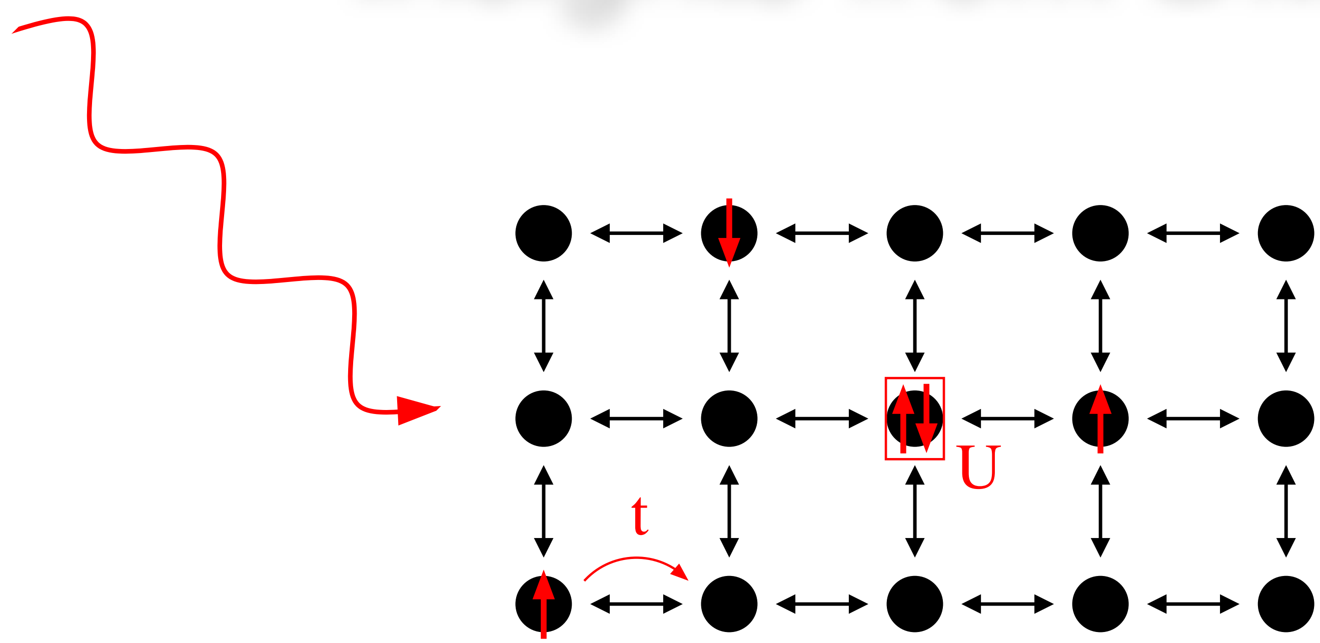
The Hubbard model out of equilibrium
- Insights from DMFT -



Philipp Werner

University of Fribourg, Switzerland

KITP, October 2012

The Hubbard model out of equilibrium
- Insights from DMFT -

In collaboration with:

Naoto Tsuji (Fribourg / Tokyo)

Takashi Oka, Hideo Aoki (Tokyo University)

Martin Eckstein (Hamburg)

KITP, October 2012

Motivation

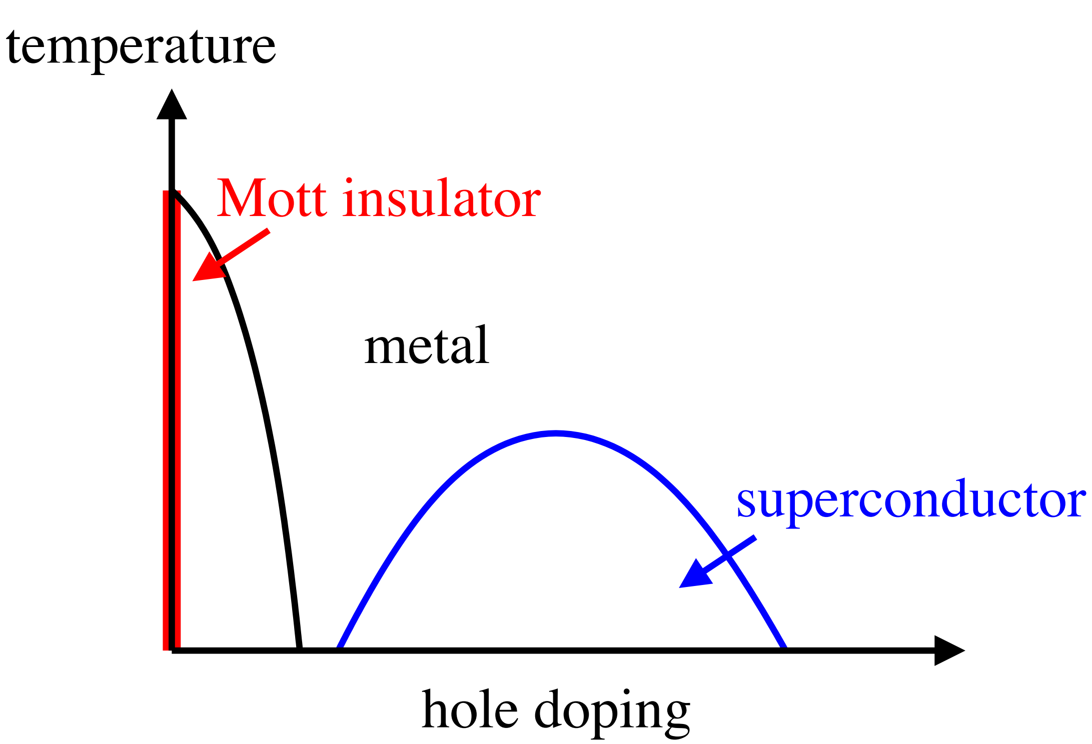
Explore nonequilibrium properties of correlated electron systems

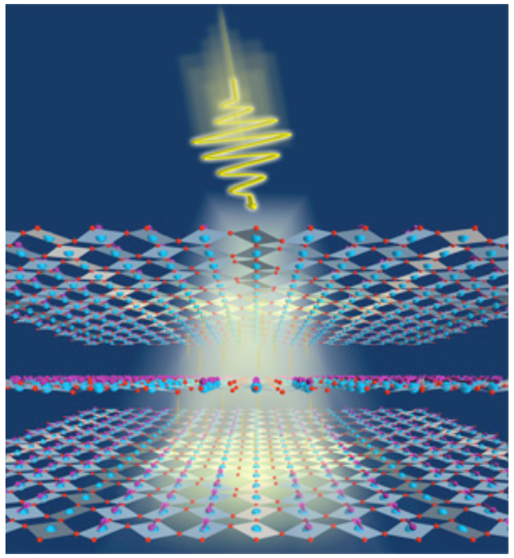
- Tune material properties by external fields

  → e. g. *photo-doping* *S. Iwai et al. (2003), H. Okamoto et al. (2007), ...*

- Create long-lived transient states with novel properties

  → e. g. *light-induced room temperature superconductivity*





D. Fausti et al. (2010)

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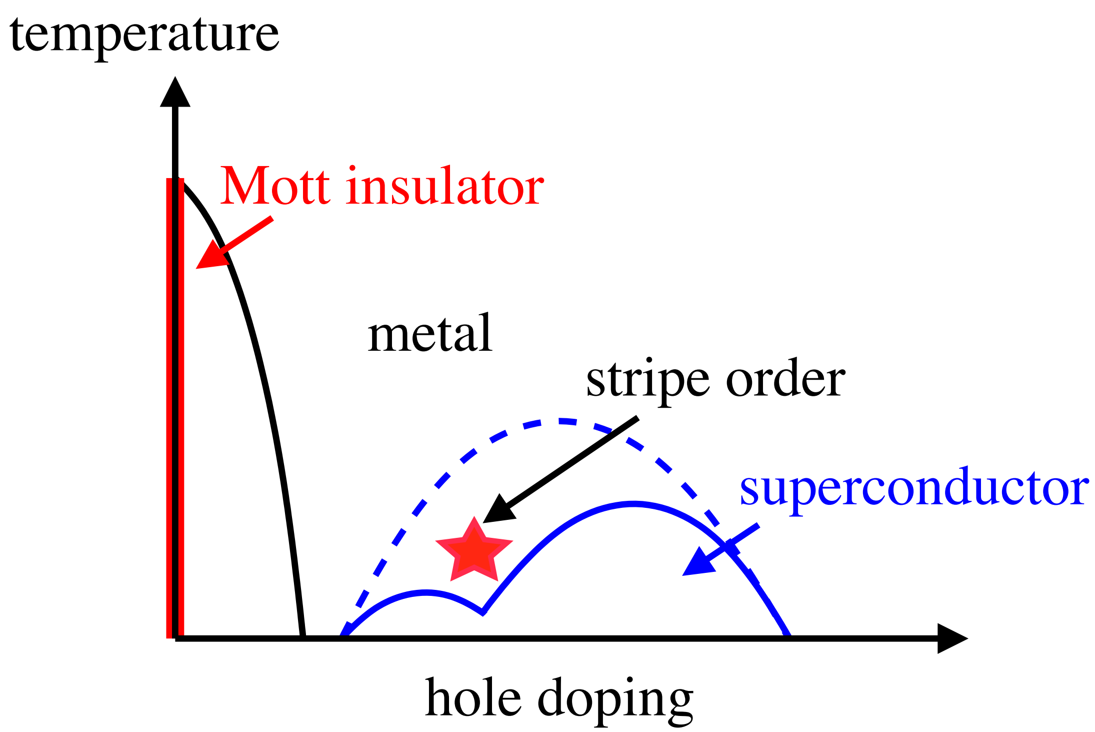

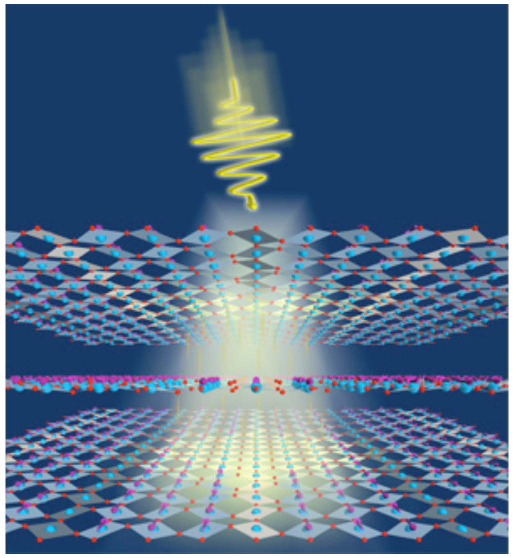

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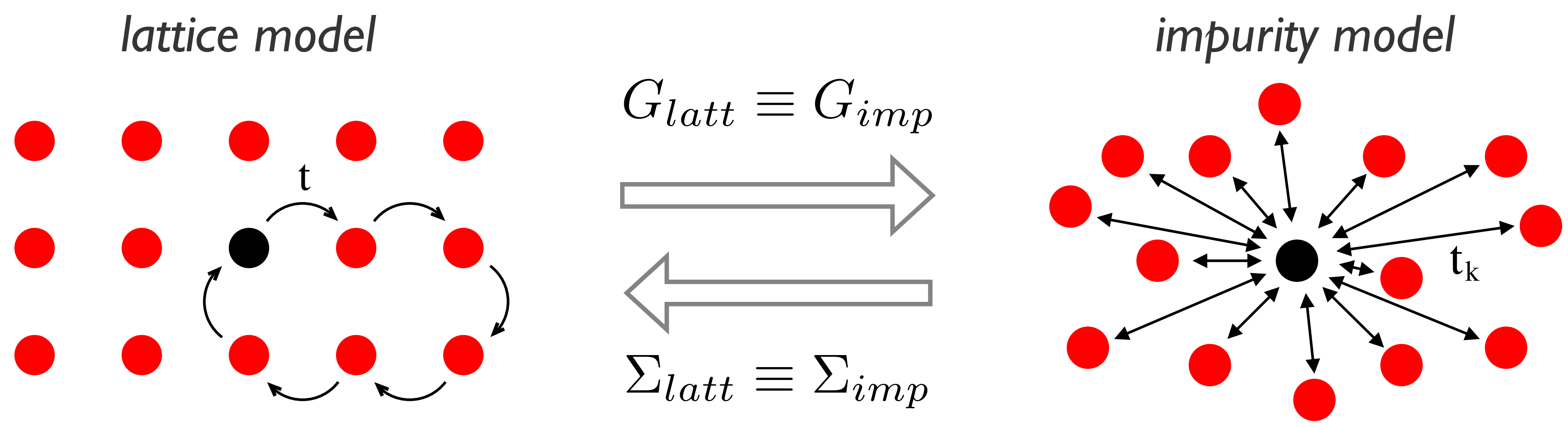
Model and method

- Dynamical mean field theory DMFT: mapping to an impurity problem

  Metzner & Vollhardt (1989); Georges & Kotliar (1992)



- Impurity solver: computes the dynamics on the correlated site

  QMC: Werner et al. (2009), Perturbation theory: Eckstein et al. (2009, 2010)

- Formalism can be extended to nonequilibrium systems

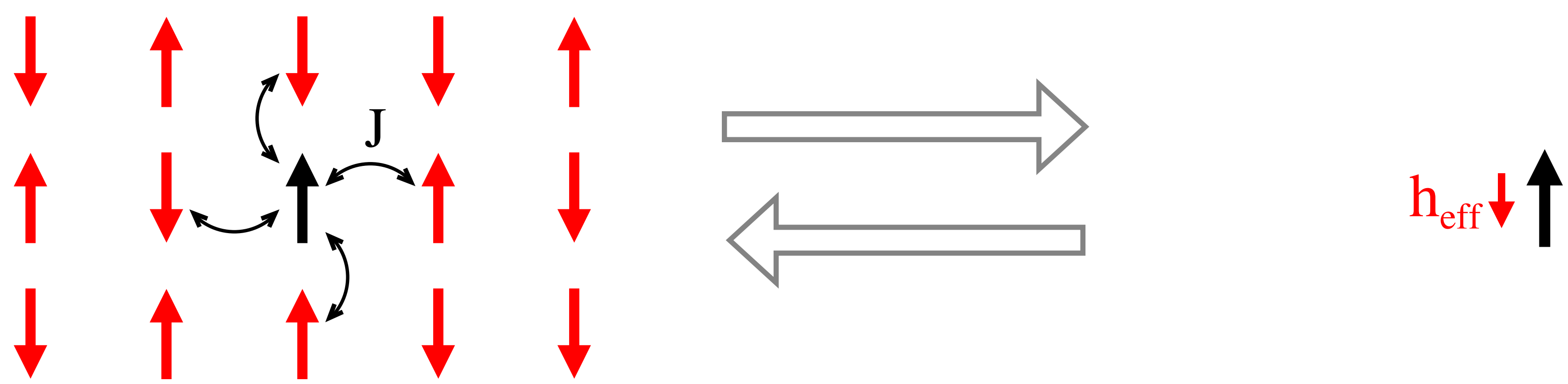
  Schmidt & Monien (2002); Freericks et al. (2006)

Model and method

- Dynamical mean field theory DMFT: mapping to an impurity problem

  Metzner & Vollhardt (1989); Georges & Kotliar (1992)

lattice model $M_{latt} \equiv M_{eff}$ *single-site effective model*



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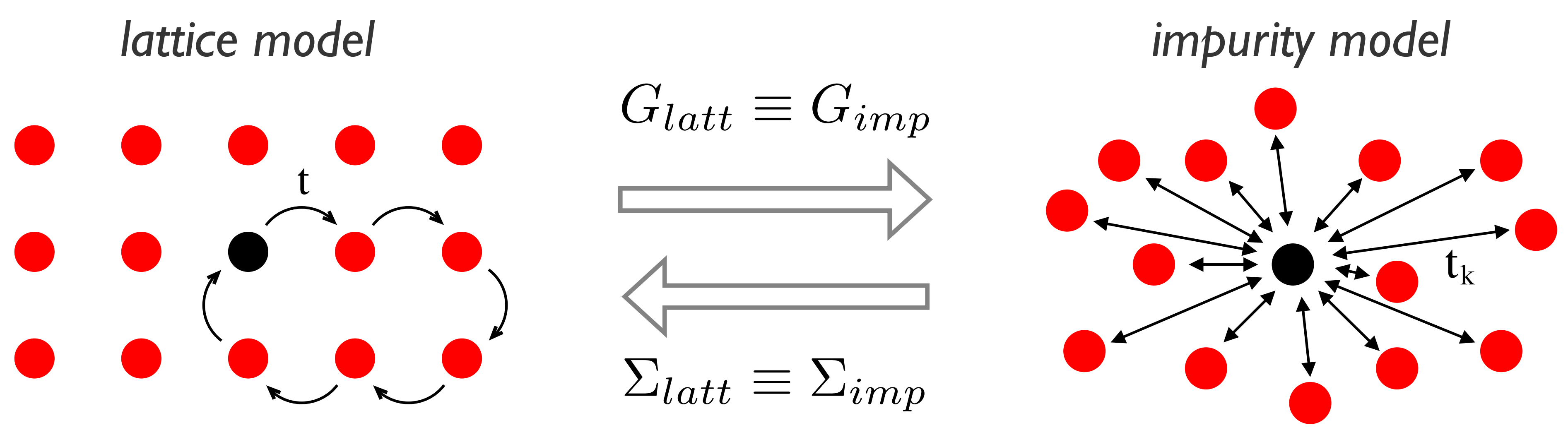

