Nonequilibrium dynamical mean field theory

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Motivation

Ultrafast pump-probe spectroscopy

- Time resolution: ~10 fs $\longrightarrow$ measures excitation and relaxation processes on the intrinsic timescale of the electrons
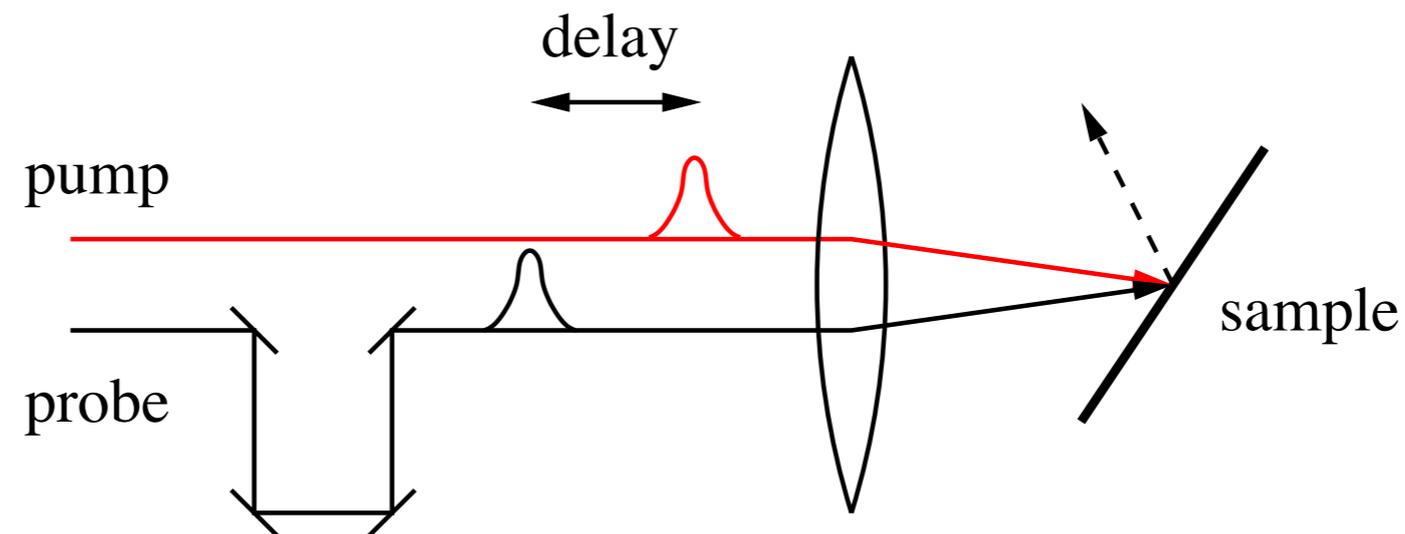

- Pump pulse drives system out of equilibrium
- Time evolution measured by subsequent probe pulses

- Possibility to "disentangle" competing effects on the time-axis

Motivation

"Tuning" of material properties by external driving

- Ultra-fast insulator-metal transition ("photo-doping")

