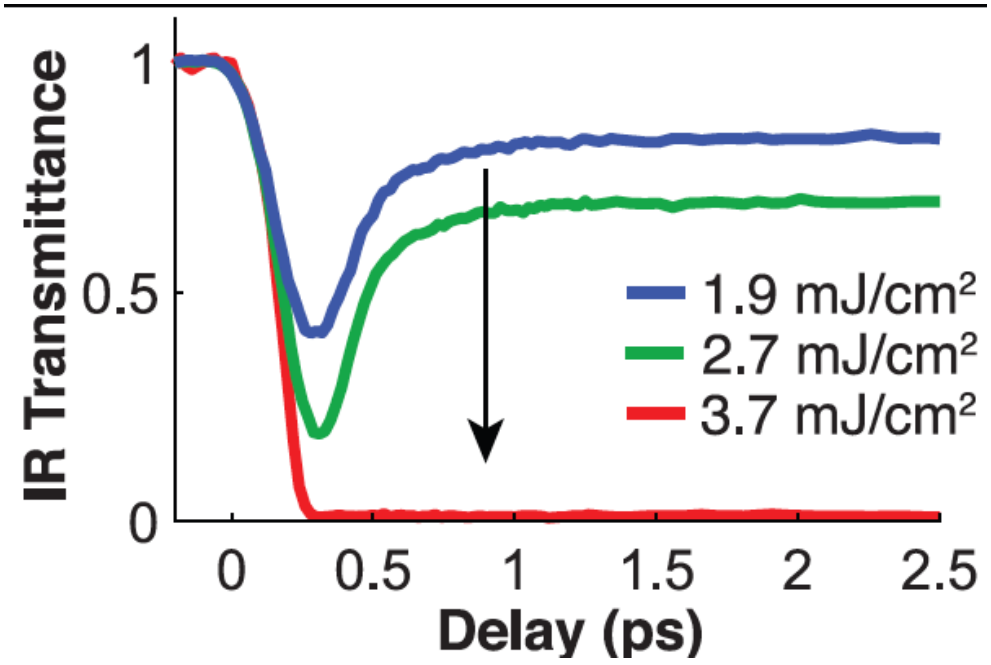
Experimental result not fully compatible with this picture.



Long-lived metallic state only for sufficiently high degree of excitation

is there a nonequilibrium phase

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Long time behavior

- **Partition function <=> path integral**

$$\mathbf{Z}\text{“}=\text{”}\int \mathcal{D}\{\phi\}\ \mathbf{e}^{-\mathbf{S}[\{\phi(\tau)\}]}$$

- **path integral dominated by most probably path (saddle point) +gaussian fluctations**

$$\mathbf{Z}\rightarrow \mathbf{e}^{-\mathbf{S}^*}\int \mathcal{D}\psi_{\mathbf{a}}\mathcal{D}\psi_{\mathbf{b}}\ldots\ \mathbf{e}^{-\frac{\mathbf{1}}{\mathbf{2}}\int \mathbf{d}\tau_{\mathbf{1}}\mathbf{d}\tau_{\mathbf{2}}\sum_{\mathbf{ab}}\psi_{\mathbf{a}}(\tau_{\mathbf{1}})\chi^{-\mathbf{1}}(\tau_{\mathbf{1}}-\tau_{\mathbf{2}})\psi_{\mathbf{b}}(\tau_{\mathbf{2}})}$$

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thus

$$\mathbf{S_{gaussian}} = -\frac{\mathbf{1}}{\mathbf{2}} \int \mathbf{d}\tau_1 \mathbf{d}\tau_2 \sum_{\mathbf{ab}} \psi_{\mathbf{a}}(\tau_1) \chi^{-1}(\tau_1 - \tau_2) \psi_{\mathbf{b}}(\tau_2)$$

- **Identify fixed point (`phase')**
- **Identify important fluctuations (quasiparticles)**
- **quasiparticle propagators <=> linear response susceptibilies**

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Path Integrals out of Equilibrium (Schwinger, Kamenev)

To describe result of measurement of operator O at time t in system described by initial density matrix ρ_{init}

Compute:

$$\langle \mathcal{O}(t) \rangle = Tr\left[e^{-iHt}\mathcal{O}e^{iHt}\rho_{init}\right]$$

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Two time evolution operators implies two contours (Schwinger, Keldysh)