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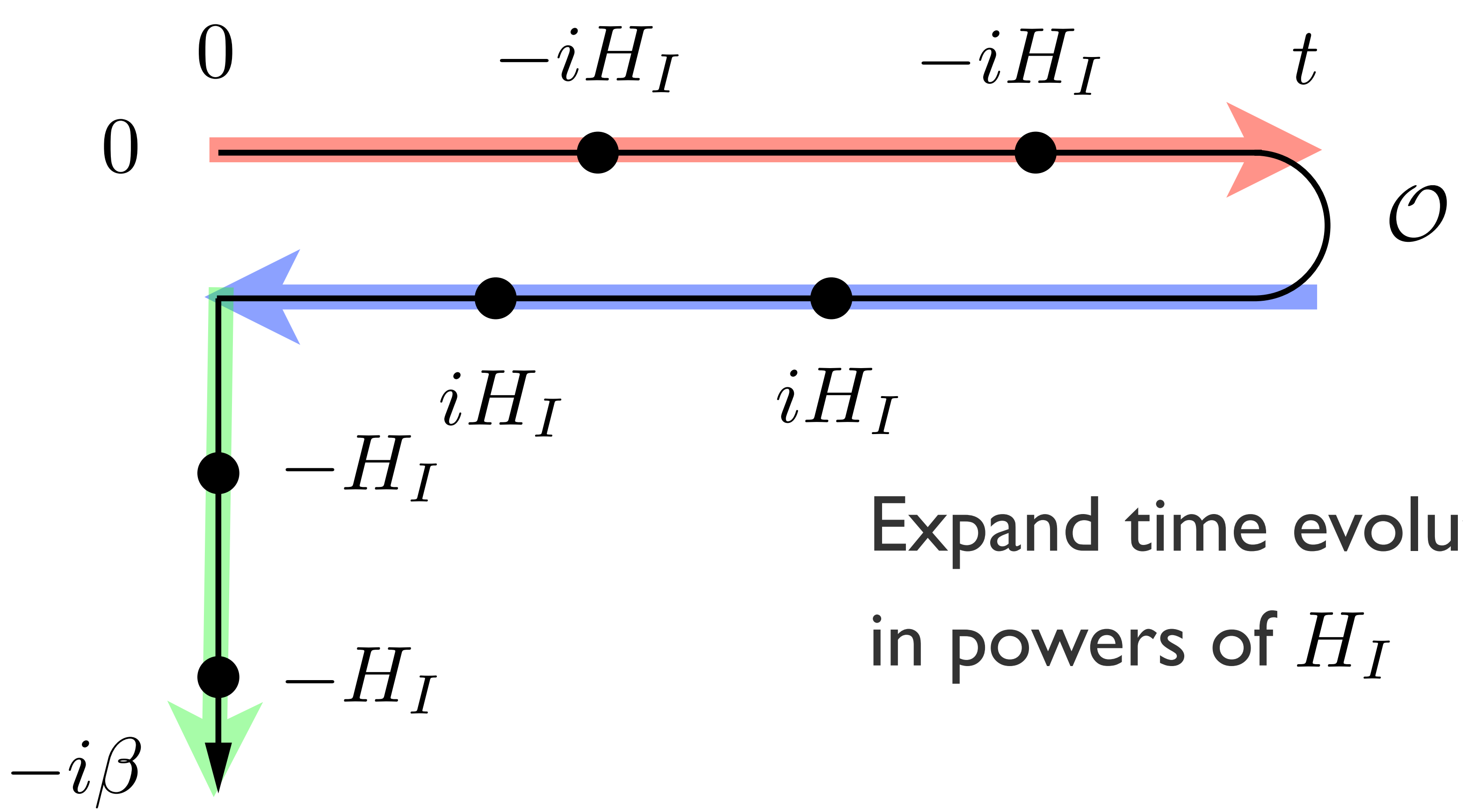
Model and method

Muehlbacher & Rabani (2008)
Werner, Oka & Millis (2009)

- Continuous-time QMC

$$\langle \mathcal{O} \rangle(t) = Tr\left[\frac{1}{Z} e^{-\beta H} U(0,t) \mathcal{O} U(t,0)\right]$$

$$= Tr\left[\frac{1}{Z} e^{-\beta H_0} \left(T_\tau e^{-\int_0^\beta d\tau H_I(\tau)}\right) \left(\tilde{T} e^{i\int_0^t ds H_I(s)}\right) \mathcal{O}(t) \left(T e^{-i\int_0^t ds H_I(s)}\right)\right]$$



Expand time evolution operators in powers of H_I

Model and method

Muehlbacher & Rabani (2008)
Werner, Oka & Millis (2009)

- Continuous-time QMC: weak-coupling formalism

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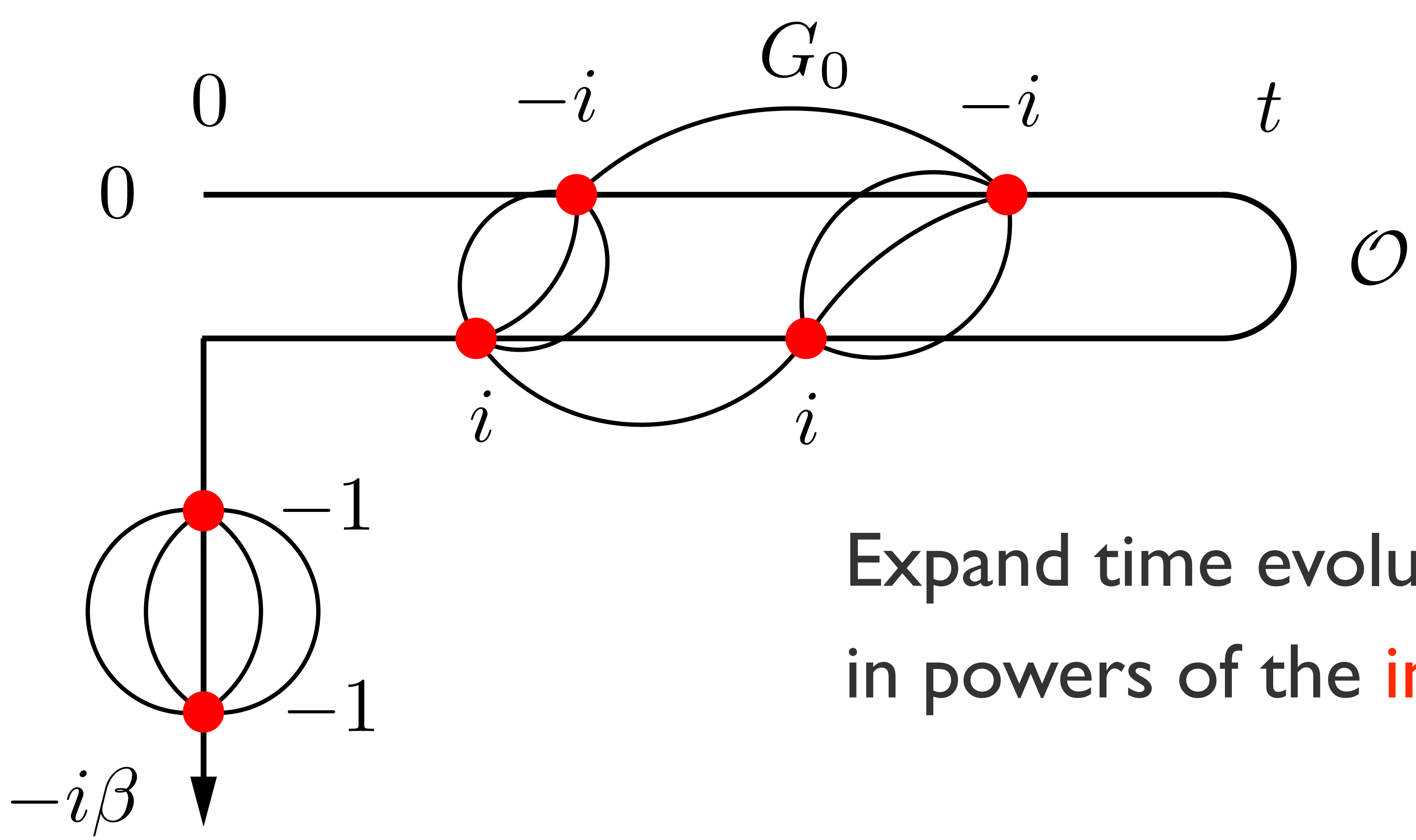
$$= Tr\left[\frac{1}{Z} e^{-\beta H_0} \left(T_\tau e^{-\int_0^\beta d\tau H_I(\tau)}\right) \left(\tilde{T} e^{i\int_0^t ds H_I(s)}\right) \mathcal{O}(t) \left(T e^{-i\int_0^t ds H_I(s)}\right)\right]$$

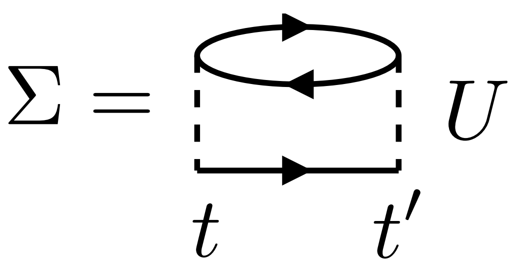


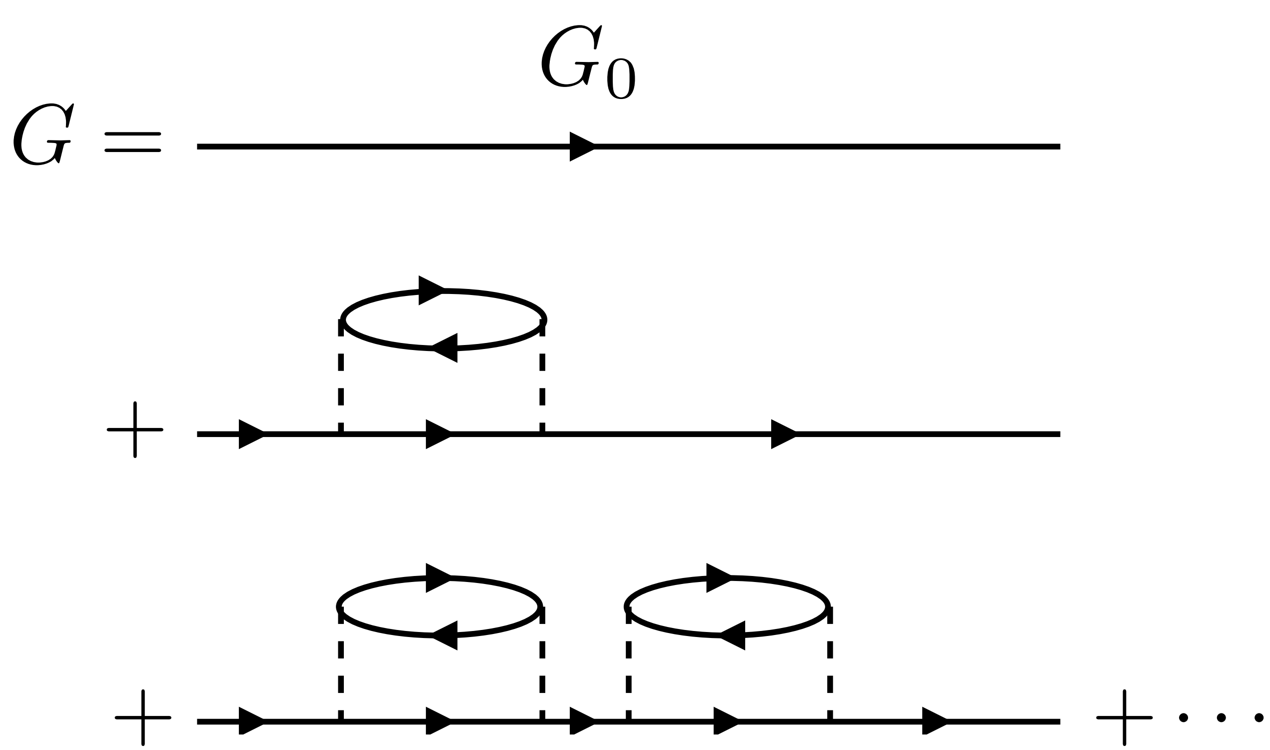
Expand time evolution operators in powers of the interaction term

Model and method

Georges & Kotliar (1992)

- Perturbative weak-coupling formalism: Generate a subset of all weak-coupling diagrams by approximating the self-energy
- Truncation at second order: *Iterated Perturbation Theory (IPT)*



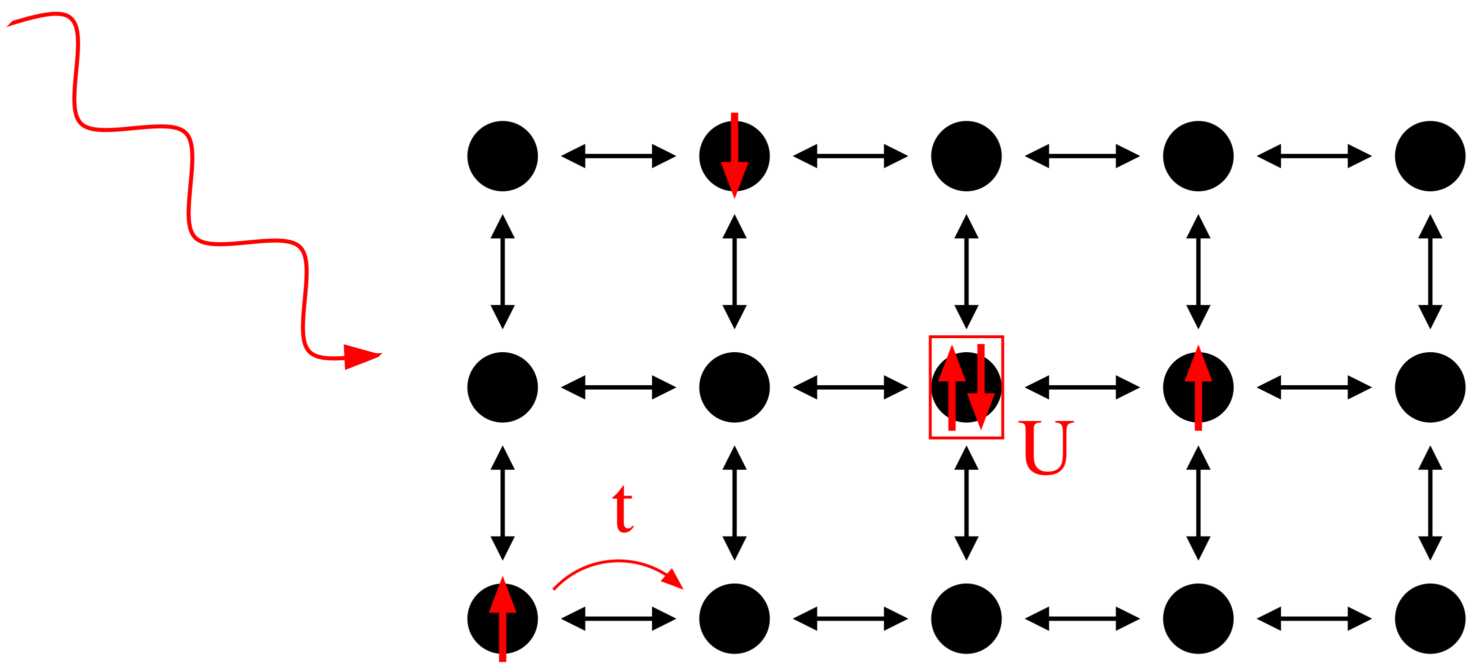


$$G = G_0 + G_0 \star \Sigma \star G$$

Model and method

Freericks & Turkowski (2005)

- Field E(t) in the body diagonal, applied at t=0
- Choose gauge with pure vector potential: $E(t) = -\partial_t A(t)$



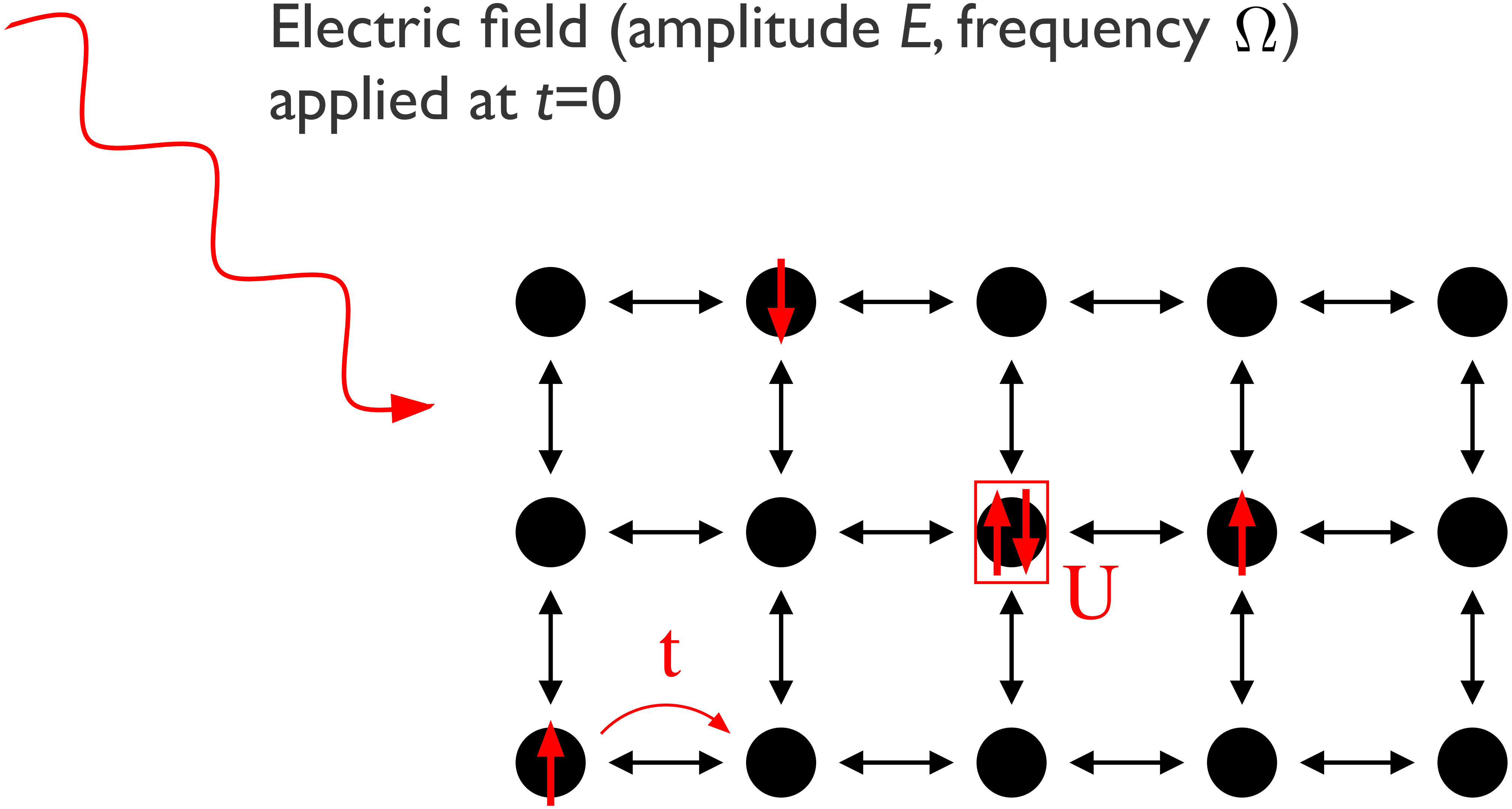
- Peierls substitution: $\varepsilon(k) \to \varepsilon(k - eA(t))$
- Lattice: hybercubic, infinite-d limit $\rho(\varepsilon) = \frac{1}{\sqrt{\pi}W}\exp(-\varepsilon^2/W^2)$

Periodic fields

Tsuji, Oka, Werner & Aoki (2011)