Iwai et al. (2003)
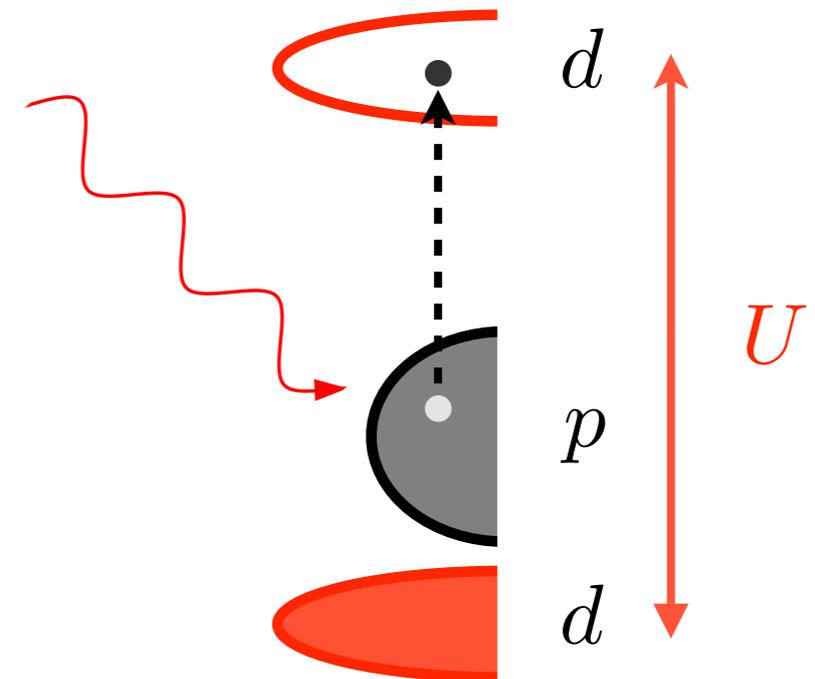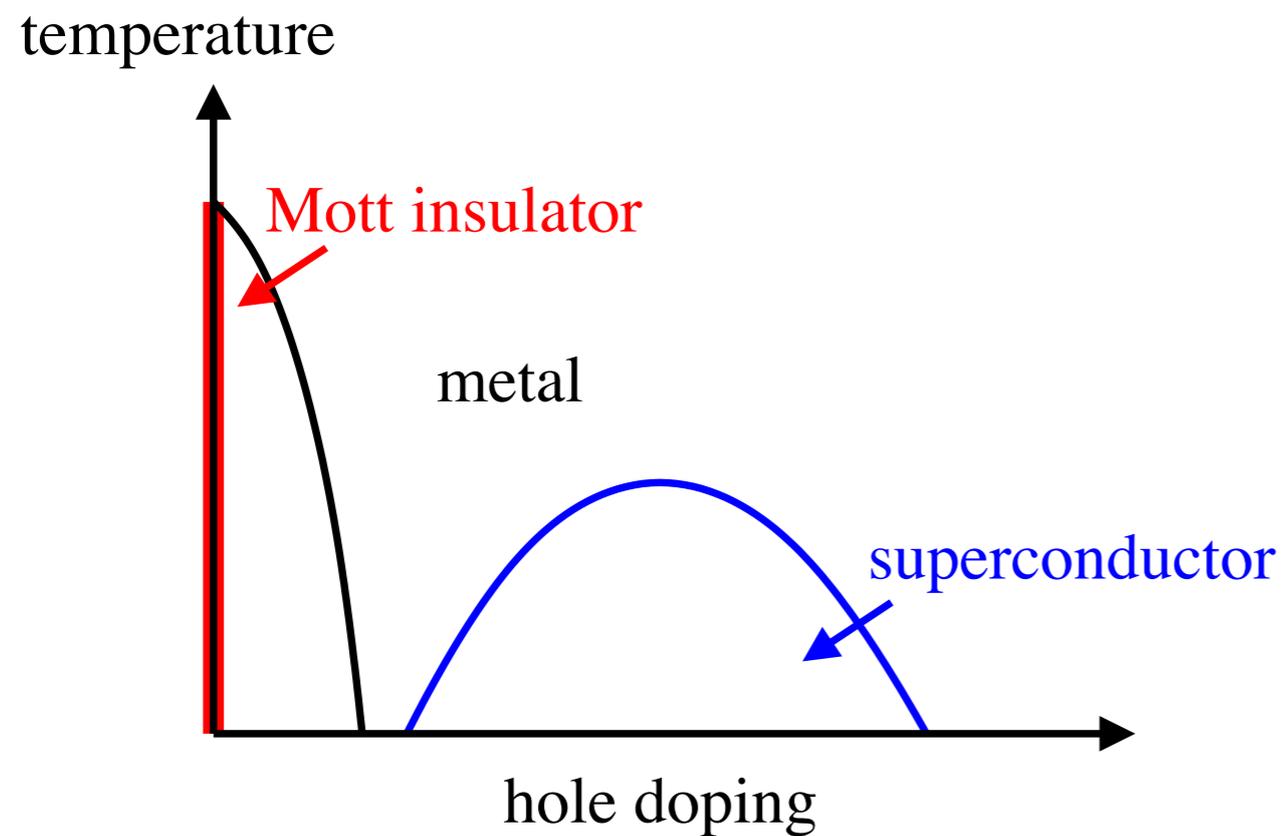
Motivation