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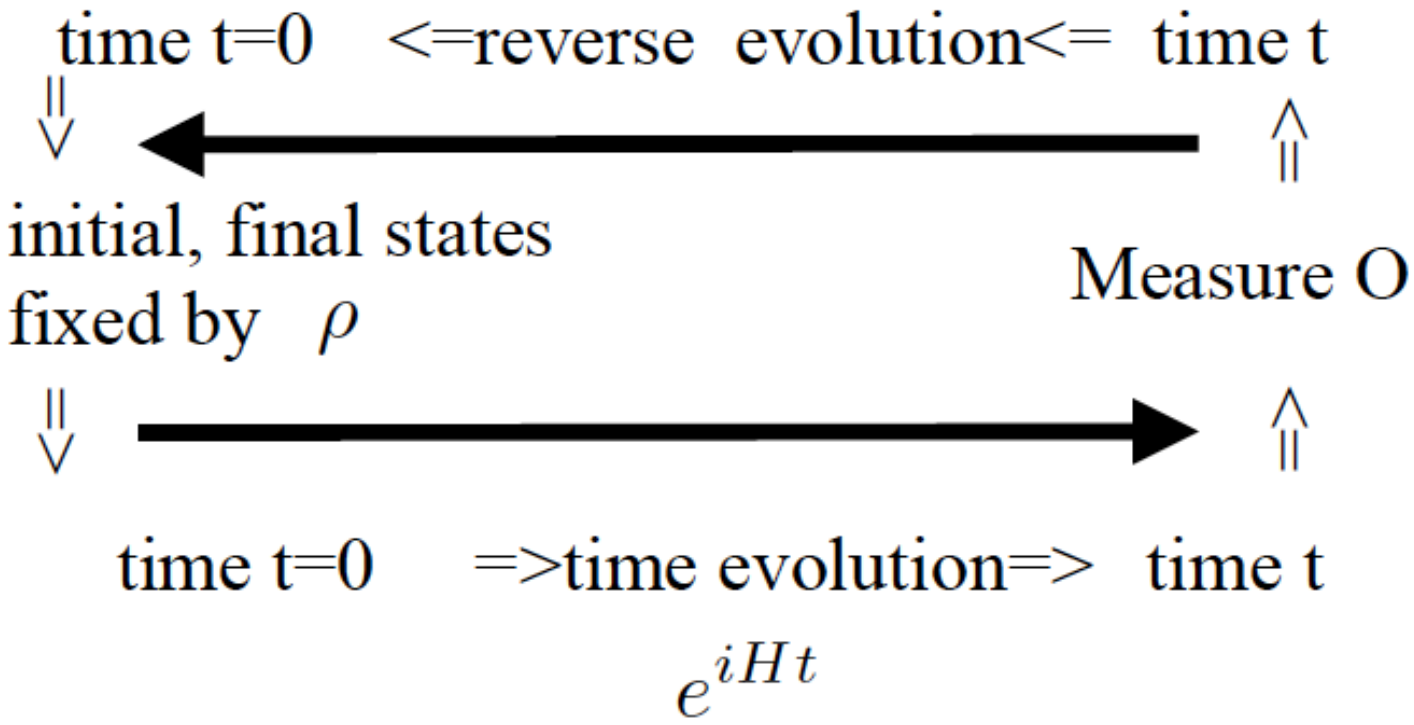
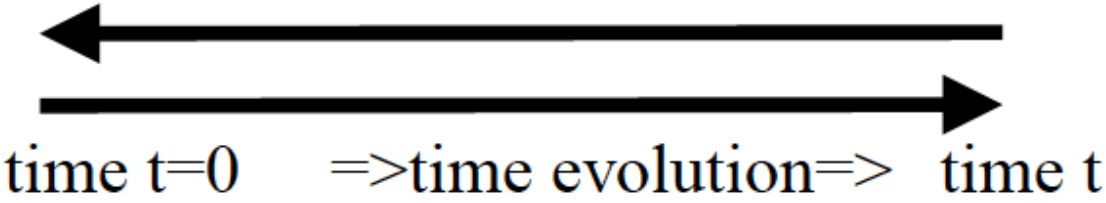