- AC-field quench in the Hubbard model

Electric field (amplitude E, frequency Ω)
applied at t=0



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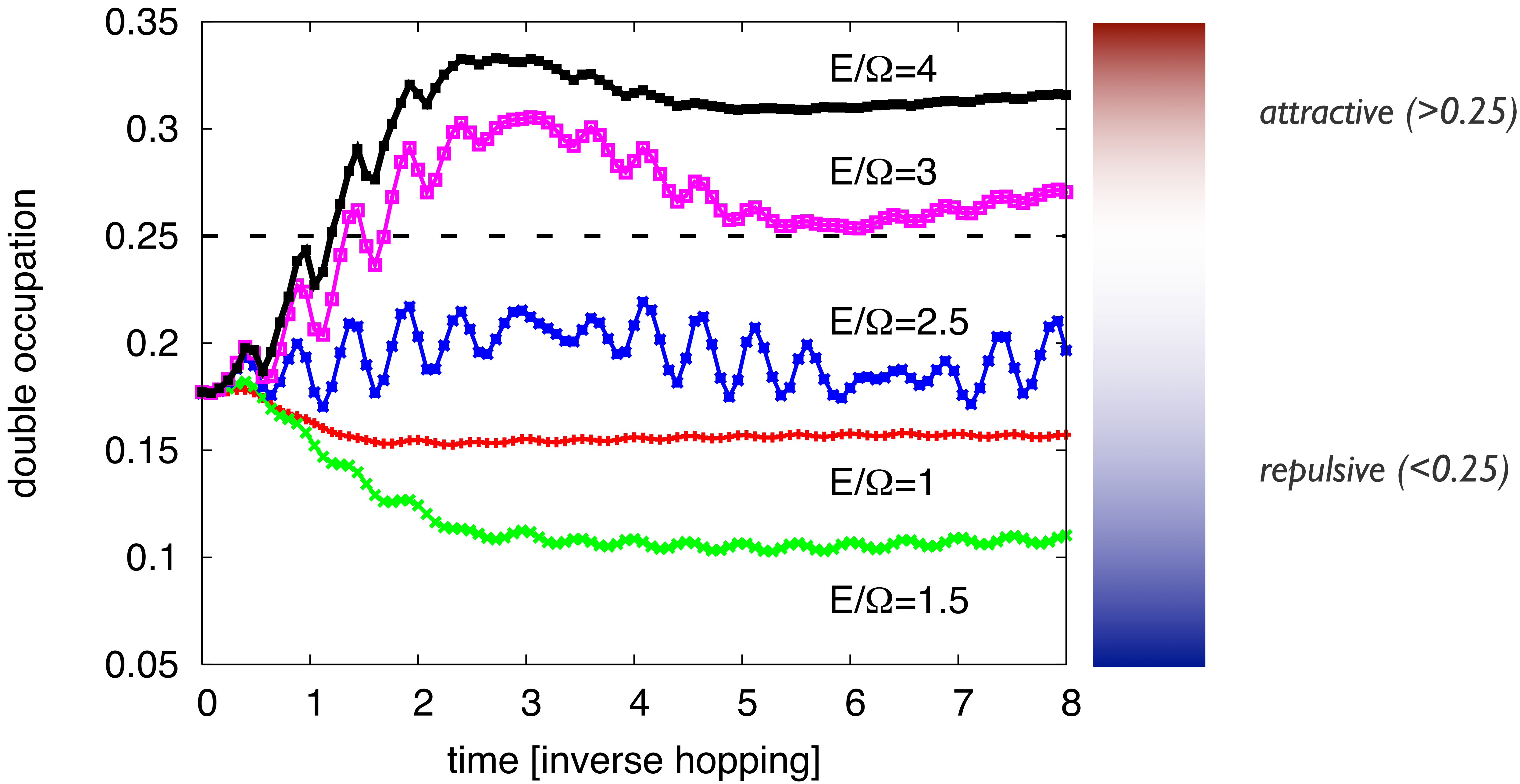
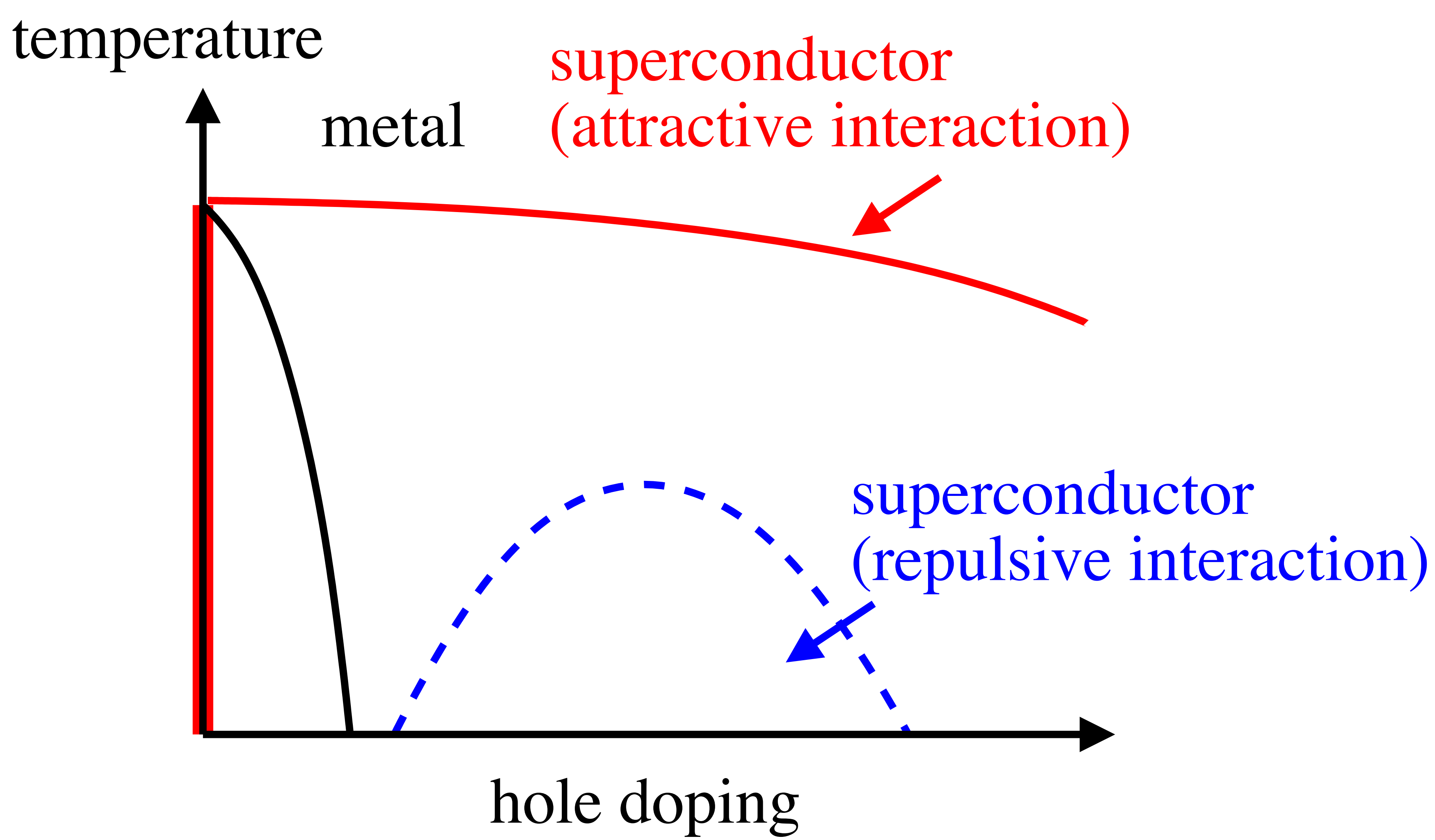


Periodic fields

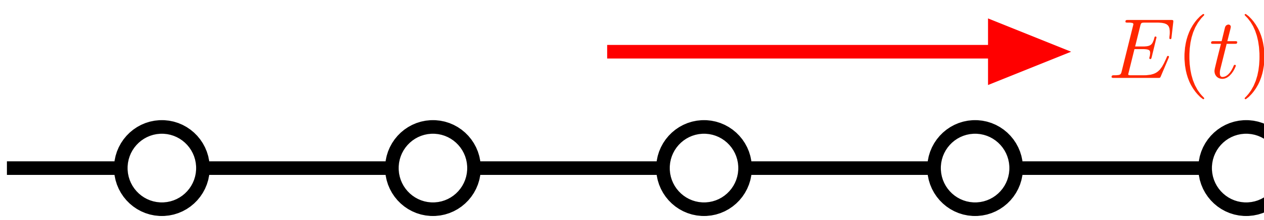
Tsuji, Oka, Werner & Aoki (2011)

- AC-field quench in the Hubbard model
  - Sign inversion of the interaction: repulsive ↔ attractive
  - *Dynamically generated* high-Tc superconductivity?



Origin of the attractive interaction

- Periodic E-field leads to a population inversion



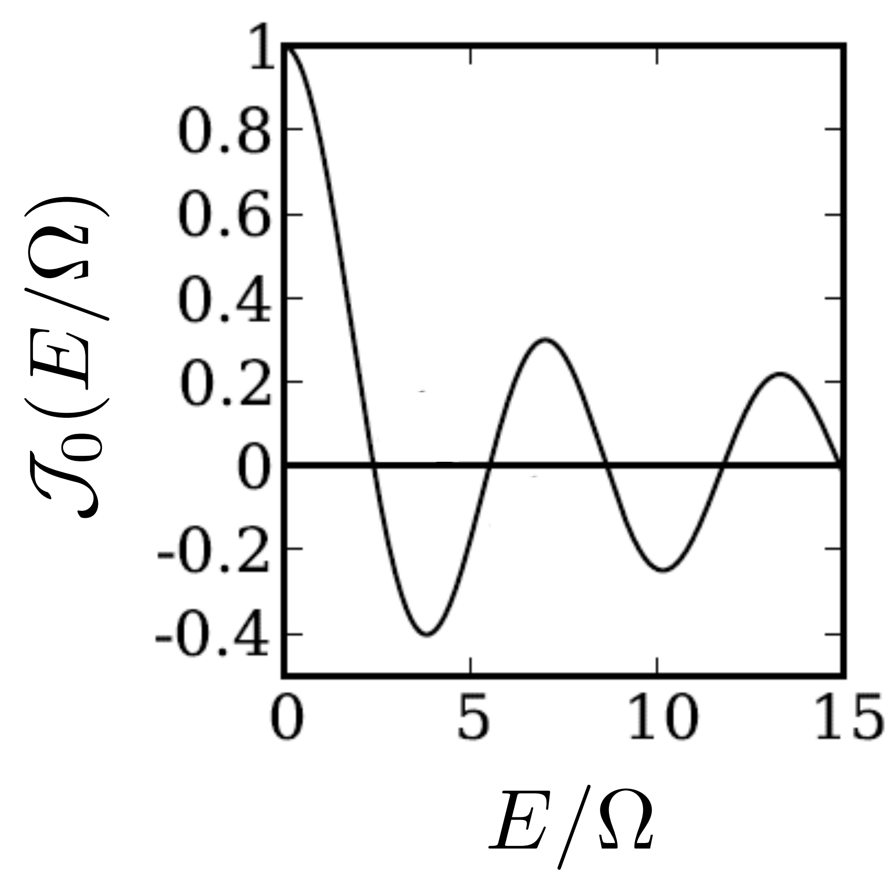
- Gauge with pure vector potential

$$E(t) = E\cos(\Omega t) = -\partial_t A(t)$$
$$\Rightarrow A(t) = -(E/\Omega)\sin(\Omega t)$$

- Peierls substitution $\epsilon_k \longrightarrow \epsilon_{k-A(t)}$

- Renormalized dispersion

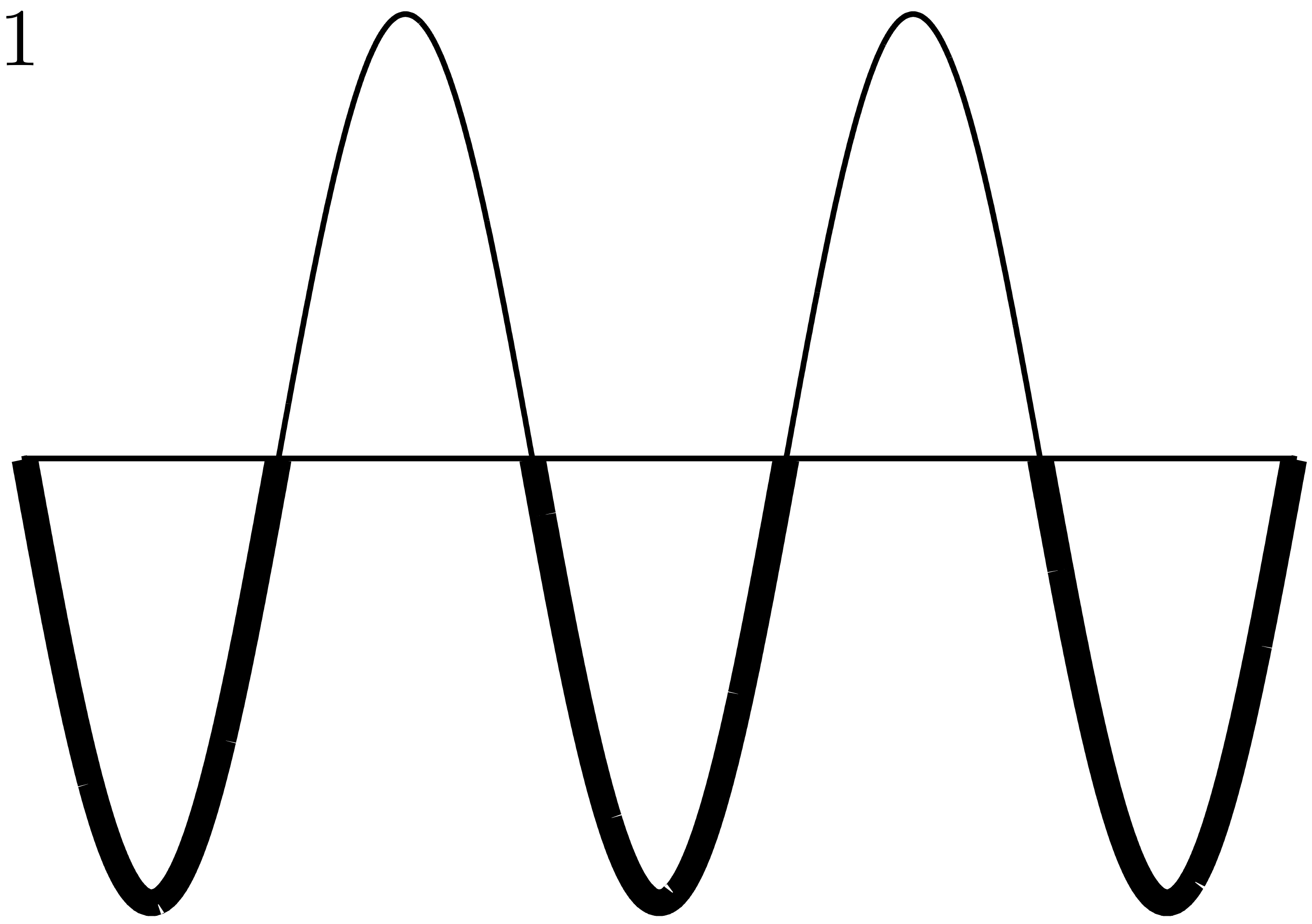
$$\overline{\epsilon_k} = \frac{\Omega}{2\pi}\int_0^{2\pi/\Omega} dt\,\epsilon_{k-A(t)} = \mathcal{J}_0(E/\Omega)\epsilon_k$$



Origin of the attractive interaction

- Periodic E-field leads to a population inversion

$\mathcal{J}_0(E/\Omega) = 1$



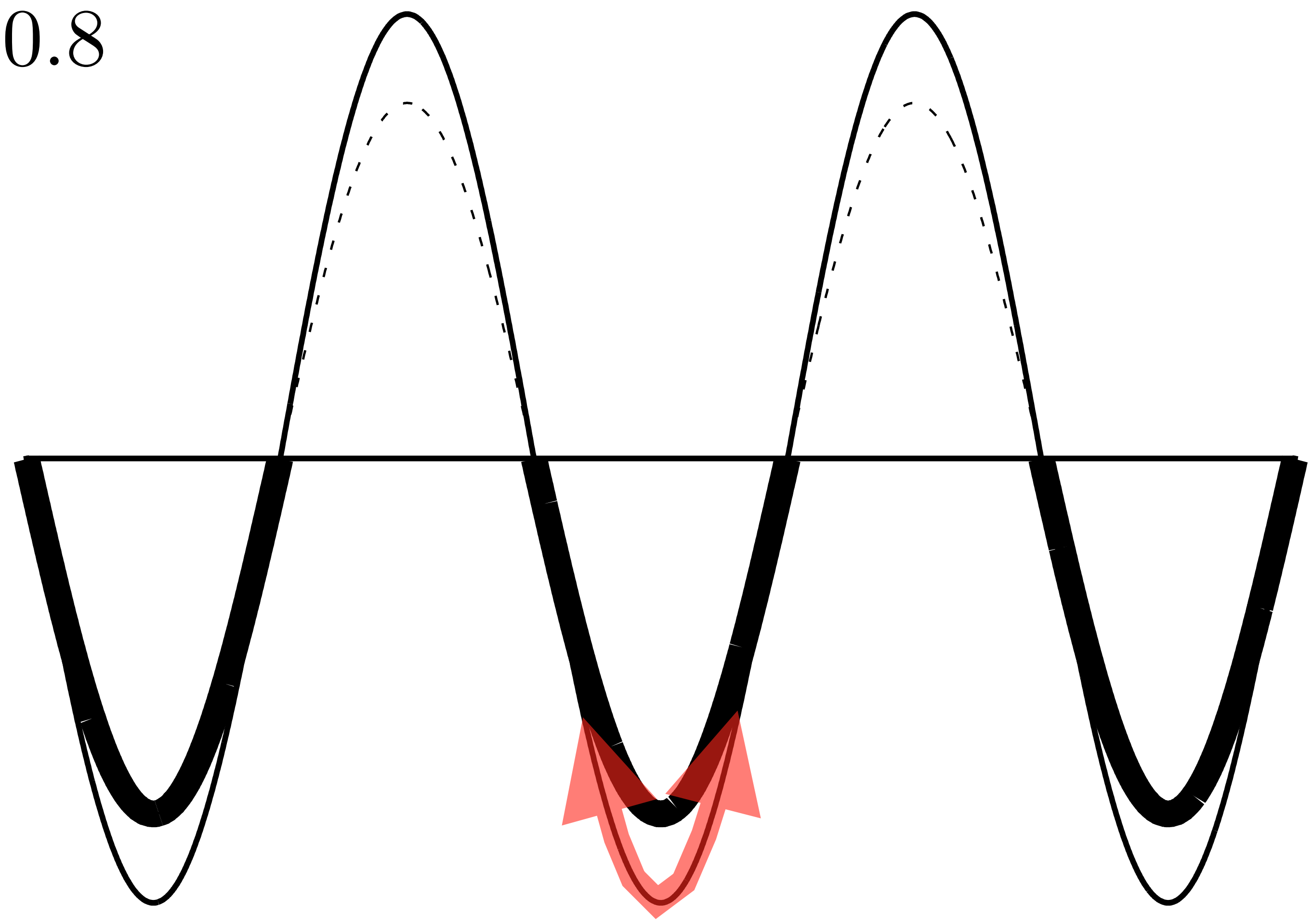
- Renormalized dispersion

$$\overline{\epsilon_k} = \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} dt \epsilon_{k-A(t)} = \mathcal{J}_0(E/\Omega) \epsilon_k$$