"Tuning" of material properties by external driving

- Create long-lived transient states with novel properties

  e. g. light-induced high-temperature superconductivity

  Fausti et al. (2010), Kaiser et al. (2013)
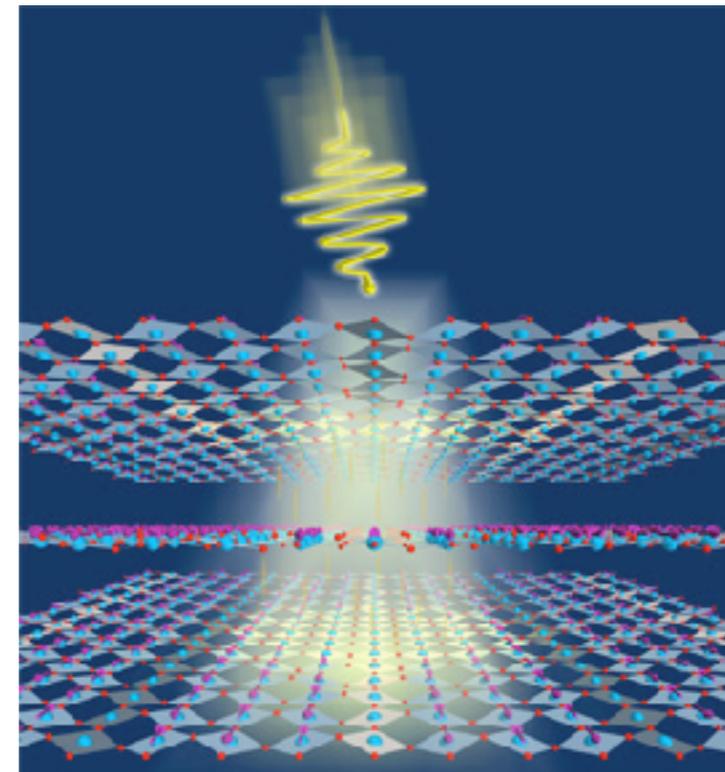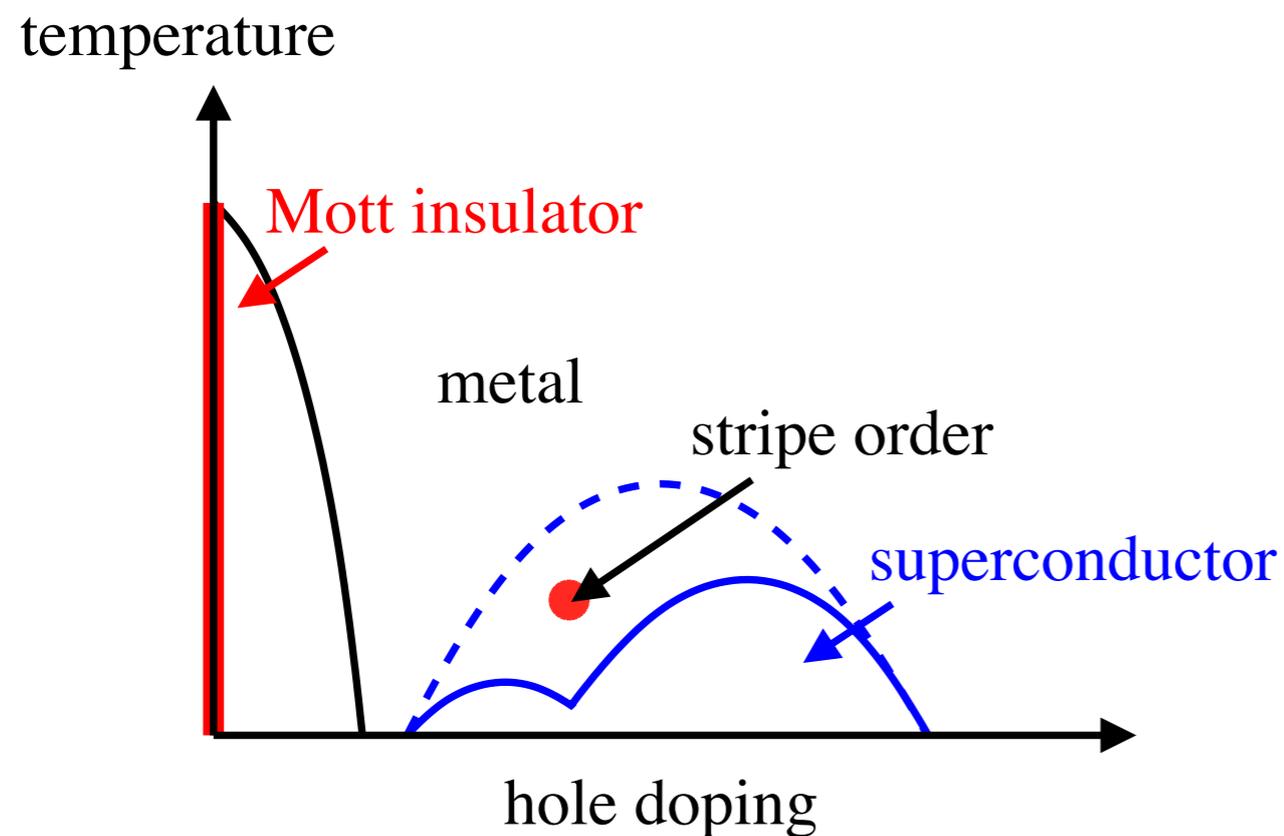