Path integral interpretation: coherent states on each contour (Schwinger, Kamenev)



$$e^{iHt} = \Pi_{i=1....N} \int \quad d\phi_N^+ ... d\phi_1^+ |\phi_N^+ >< \phi_N^+ | e^{i\Delta t H} | . \phi_{N-1}^+ > .$$

$$\times \quad < \phi_{N-1}^+ | e^{i\Delta t H} | .... \phi_1^+ >< \phi_1^- +$$

$$e^{-iHt} = \Pi_{i=1....N} \int \quad d\phi_1^- ... d\phi_N^- | \phi_1^- >< \phi_1^- | e^{-i\Delta t H} | .....$$

$$\times \quad | \phi_{N-1}^- >< \phi_{N-1}^- | e^{-i\Delta t H} | \phi_N^- >< \phi_N^- |$$

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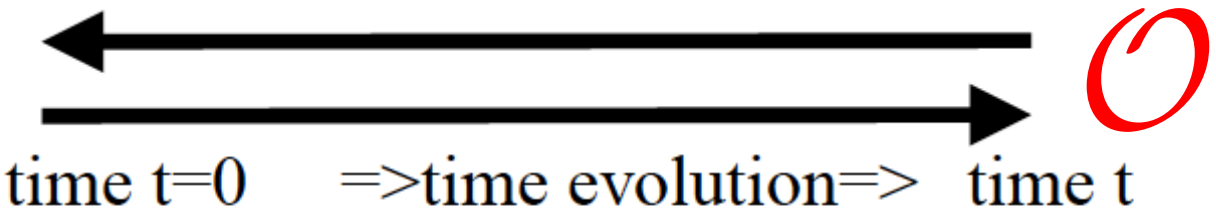
Measure operator



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$$e^{-iHt} = \Pi_{i=1....N} \int d\phi_1^- ... d\phi_N^- |\phi_1^- >< \phi_1^- | e^{-i\Delta t H} | .....$$

$$\times \quad |\phi_{N-1}^- >< \phi_{N-1}^- | e^{-i\Delta t H} | \phi_N^- >< \phi_N^- |$$

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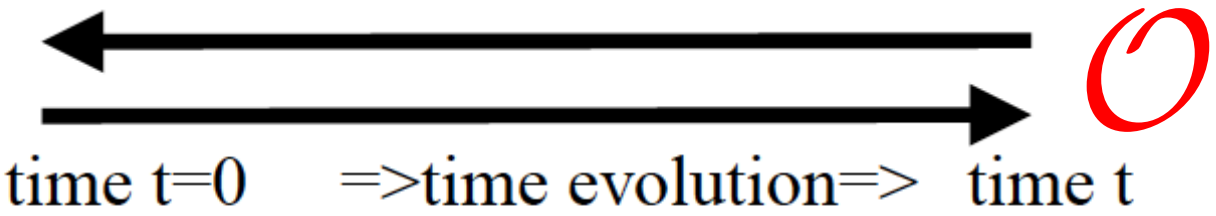
Measure operator



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$$e^{-iHt} = \Pi_{i=1....N} \int d\phi_1^- ... d\phi_N^- |\phi_1^- >< \phi_1^- | e^{-i\Delta t H} | .....$$
$$\times \quad |\phi_{N-1}^- >< \phi_{N-1}^- | e^{-i\Delta t H} |\phi_N^- >< \phi_N^-|$$

$$\langle \mathcal{O}(t) \rangle = Tr \left[e^{-iHt} \mathcal{O} e^{iHt} \rho_{init} \right]$$

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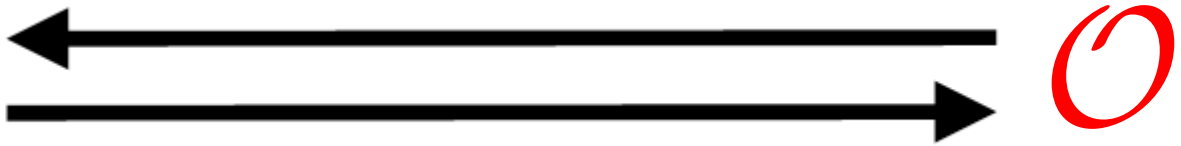
Measure operator



$$e^{iHt} = \Pi_{i=1....N} \int d\phi_N^+ ... d\phi_1^+ |\phi_N^+ >< \phi_N^+ | e^{i\Delta t H} | . \phi_{N-1}^+ > .$$
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Crucial factor $< \phi_N^- | \mathcal{O} | \phi_N^+ >$