Origin of the attractive interaction

- Periodic E-field leads to a population inversion

$\mathcal{J}_0(E/\Omega) = 0.8$



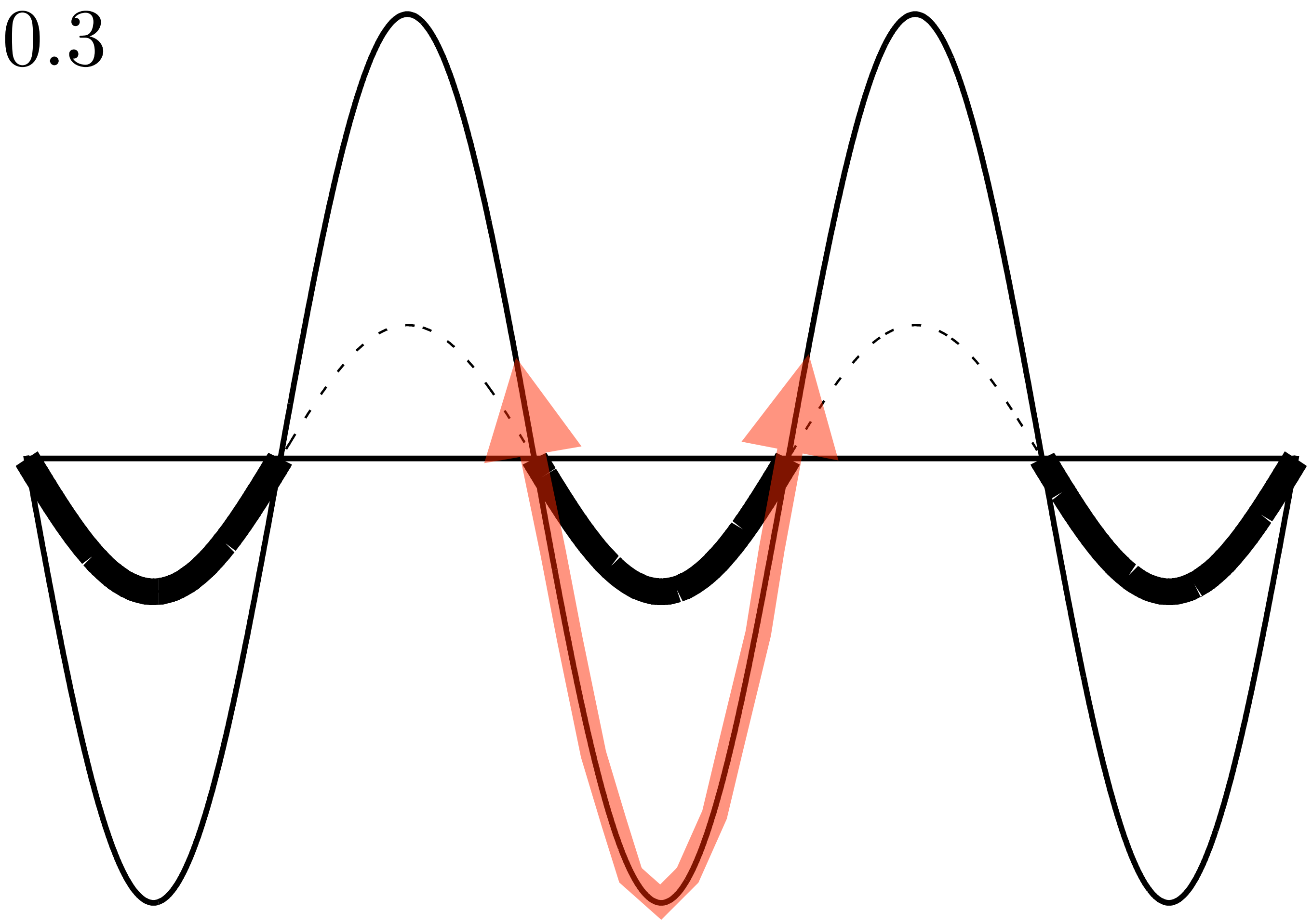
- Renormalized dispersion

$$\overline{\epsilon_k} = \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} dt \epsilon_{k-A(t)} = \mathcal{J}_0(E/\Omega)\epsilon_k$$

Origin of the attractive interaction

- Periodic E-field leads to a population inversion

$\mathcal{J}_0(E/\Omega) = 0.3$



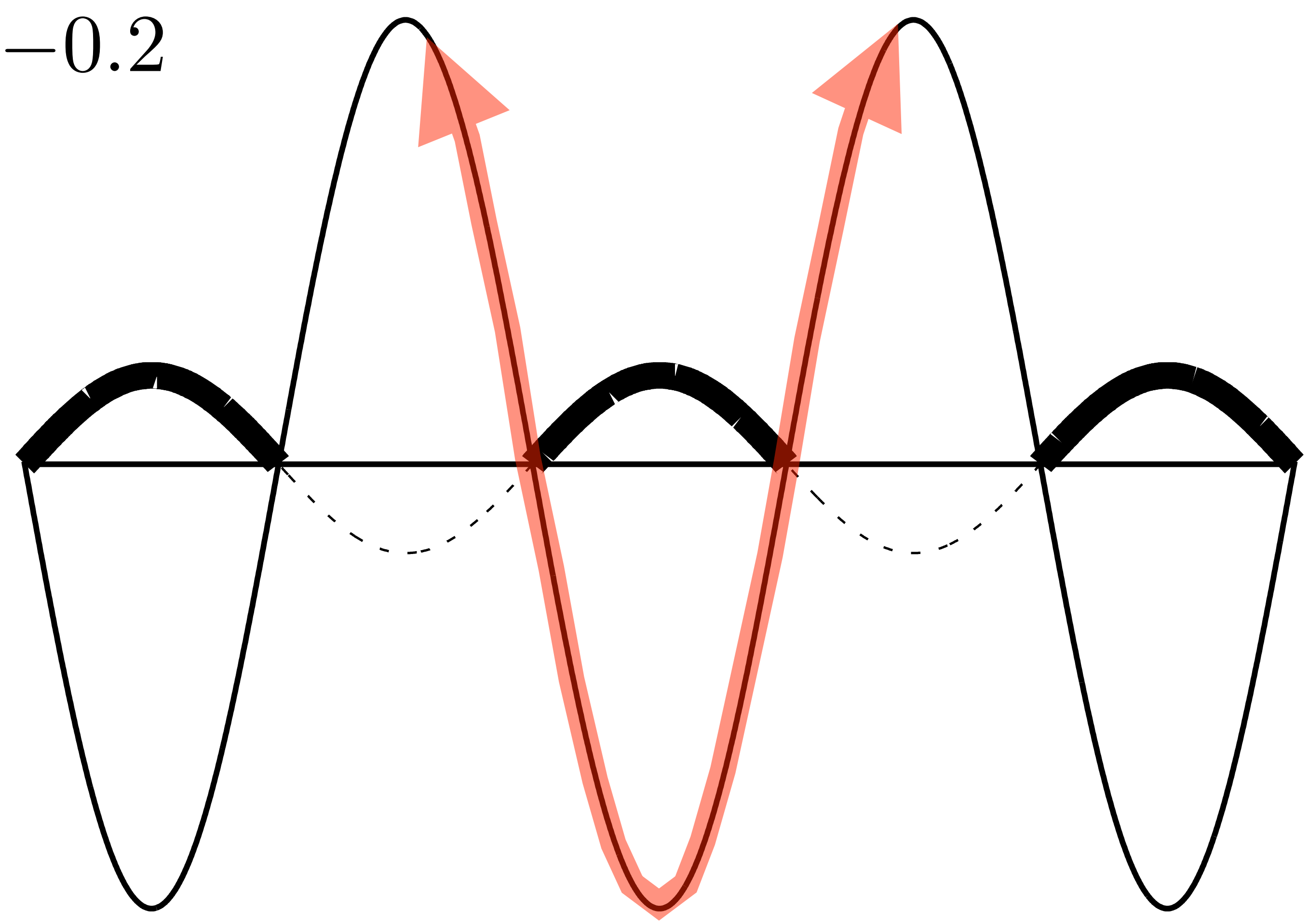
- Renormalized dispersion

$$\overline{\epsilon_k} = \frac{\Omega}{2\pi}\int_0^{2\pi/\Omega} dt \epsilon_{k-A(t)} = \mathcal{J}_0(E/\Omega)\epsilon_k$$

Origin of the attractive interaction

- Periodic E-field leads to a population inversion

$\mathcal{J}_0(E/\Omega) = -0.2$



- Renormalized dispersion

$$\overline{\epsilon_k} = \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} dt \epsilon_{k-A(t)} = \mathcal{J}_0(E/\Omega)\epsilon_k$$

Origin of the attractive interaction

- Inverted population = negative temperature

- State with $U > 0, T < 0$ is equivalent to state with $U < 0, T > 0$

$$\tilde{T} < 0, \mathcal{J}_0 < 0 \qquad \rho \propto \exp\left(-\frac{1}{\tilde{T}}\left[\sum_{k\sigma} \mathcal{J}_0 \epsilon_k n_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}\right]\right)$$

$$T_{\text{eff}} = \frac{\tilde{T}}{\mathcal{J}_0} > 0 \qquad = \exp\left(-\frac{1}{T_{\text{eff}}}\left[\sum_{k\sigma} \epsilon_k n_{k\sigma} + \frac{U}{\mathcal{J}_0} \sum_i n_{i\uparrow} n_{i\downarrow}\right]\right)$$

- Effective interaction of the $T_{\text{eff}} > 0$ state

$$U_{\text{eff}} = \frac{U}{\mathcal{J}_0(E/\Omega)}$$

Summary I

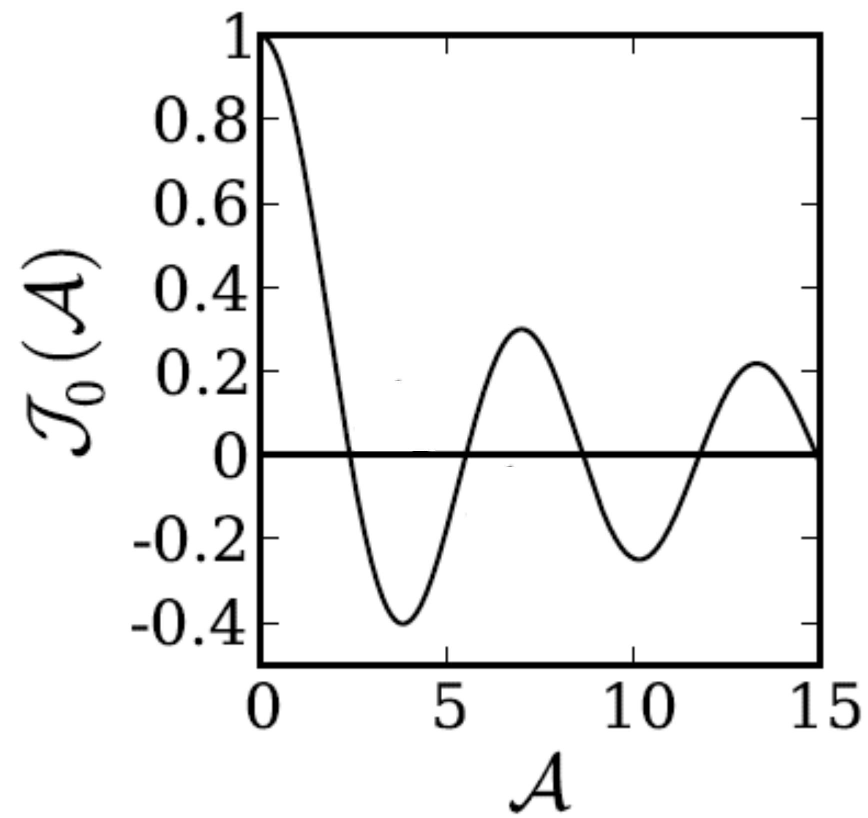
Tsuji, Oka, Werner & Aoki (2011)

- Controlling the Coulomb interaction by ac fields

- Advantages
  - Interaction continuously tunable

$$U_{\mathrm{eff}} = \frac{U}{\mathcal{J}_0(E/\Omega)}$$

  - Reversible

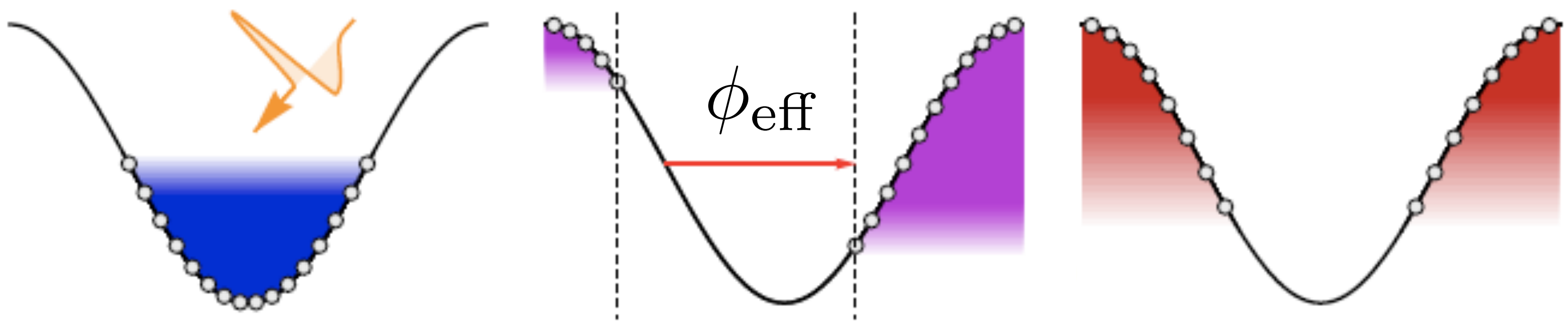


- Disadvantages
  - Need high frequency ac field (interband transitions?)
  - Effect lasts only during irradiation
  - Strong heating effect

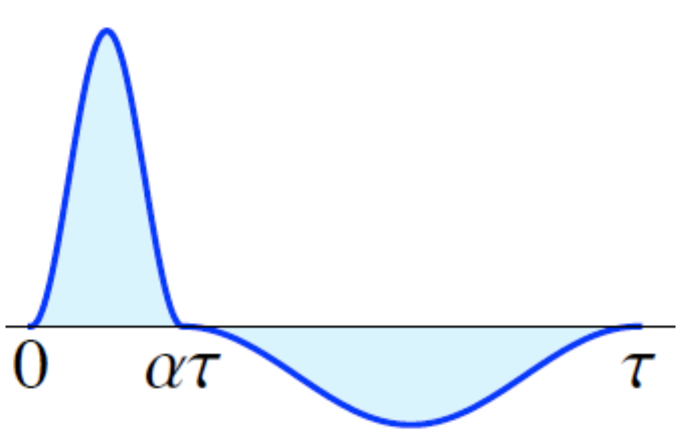
Pulsed field

Tsuji, Oka, Aoki & Werner (2012)

- Shift the population using an asymmetric mono-cycle pulse



- Consider a physical pulse with $\phi = \int E(t)dt = 0$
- Interacting electrons: $\phi_{\rm eff} \neq \phi$ (depends sensitively on pulse-shape)
- By combining fast and slow half-cycle pulses can achieve $\phi = 0, \quad \phi_{\rm eff} \approx \pi$



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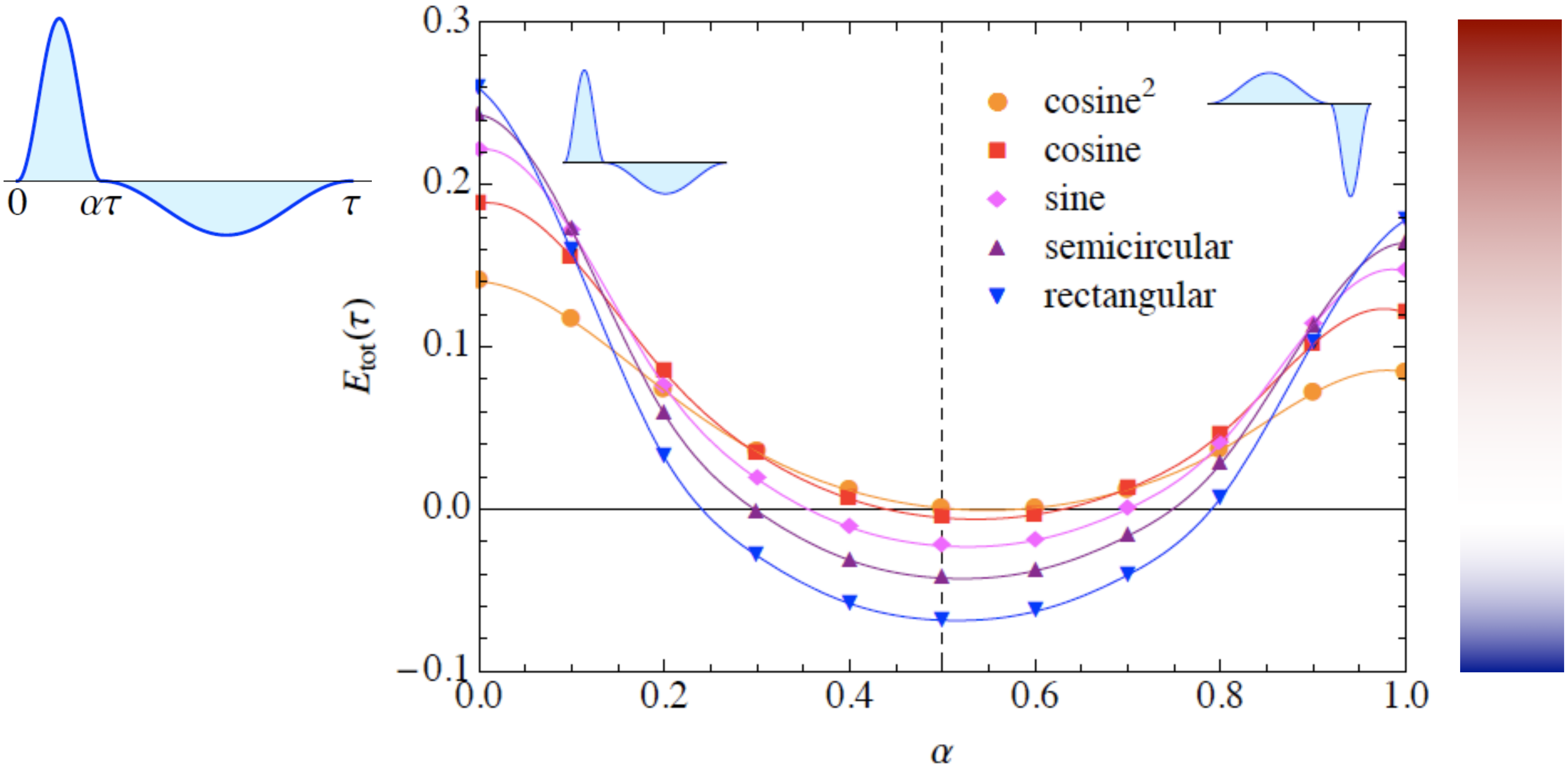