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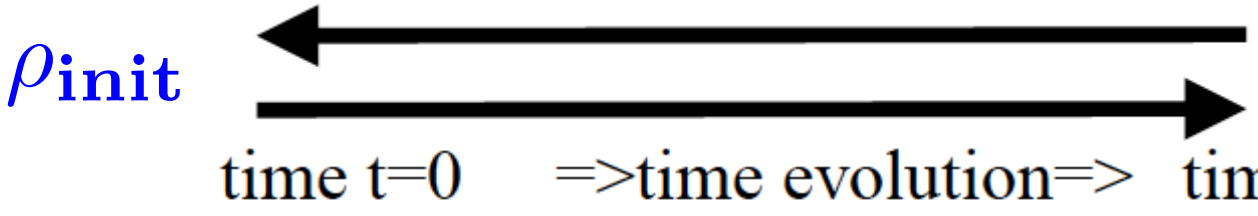
Initial density matrix



$$e^{iHt} = \Pi_{i=1....N} \int d\phi_N^+ ... d\phi_1^+ |\phi_N^+ >< \phi_N^+ | e^{i\Delta t H} | . \phi_{N-1}^+ > .$$
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Crucial factor $< \phi_1^+ | \rho_{init} | \phi_1^- >$

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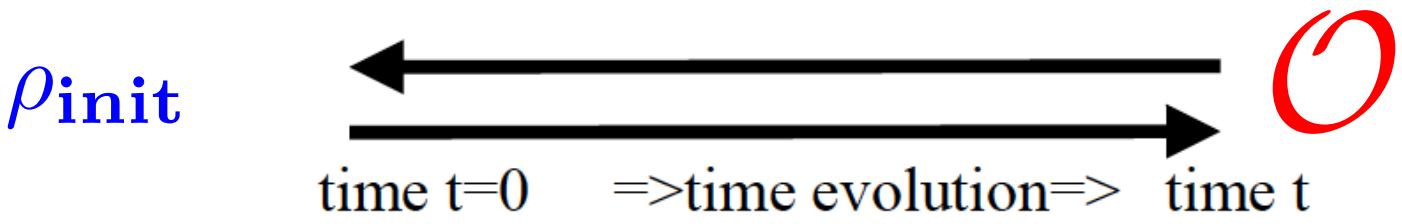
Path integral



$$\langle \mathcal{O} \rangle = \int \mathbf{d}\phi_+ \mathbf{d}\phi_- \rho_{\mathbf{init}}(\phi_+, \phi_-) \int \mathcal{D}\phi_+(\mathbf{t}) \mathcal{D}\phi_-(\mathbf{t}) \mathbf{W_O}(\{\phi_+, \phi_-\})$$

(1) Fix start (on + line) and stop (on -) values $\phi^{\pm}$
(2) Sum over all paths connecting start and stop values.
Weight paths by action W (dep on operator O)
(3) Sum over all start and stop values, weighted by ρ_{init}

Steady State

At long times: system forgets initial condition
=>?
replace initial density matrix by steady state one

$$\langle \mathcal{O} \rangle = \int \mathbf{d}\phi_+ \mathbf{d}\phi_- \rho_{\mathbf{SS}}(\phi_+, \phi_-) \int \mathcal{D}\phi_+(\mathbf{t}) \mathcal{D}\phi_-(\mathbf{t}) \mathbf{W_O}(\{\phi_+, \phi_-\})$$

Notes:

- **steady state density matrix must be determined**
- **Initial conditions may not be (fully) forgotten**

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Steady State

At long times: system forgets initial condition

=>?

replace initial density matrix by steady state one

$$\langle \mathcal{O} \rangle = \int \mathbf{d}\phi_+ \mathbf{d}\phi_- \rho_{\mathbf{SS}}(\phi_+, \phi_-) \int \mathcal{D}\phi_+(\mathbf{t}) \mathcal{D}\phi_-(\mathbf{t}) \mathbf{W_O}(\{\phi_+, \phi_-\})$$

Steady state density matrix must be determined e.g. as solution of kinetic equation

$$\rho_{\mathbf{SS}} = \mathbf{e}^{\mathbf{iHt}} \rho_{\mathbf{SS}} \mathbf{e}^{-\mathbf{iHt}}$$

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Identification of Important Paths