pulse asymmetry

Pulsed field

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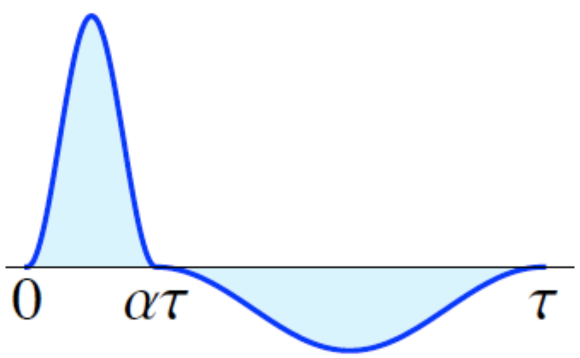
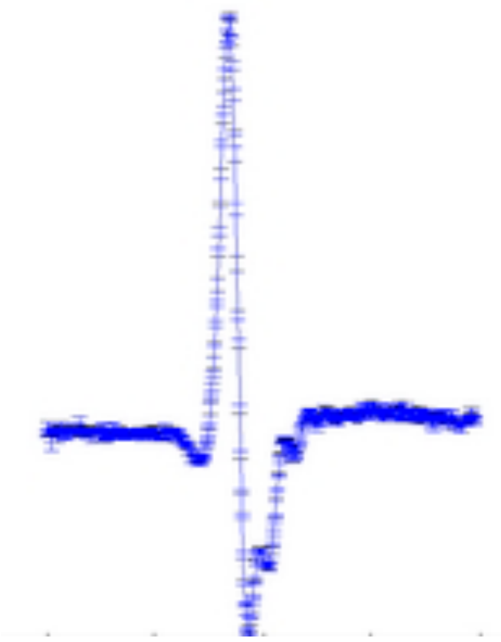
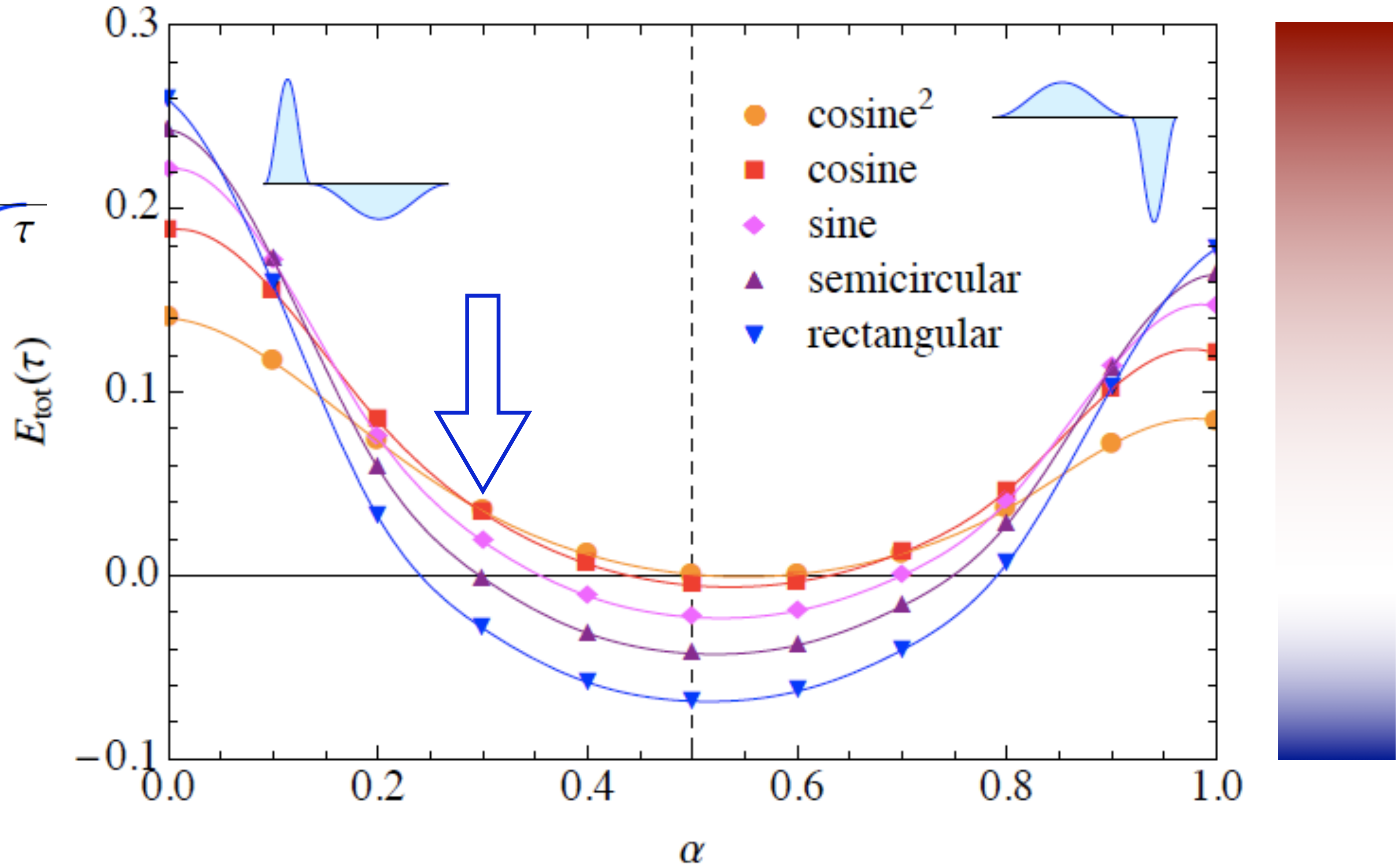




example of a realistic pulse
Christoph Hauri (PSI)

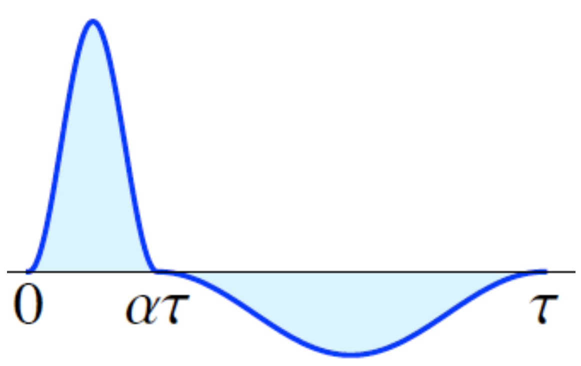


pulse asymmetry

Pulsed field

Tsuji, Oka, Aoki & Werner (2012)

- Shift the population using an asymmetric mono-cycle pulse
- Desired material properties:
  - Metallic system with weak to moderate correlations
  - Single band crossing the Fermi level
  - Large gaps to other bands
- Desired properties of the field pulse:
  - ~10 fs monocycle pulse
  - peak asymmetry ~7:3
  - field strength $10^8 - 10^9$ V/m
- Proposed measurements:
  - Time-resolved ARPES
  - (negative) optical conductivity

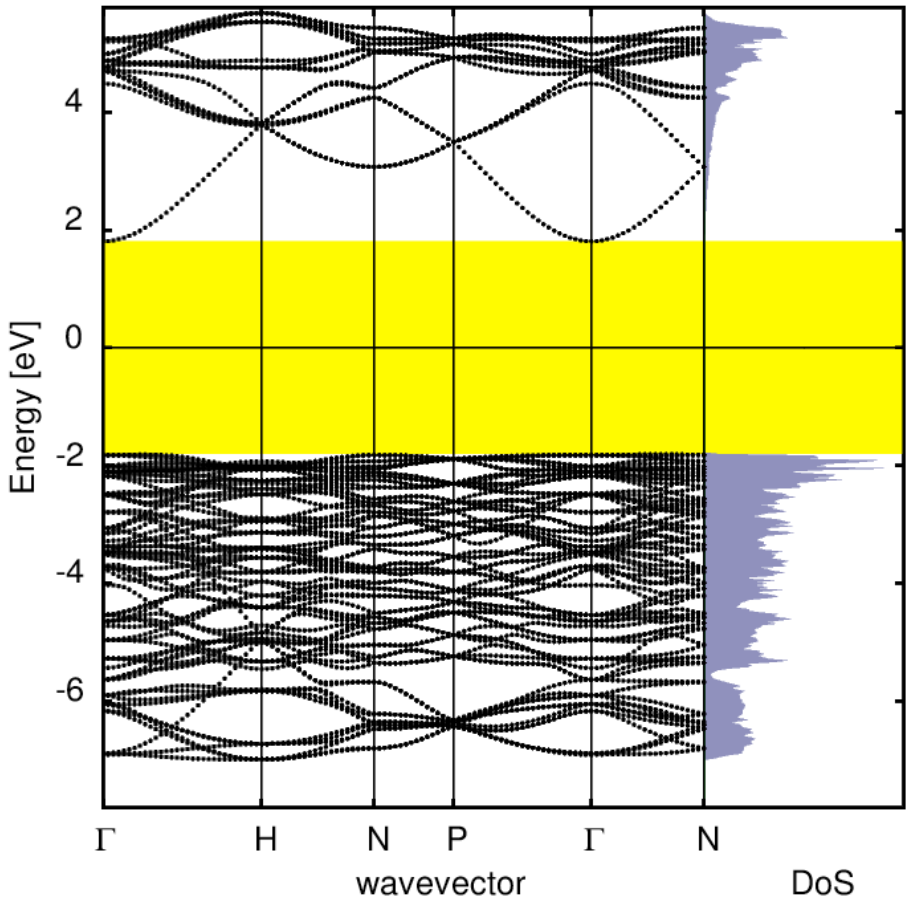


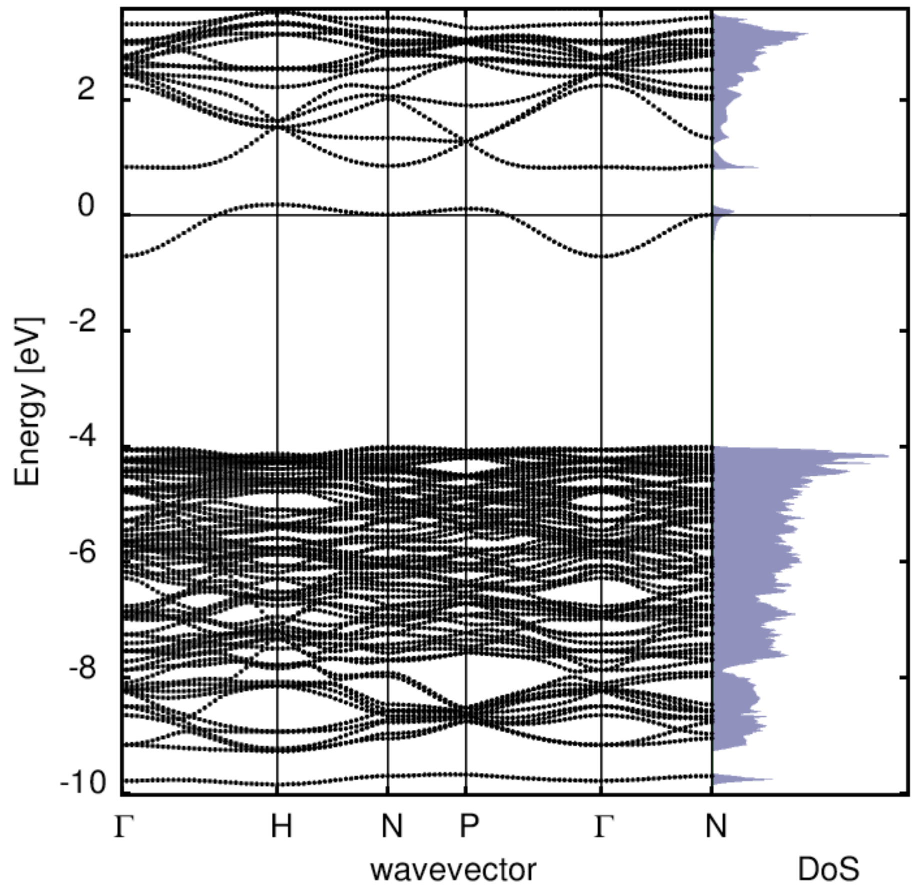
Pulsed field

Tsuji, Oka, Aoki & Werner (2012)

- Shift the population using an asymmetric mono-cycle pulse

- Potentially interesting material: *Sn* doped In_2O_3
  - Transparent conductor
  - Single *s*-band crossing the Fermi level   *band structure by Bernard Delley (PSI)*



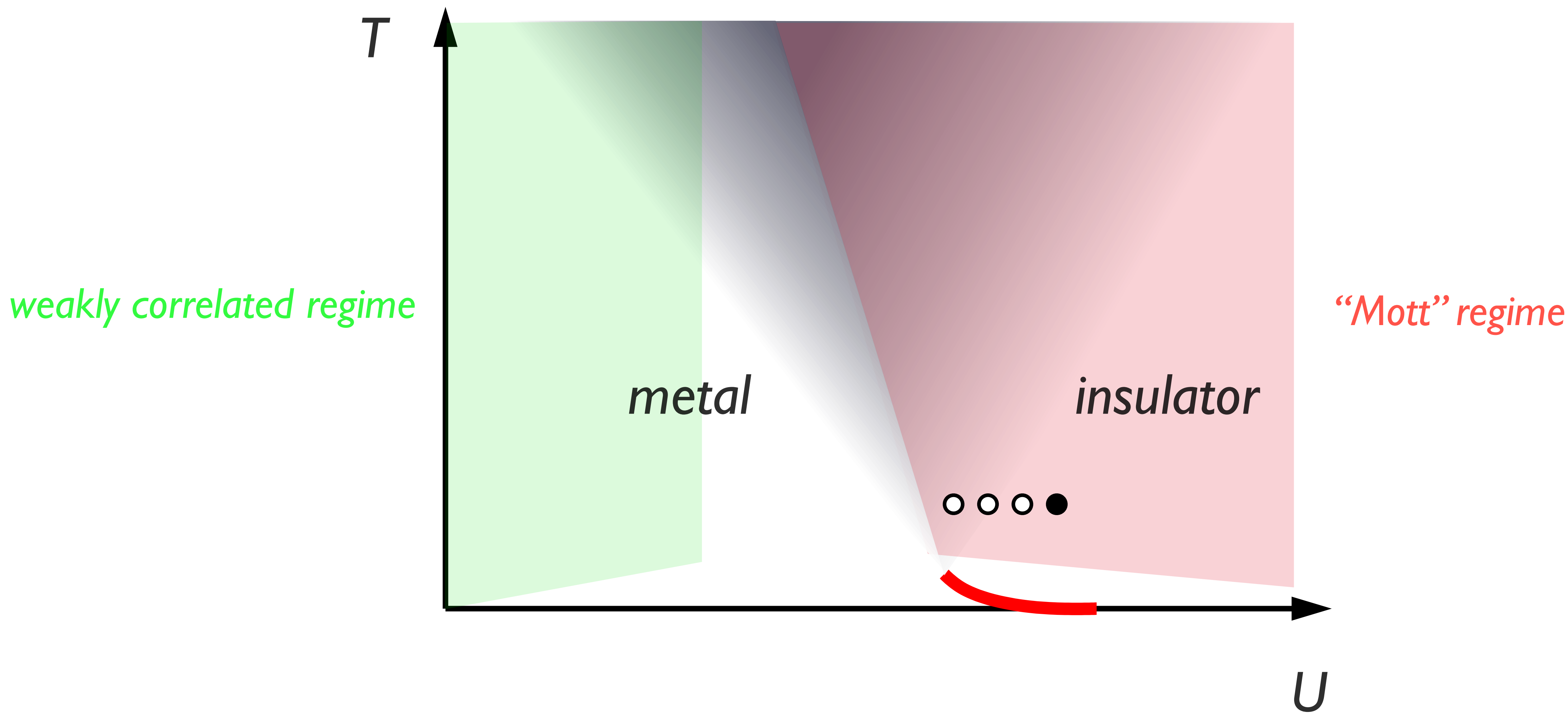


Pulse excited Mott insulator

- "Photo-excitation" of carriers across the Mott gap

  Eckstein & Werner (2011)

- Question: How quickly does the electronic system thermalize?



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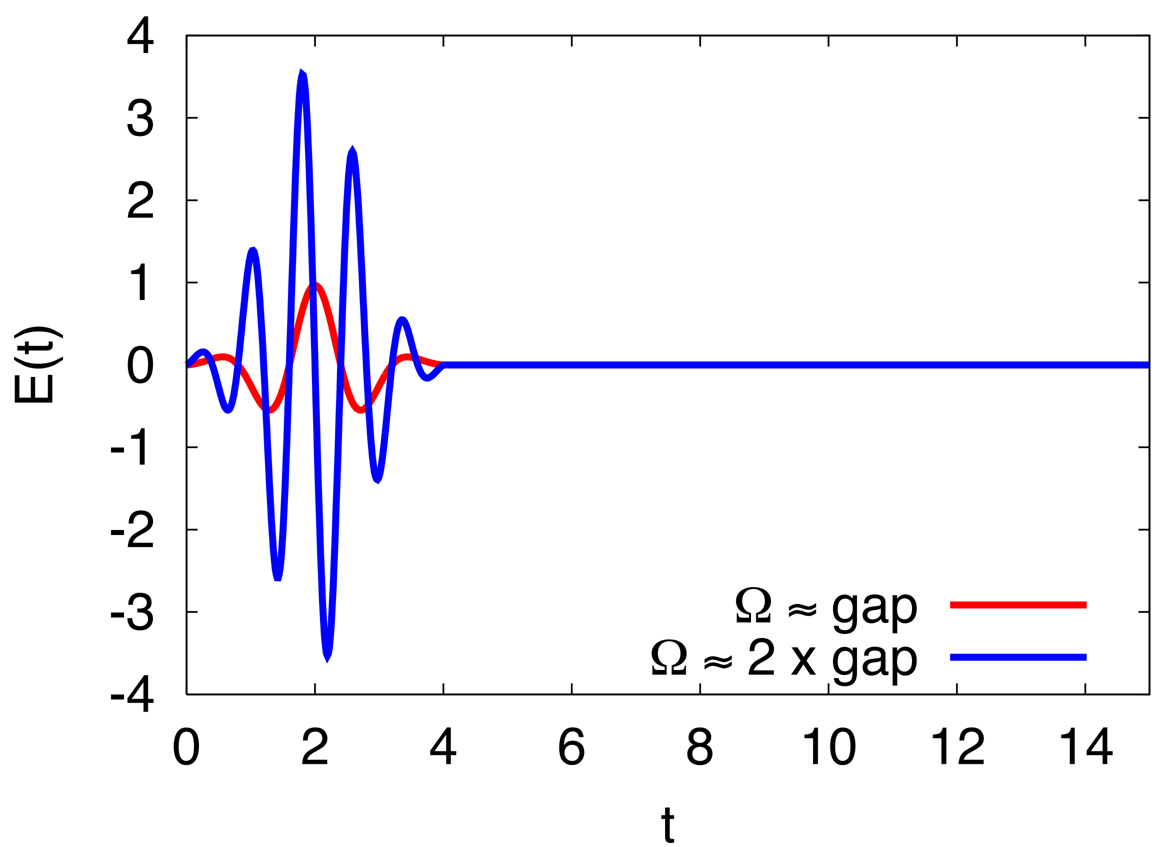
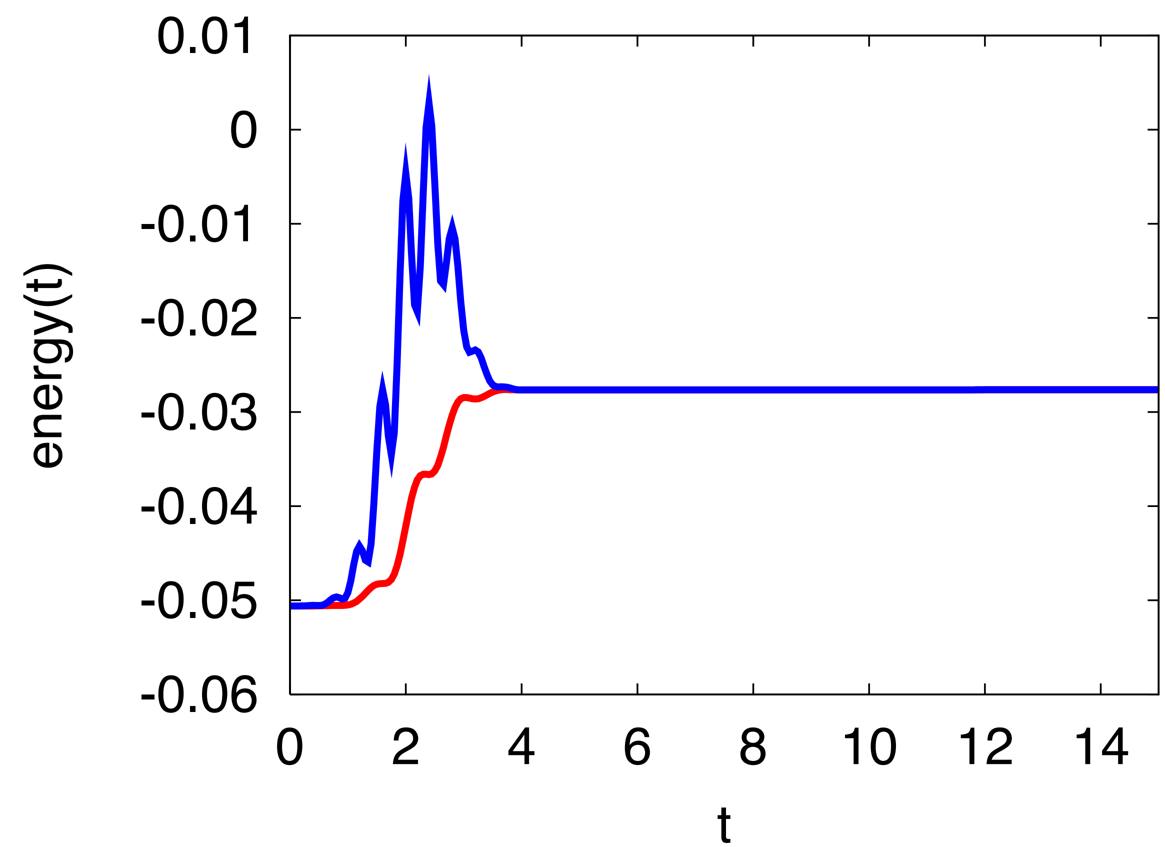
pulse form



total energy → T_{eff}



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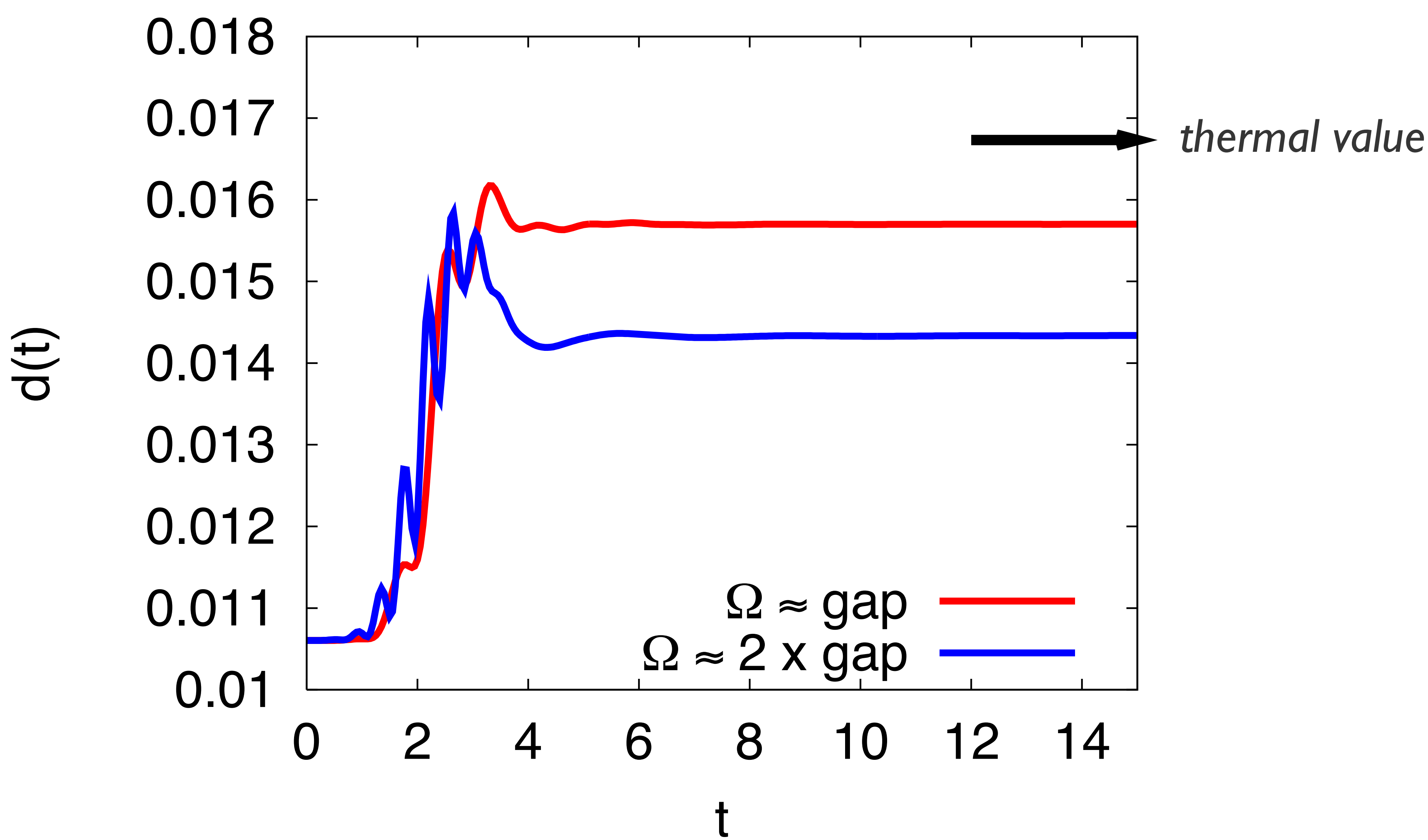

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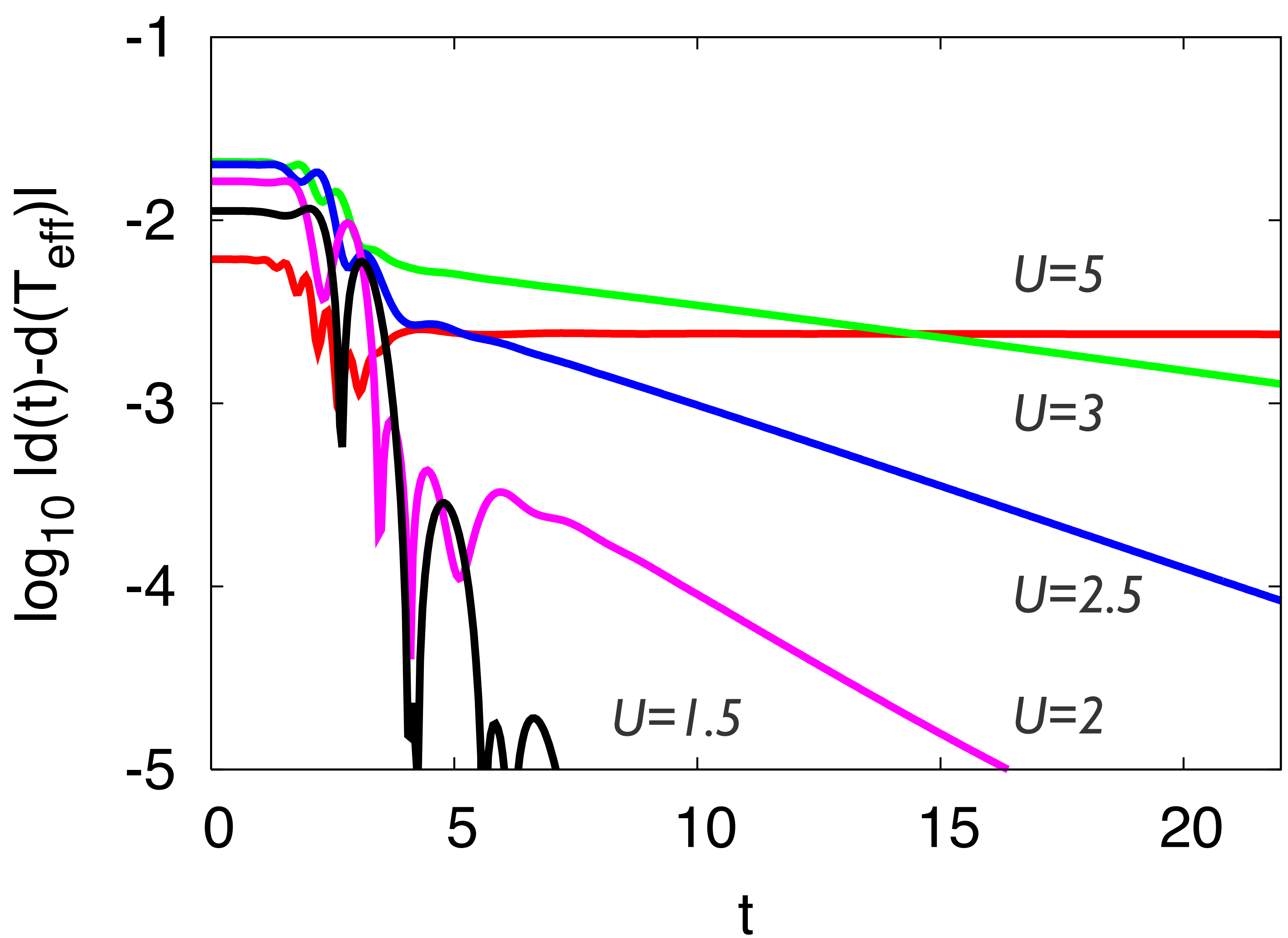

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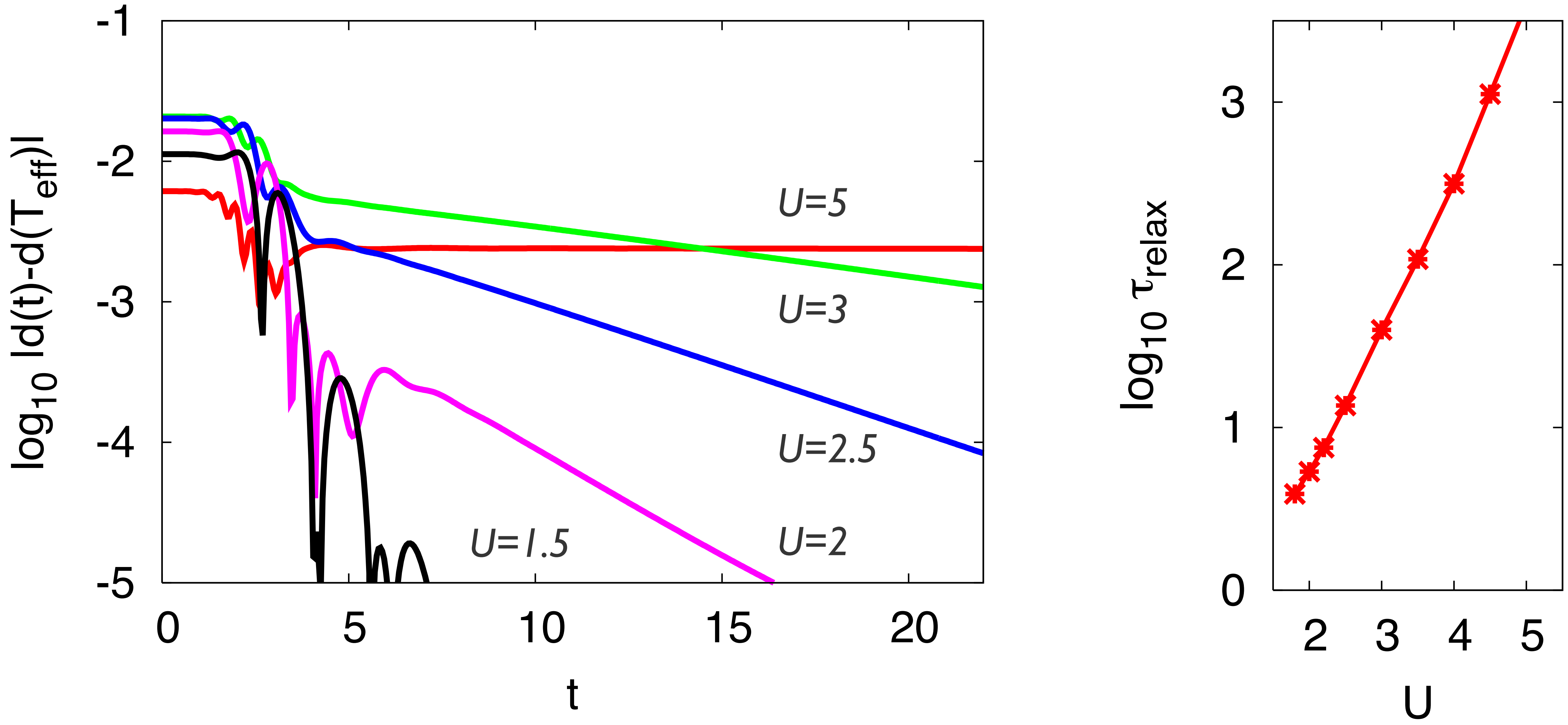

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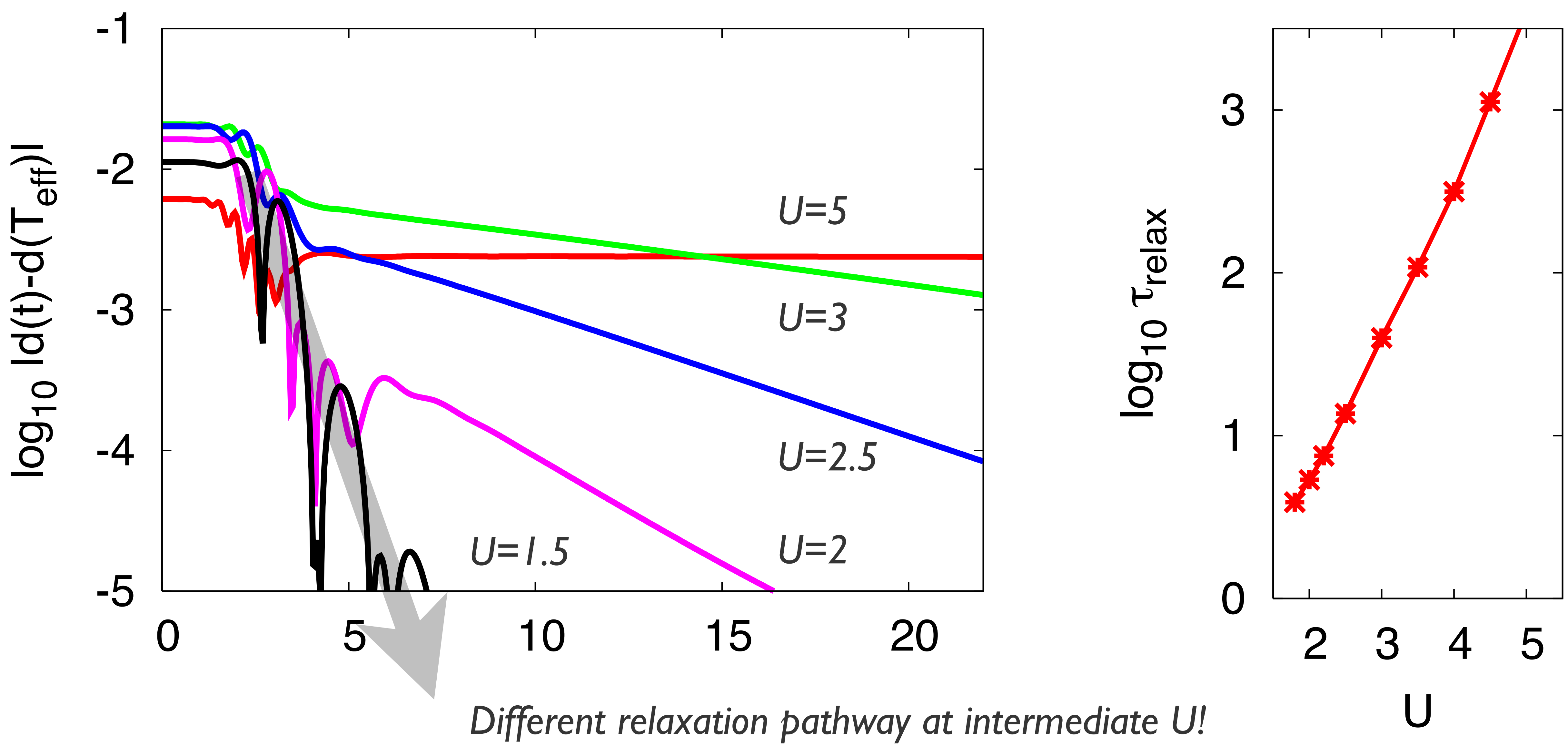


Different relaxation pathway at intermediate U!