In equilibrium

$$\mathbf{Z = Tr}\left[\mathbf{e}^{-\frac{\mathbf{H}}{\mathbf{T}}}\right]$$

Important paths are those that dominate the path integral for the partition function

$$\mathbf{Z}\text{“}=\text{”}\int \mathcal{D}\{\phi\}\ \mathbf{e}^{-\mathbf{S}[\{\phi(\tau)\}]}$$

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Out of equilibrium

If operator O=1 then

$$\langle \mathcal{O}(t) \rangle = Tr\left[e^{-iHt}\mathcal{O}e^{iHt}\rho_{init}\right] = Tr[\rho_{init}] = 1$$

No basis for selecting paths

=>"Important paths" <=> paths making important contribution to specific operator.

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Most important case: steady-state density matrix
seek paths that maximize the density matrix

$$\rho_{\mathrm{SS}} \to\approx \rho_{\mathrm{SS}}(\phi_+, \phi_-)$$

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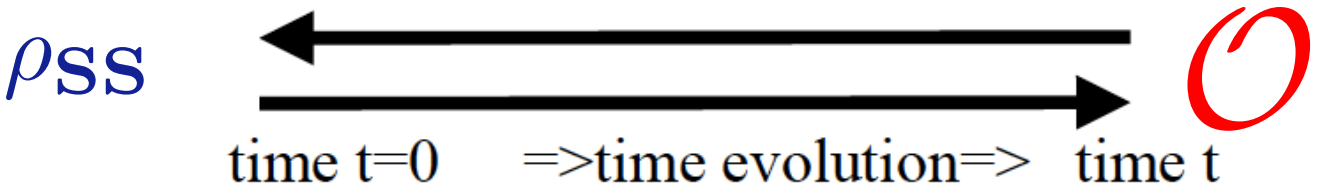
Stationary path approximation



$$\langle \mathcal{O}(t) \rangle = Tr\left[e^{-iHt}\mathcal{O}e^{iHt}\rho_{init}\right]$$

Stationary path configuration must be the same on outbound and inbound time contour (so oscillations cancel) and must extremize the diagonal component of the density matrix

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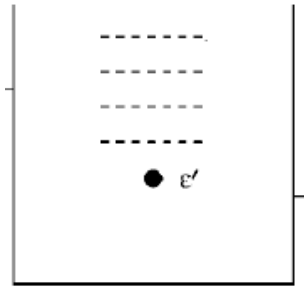
local polaron

$$H = H_{dot} + H_{lead} + H_{mix}$$

$$H_{lead} = \sum_{k,a=L,R} \varepsilon_k c^{\dagger}_{k,a} c_{k,a}.$$

$$H_{mix} = \sum_{k,a=L,R} V^a_k c^{\dagger}_{k,a} d + H.c.$$

$$H_{dot} = \varepsilon' d^{\dagger} d + \lambda q d^{\dagger} d + \frac{K}{2} q^2 + \frac{1}{2M} p^2$$



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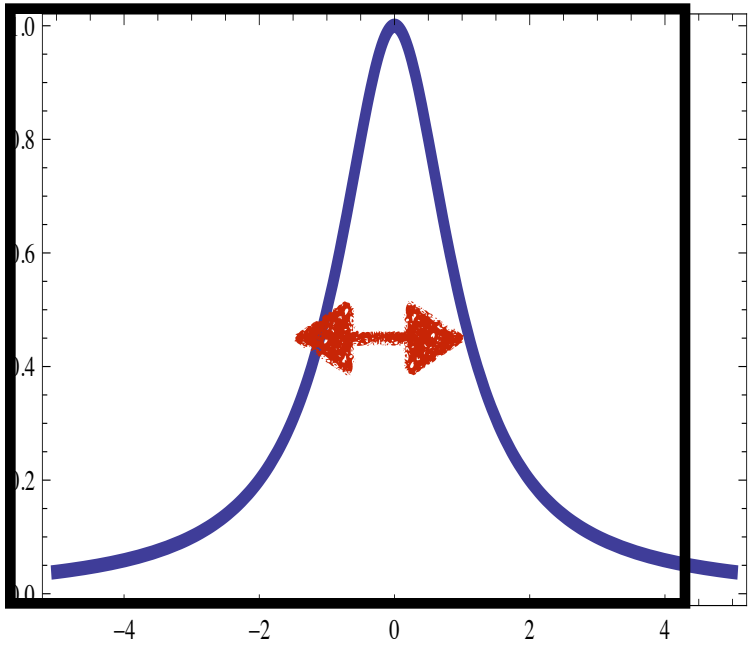
Density of states in absence of phonons