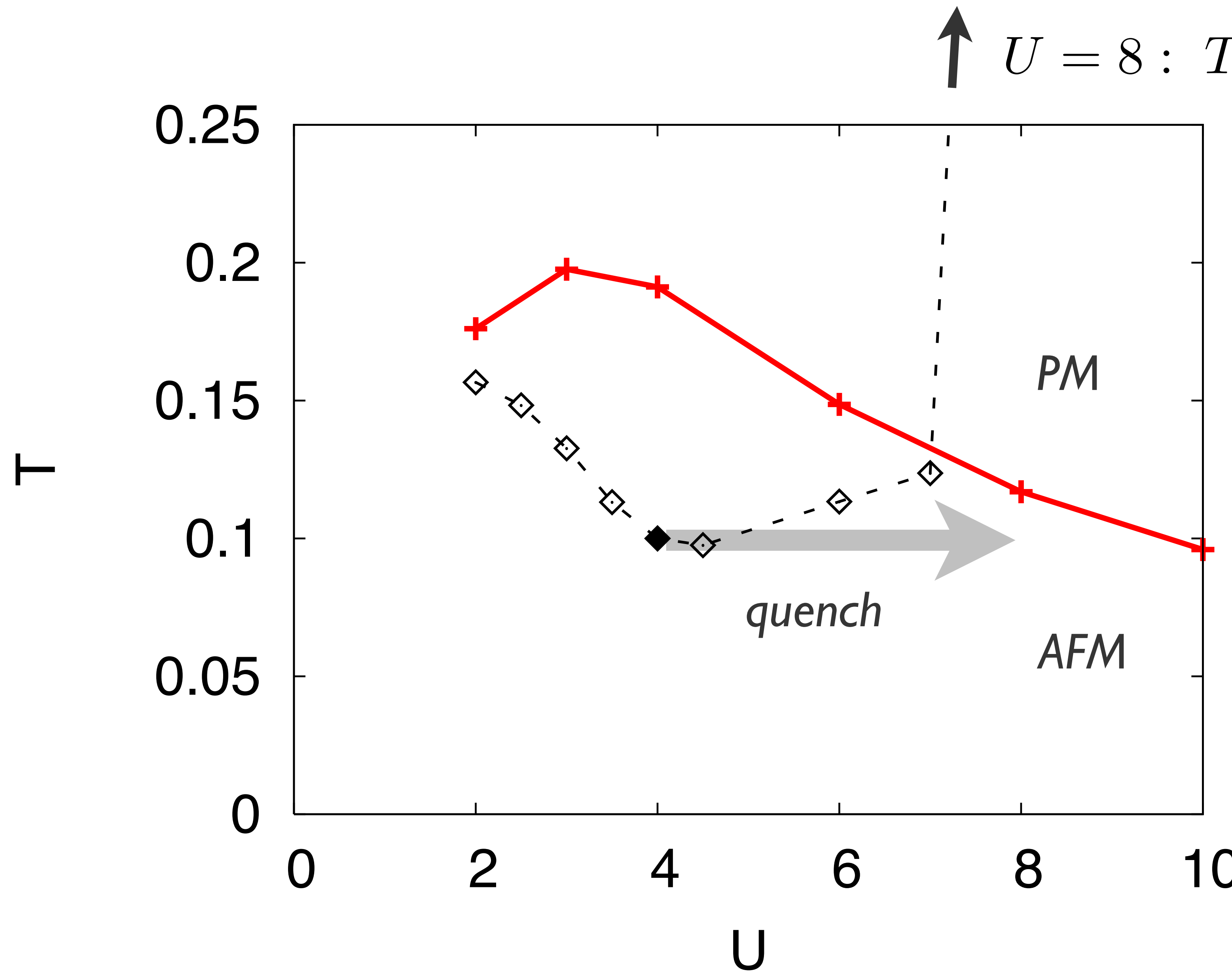
Nonthermal symmetry-broken states

- “Photo-doped” antiferromagnetic Mott insulator (*U*-quench)

  Werner, Tsuji & Eckstein (2012)

- *U*-quench into the strongly correlated regime freezes doublons / holes

$U = 8: \ T_{\text{eff}} \approx 1$

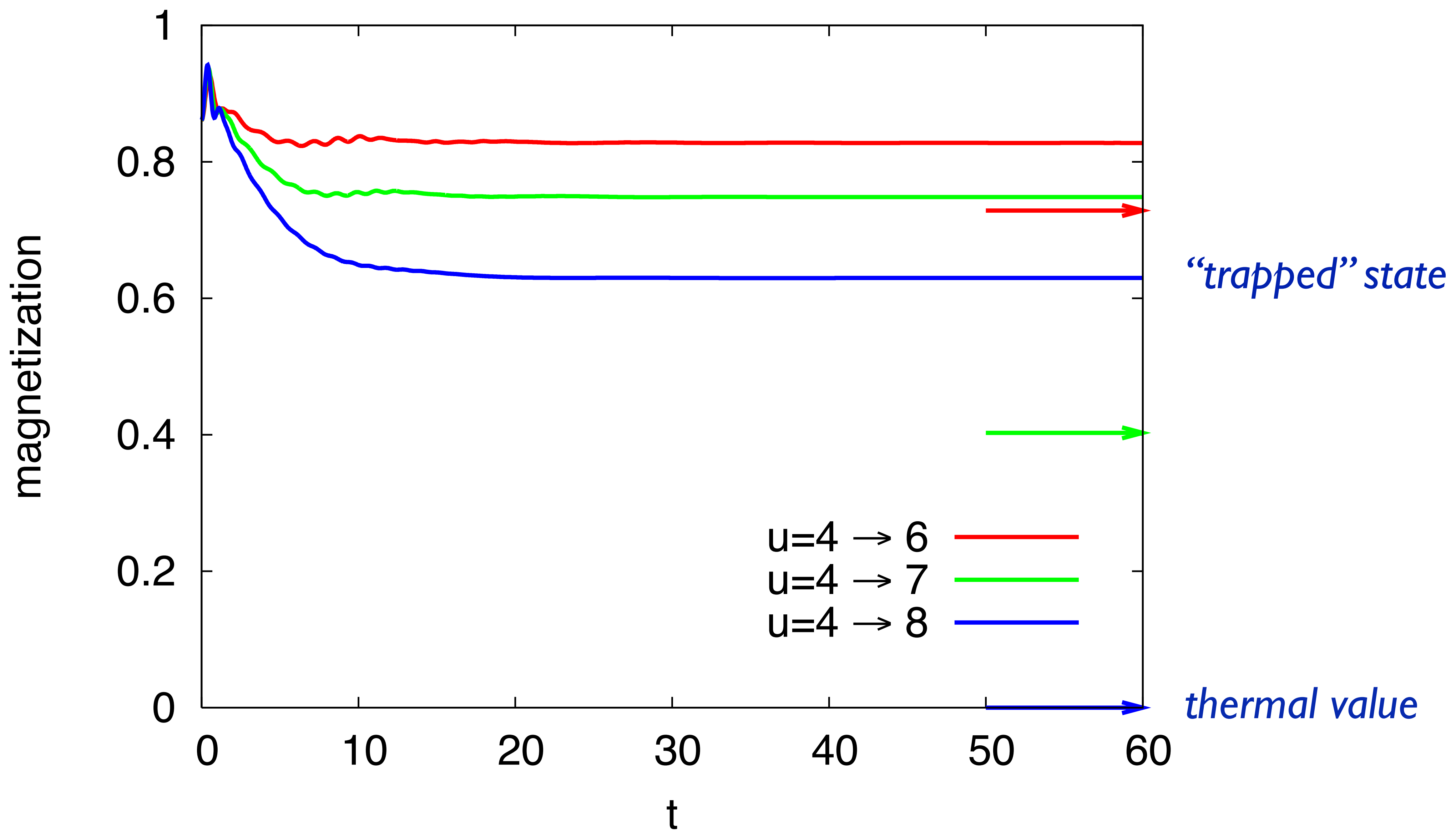


Nonthermal symmetry-broken states

- "Photo-doped" antiferromagnetic Mott insulator (*U*-quench)

  Werner, Tsuji & Eckstein (2012)

- Magnetization does not vanish, even if thermal state PM



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- "Photo-doped" antiferromagnetic Mott insulator (*U*-quench)

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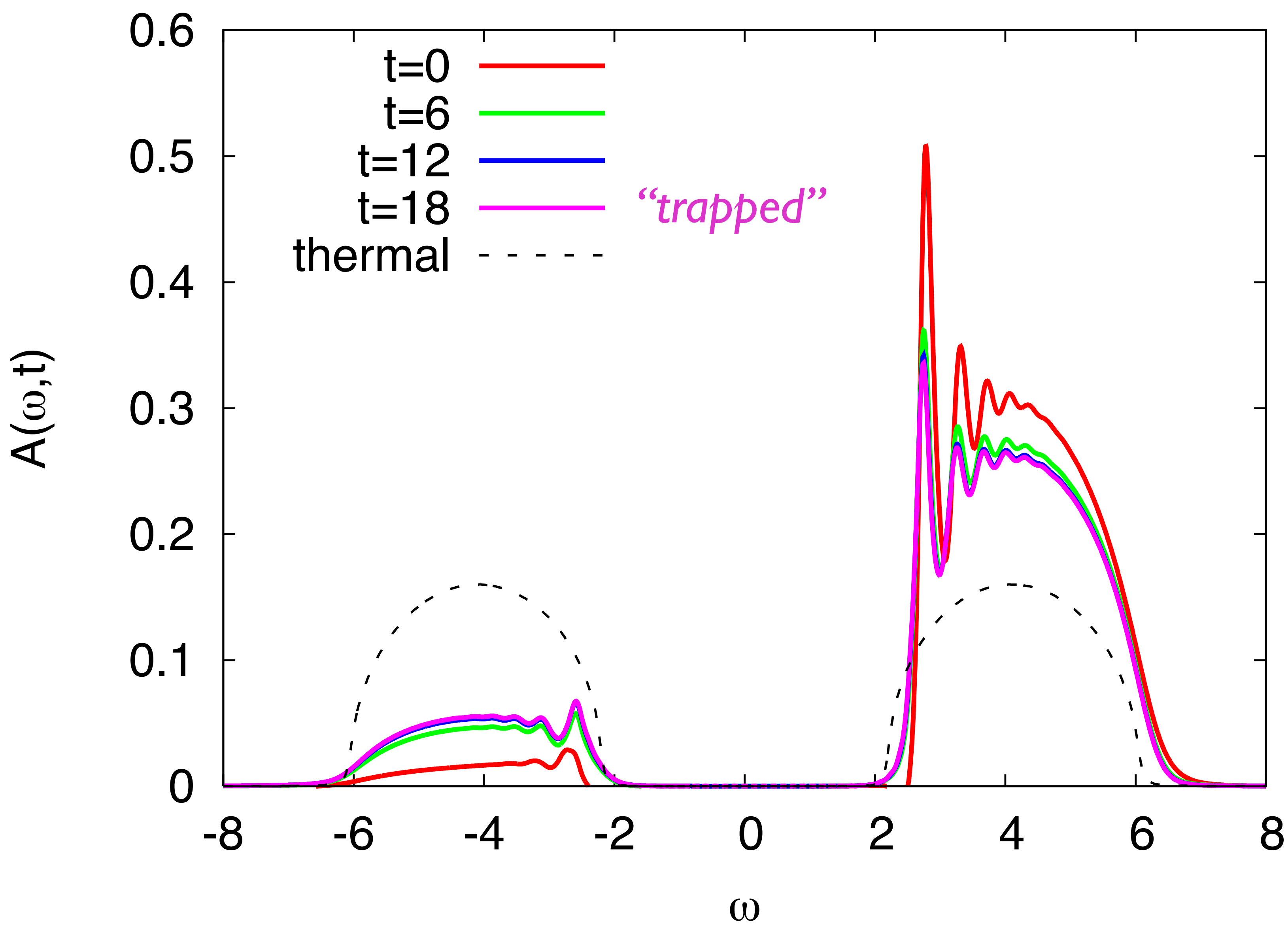
- Trapped state similar to chemically doped Mott insulator



timed-dependent spectral function (minority spin)

Nonthermal symmetry-broken states

- “Photo-doped” antiferromagnetic Mott insulator (*U*-quench)

  Werner, Tsuji & Eckstein (2012)

- Trapped state similar to chemically doped Mott insulator

- Interpretation:
  - Trapped state is a “t-J model” state with fixed doublons / holes
  - This state is protected by the slow decay of doublons
  - Effective temperature below the Neel temperature of the t-J state

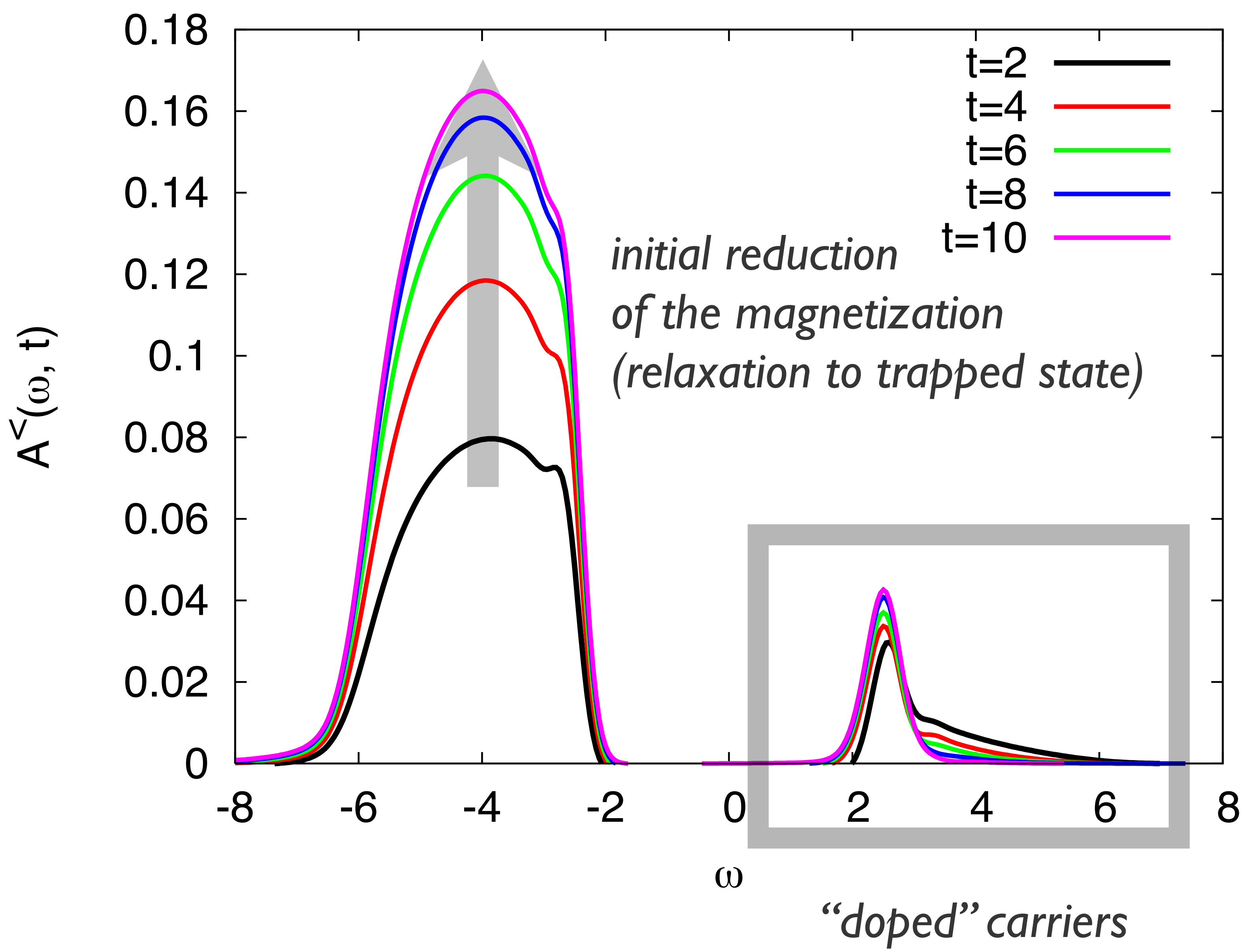
    → entropy cooling due to AFM background

Nonthermal symmetry-broken states

- “Photo-doped” antiferromagnetic Mott insulator (*U*-quench)

  Werner, Tsuji & Eckstein (2012)

- Cooling effect is evident from the time-evolution of the occupation



occupied part of the minority-spin spectral function

Nonthermal symmetry-broken states

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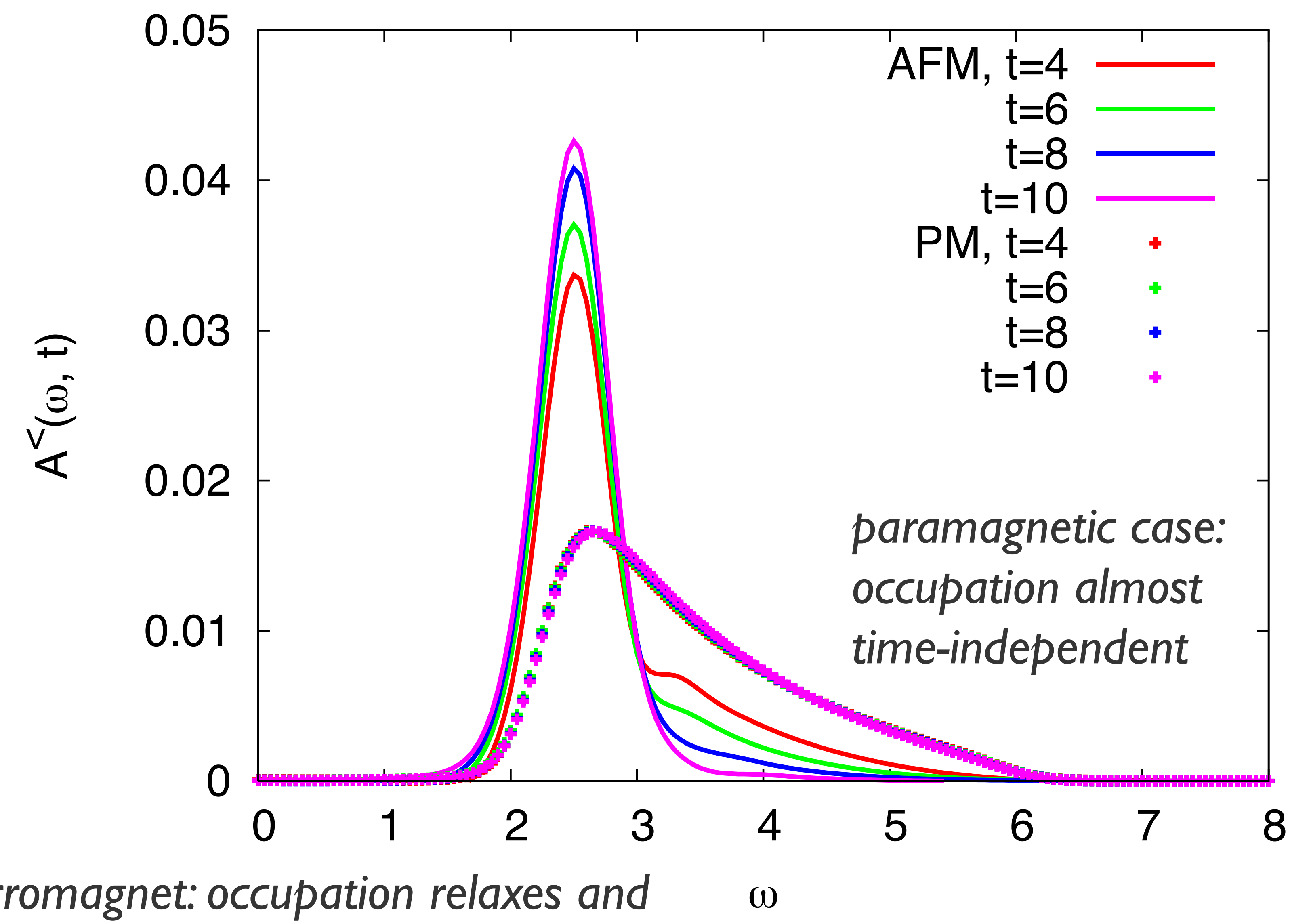
  Werner, Tsuji & Eckstein (2012)