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Energy scales

$$\Gamma^a = \pi \sum_k |V_k^a|^2 \, \delta(\omega - \varepsilon_k) \quad \text{1/(electron escape time)}$$

$$\omega_{phonon} = \sqrt{\frac{K}{M}} \quad << \Gamma \quad \text{(adiabatic approx)}$$

polaron shift at $\Gamma = 0$: $\dfrac{\lambda^2}{K}$

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Polaron shift

Energy of isolated dot $\lambda q d^\dagger d + \frac{K}{2} q^2$

Implies extremum $\frac{\lambda \left\langle \mathbf{d}^\dagger \mathbf{d} \right\rangle}{\mathbf{K}} = \mathbf{q}^\star$

$$\Rightarrow \varepsilon \rightarrow \varepsilon - \frac{\lambda^2 \left\langle \mathbf{d}^\dagger \mathbf{d} \right\rangle^2}{\mathbf{2K}}$$

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In equilibrium

If $\dfrac{\lambda^2}{K} \gtrsim \Gamma$ Then 2 extrema

$$\varepsilon > \mu: \quad \langle d^\dagger d \rangle \approx 0; \quad q^\star \approx 0$$

$$\varepsilon < \mu: \quad \langle d^\dagger d \rangle \approx 1; \quad q^\star \approx \frac{\lambda}{K}$$

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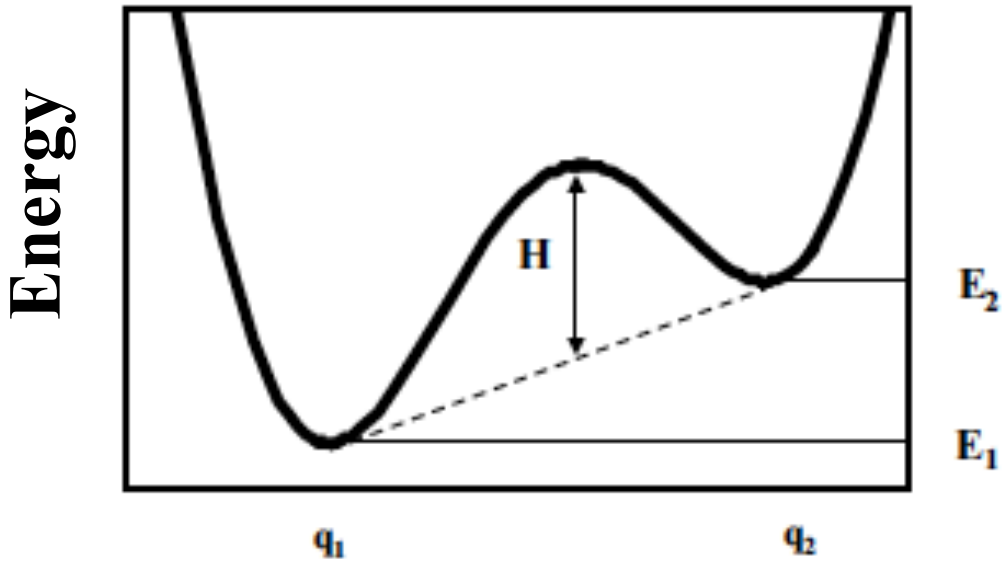
Equilibrium: two states for oscillator



$$P_2 \sim e^{-\frac{E_2 - E_1}{T}}$$

$$P(q - q_1) \sim e^{-\frac{K(q-q_1)^2}{\omega_0 \coth \frac{\omega_0}{2T}}}$$

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Nonequilibrium local polaron

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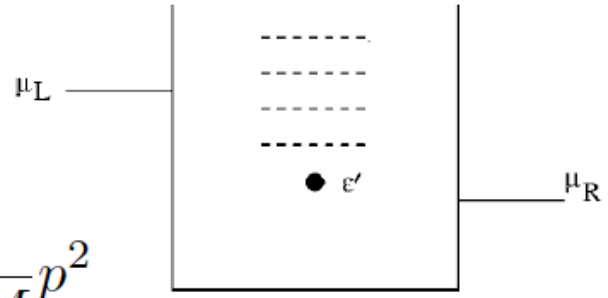

Can be more or less completely solved

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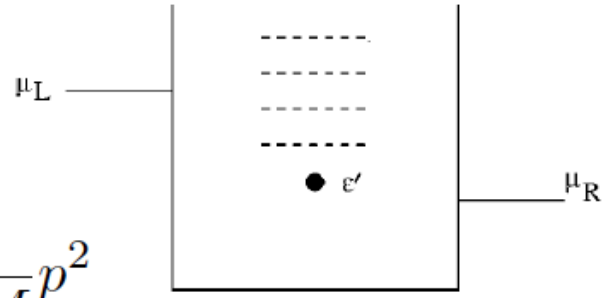

Open system: coupled to leads (reservoirs)

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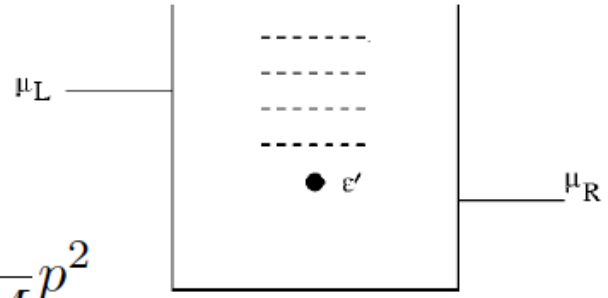

Open system: coupled to leads (reservoirs)
steady state exists and is unique

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Nonequilibrium local polaron

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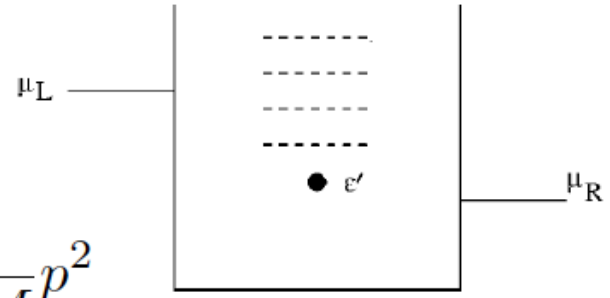

Difference in chemical potential
=> current across quantum dot

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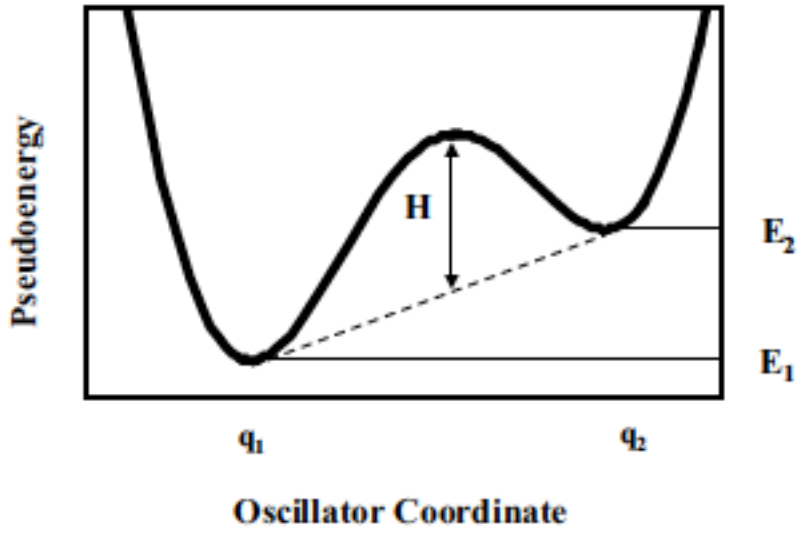
Nonequilibrium results



$$P_2 \sim e^{-\frac{E_2 - E_1}{T'_{eff}}}$$

$$T'_{eff} \approx T_{eff} \ln \frac{E_2 - E_1}{T_{eff}}$$

$$P(q - q_1) \sim e^{-\frac{K(q-q_1)^2}{\omega_0 \coth \frac{\omega_0}{2T_{eff}}}}$$

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Key point

T_{eff} a complicated function of current and T of leads

As $T_{reservoir} \Rightarrow 0$

$$T_{eff} \sim \Delta\mu$$

Effective temperature of electron system proportional to current; <u>parametrically larger than I^2R</u>
Effective temperature larger than physical temperature