- Cooling effect is evident from the time-evolution of the occupation



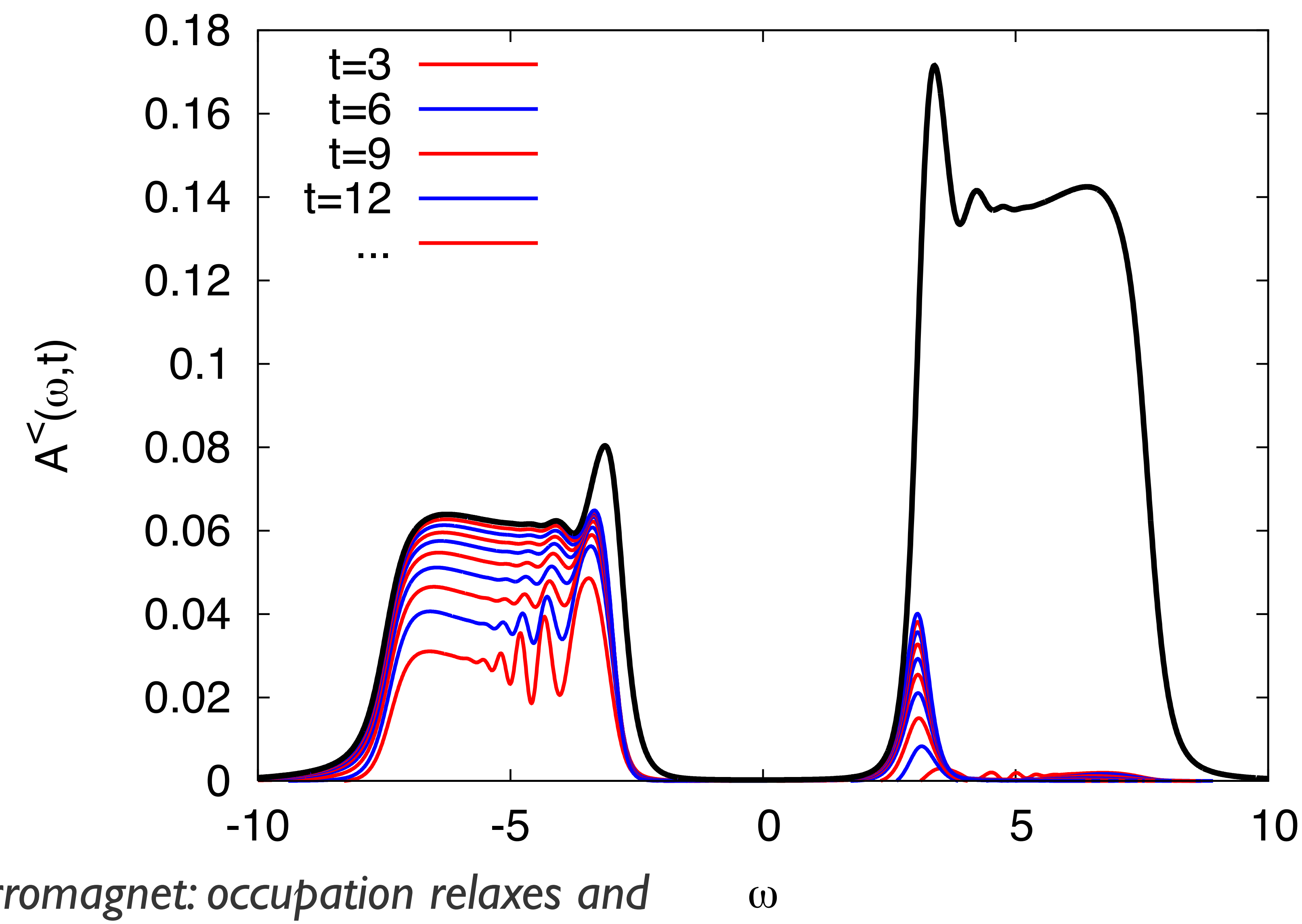
antiferromagnet: occupation relaxes and accumulates at lower band edge

Nonthermal symmetry-broken states

- Real photo-doping simulation $\Omega_{\rm pulse} \approx 12$

  work in progress

- Cooling effect is evident from the time-evolution of the occupation



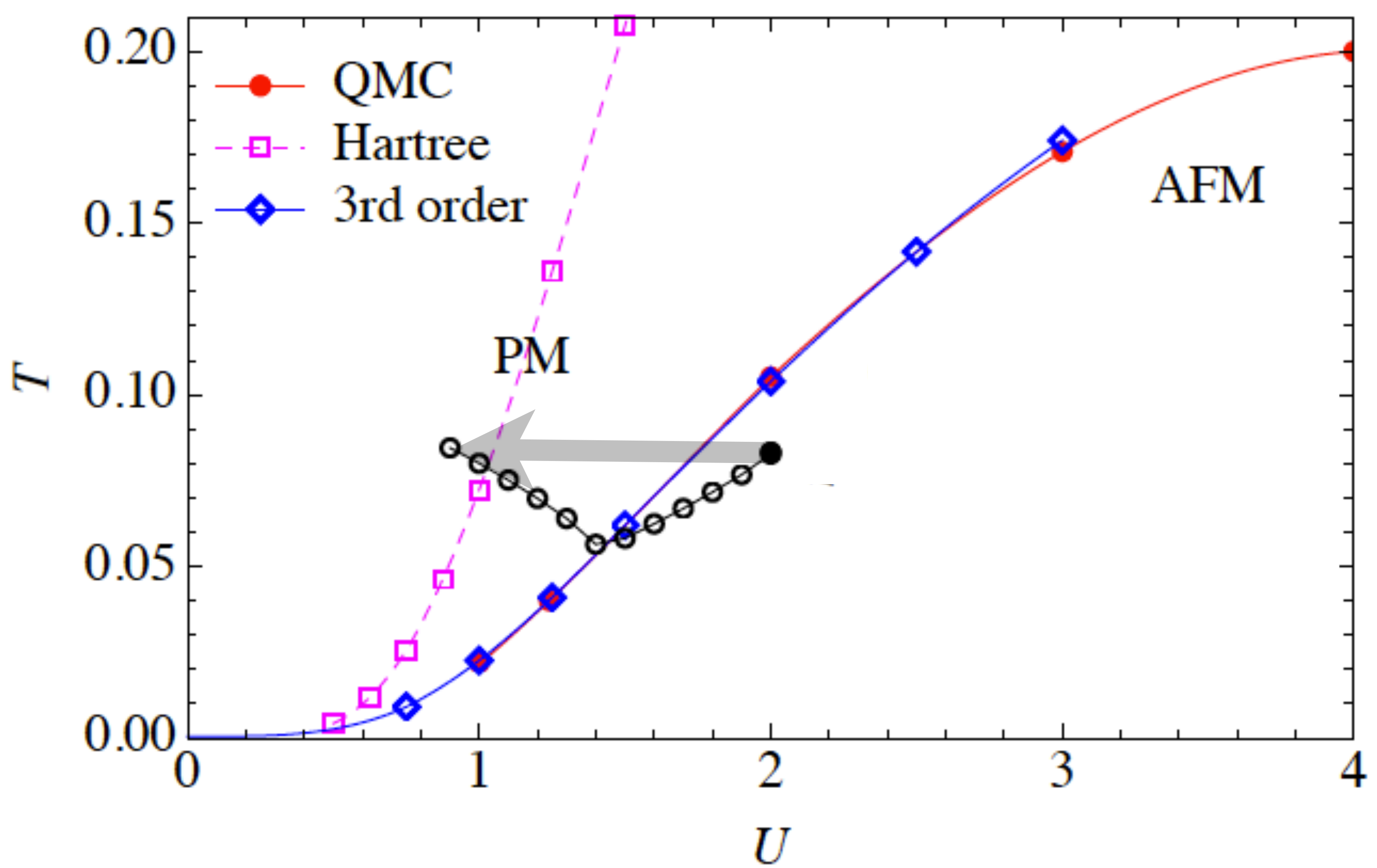
antiferromagnet: occupation relaxes and accumulates at lower band edge

Nonthermal symmetry-broken states

- Weak-coupling regime

  Tsuji, Eckstein & Werner (2012)

- Slow ramp from (Slater-)Antiferromagnet to Paramagnet

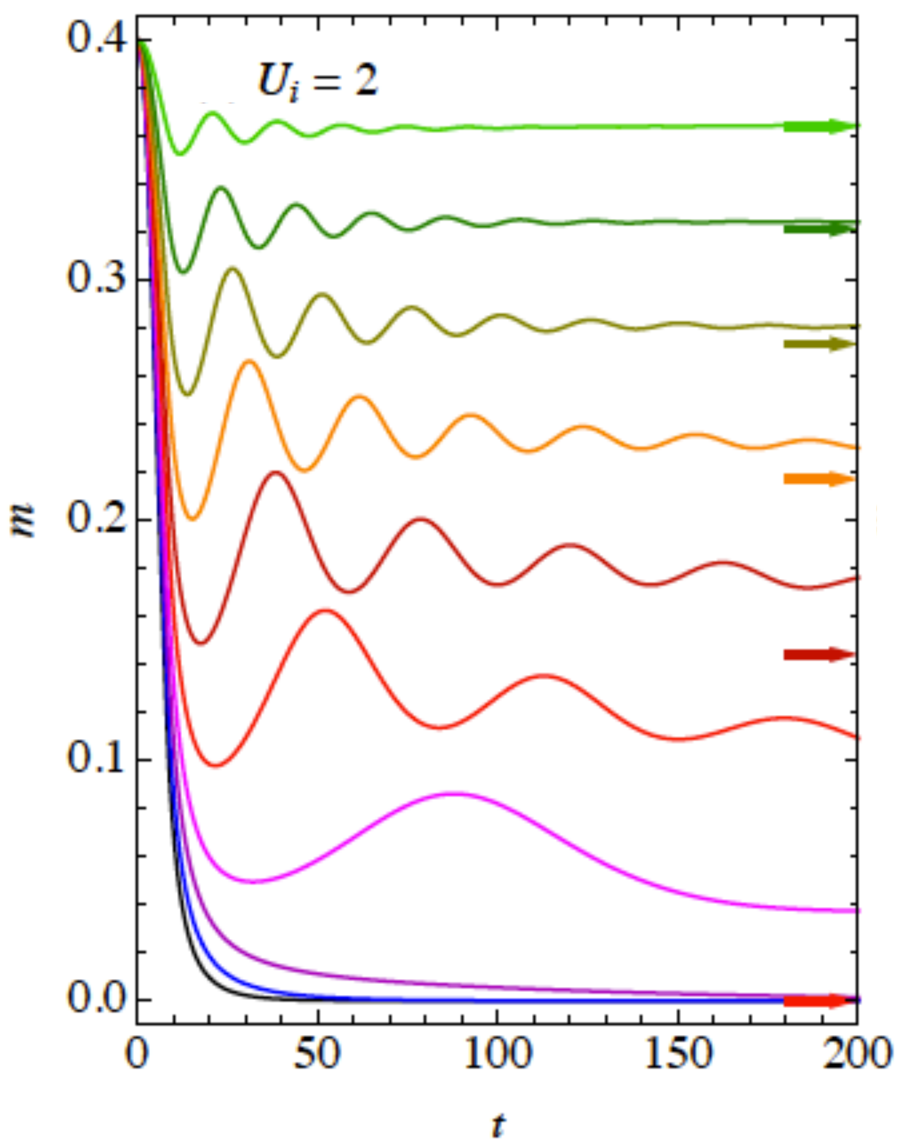


Nonthermal symmetry-broken states

- Weak-coupling regime

  Tsuji, Eckstein & Werner (2012)

- Time-evolution of the magnetization for different final *U*



arrows indicate thermal magnetization

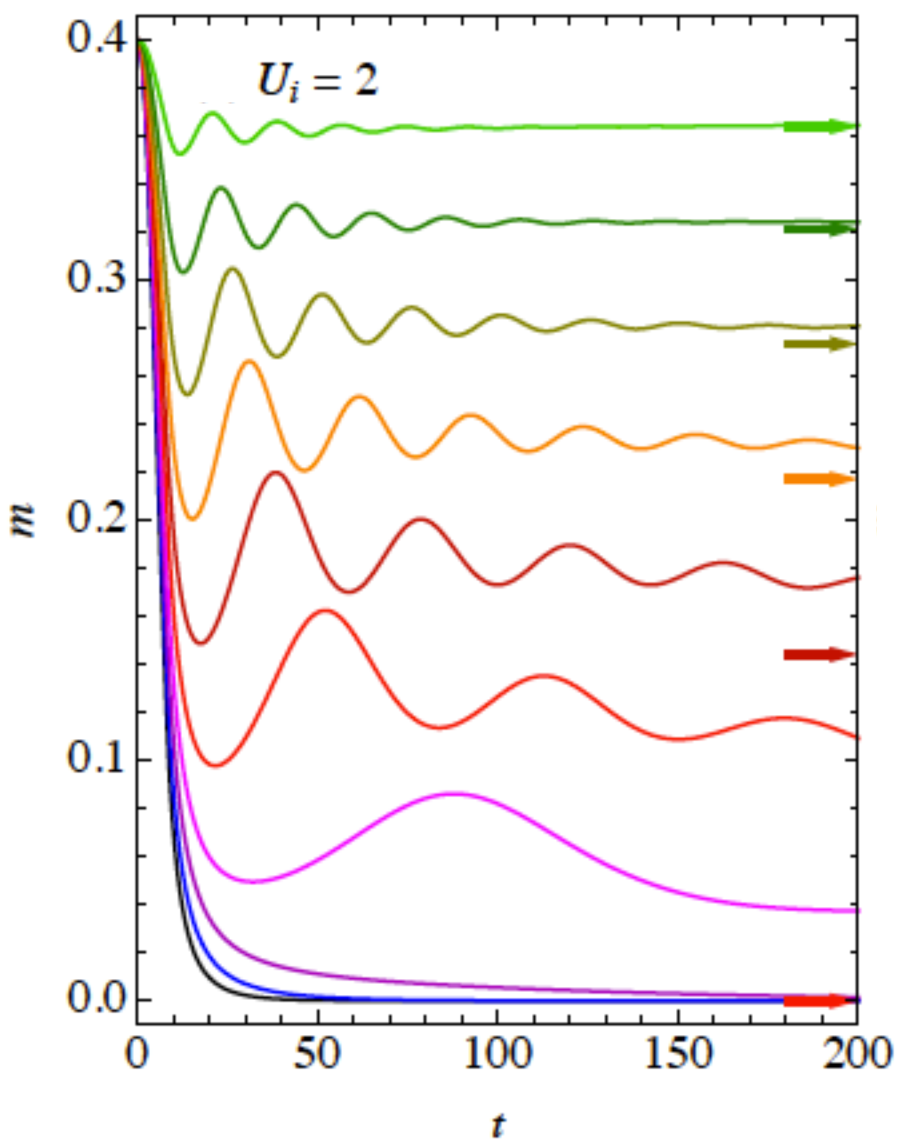
U=1.4: Oscillations around a nonthermal value (thermal magnetization=0)

Nonthermal symmetry-broken states

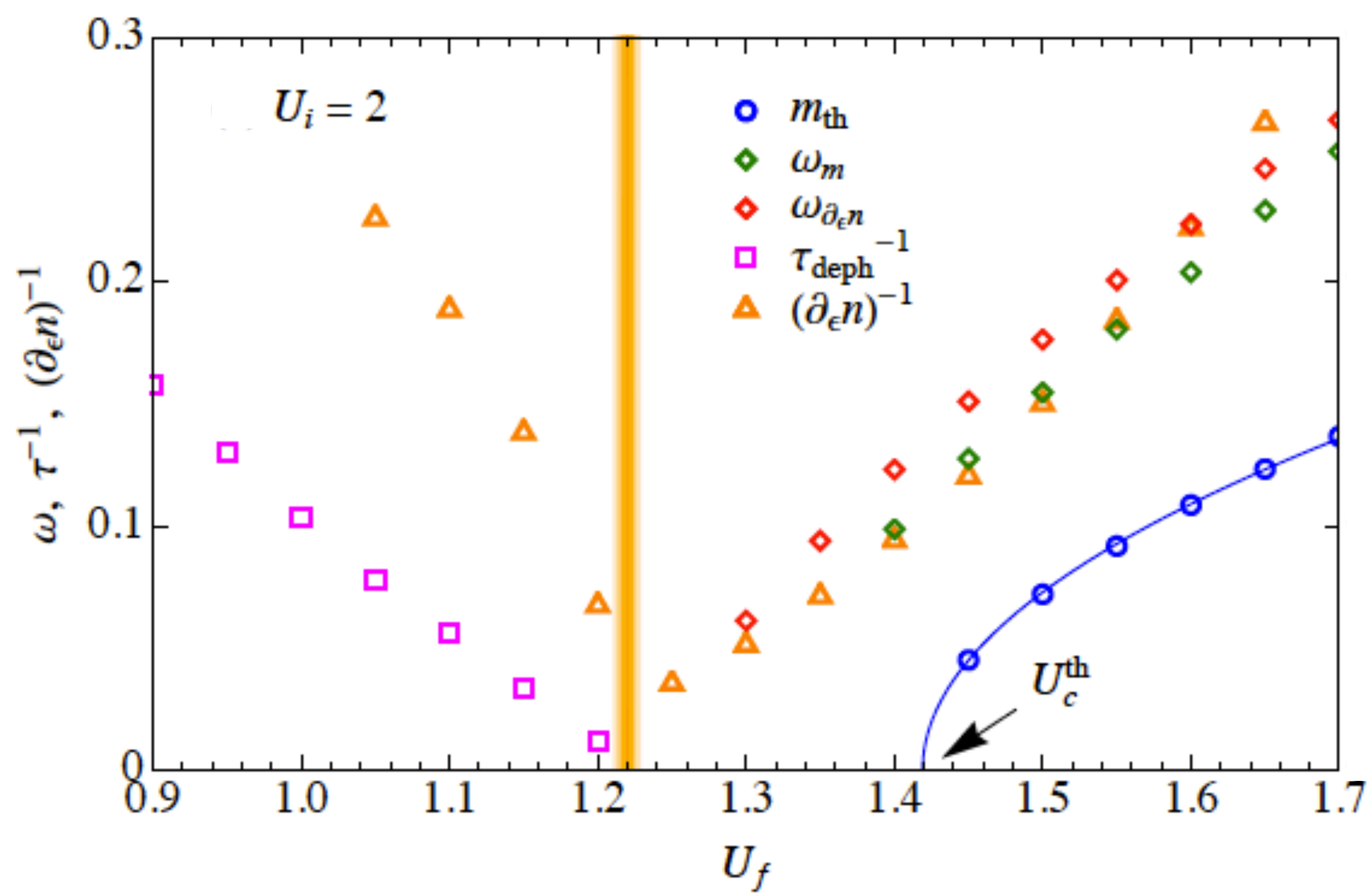
- Weak-coupling regime

  Tsuji, Eckstein & Werner (2012)

- Evidence for a nonthermal critical point (GL-description fails)



diverging timescales (period of amplitude mode, dephasing time, ...)



Summary

Nonequilibrium dynamical mean field results for Hubbard model

- *Metallic system: Population inversion by an asymmetric mono-cycle pulse*
  - *Interaction conversion:* $U \longrightarrow -U$
  - *Dynamically generated superconductivity?*

- *Antiferromagnetic insulator: Nonthermal symmetry-broken states*
  - *Thermalization delayed by slow decay of doublons*
  - *Similar effect expected in superconductors* ⟶ *experiment by Fausti et al.?*

- *Trapped states also in the weak-coupling regime*
  - *Short-time dynamics controlled by nonthermal critical points*