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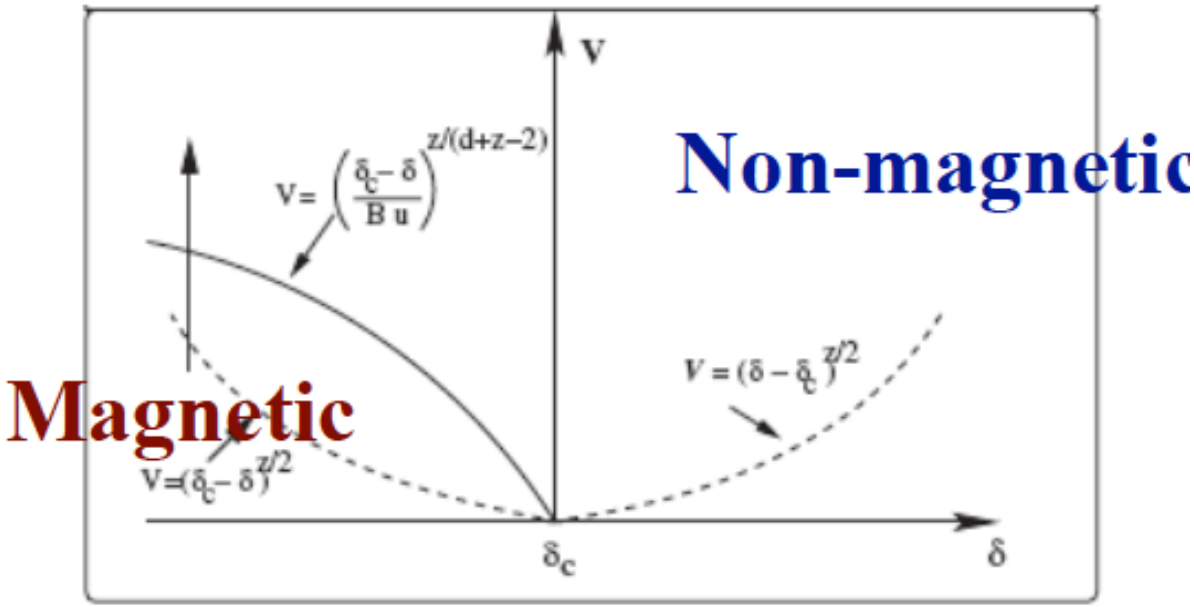
Current-driven quantum criticality nonequilibrium=>temperature without heating relative to reservoir



$$T_{eff} \sim \Delta\mu \coth \frac{\Delta\mu}{T}$$

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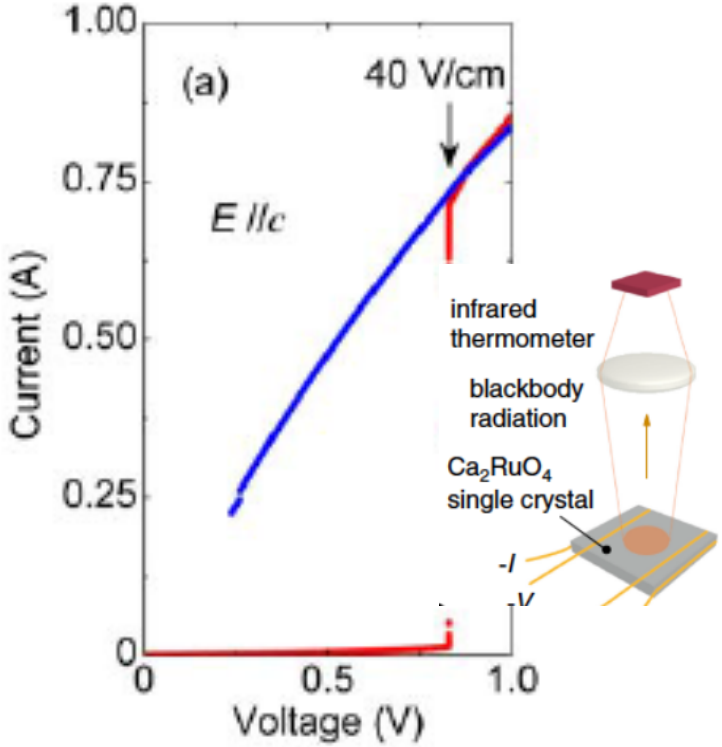
Effective temperature not equal to physical tempeature



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Important question:
how well can we solve impurity models out of equilibrium

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