*THz pulse couples to phonons*

Motivation

"Tuning" of material properties by external driving

- Create long-lived transient states with novel properties

  e. g. light-induced high-temperature superconductivity

*Mitrano et al. (2015)*

K_3C_{60}
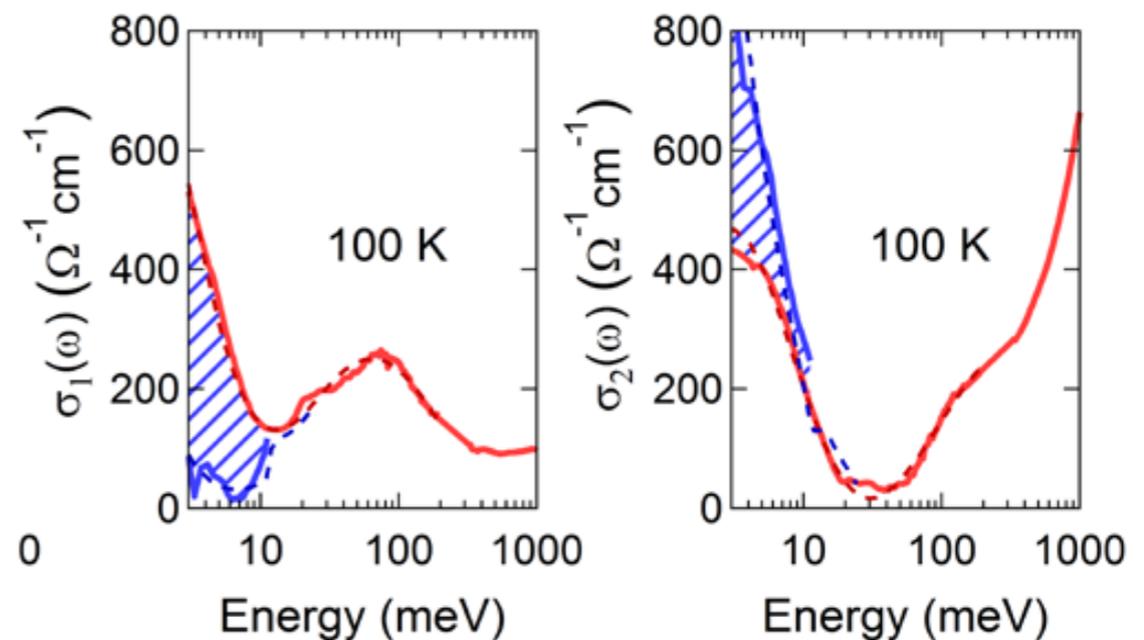
Motivation

"Tuning" of material properties by external driving

- Switching into metastable, but long-lived "hidden states"

  e. g. Reversible switching of TaS$_2$ into / out of a metallic hidden state

  Stojchevska et al. (2014)

equilibrium state (insulating)

hidden state (conducting)

Motivation

"Tuning" of   es by external driving

- Switching   but long-lived "hidden states"

e. g. Revers aS_2 into / out of a metallic hidden state

Stojchevska et al. (2014)

equilibrium state

hidden state

Resistance (Ohm)

Temperature (K)
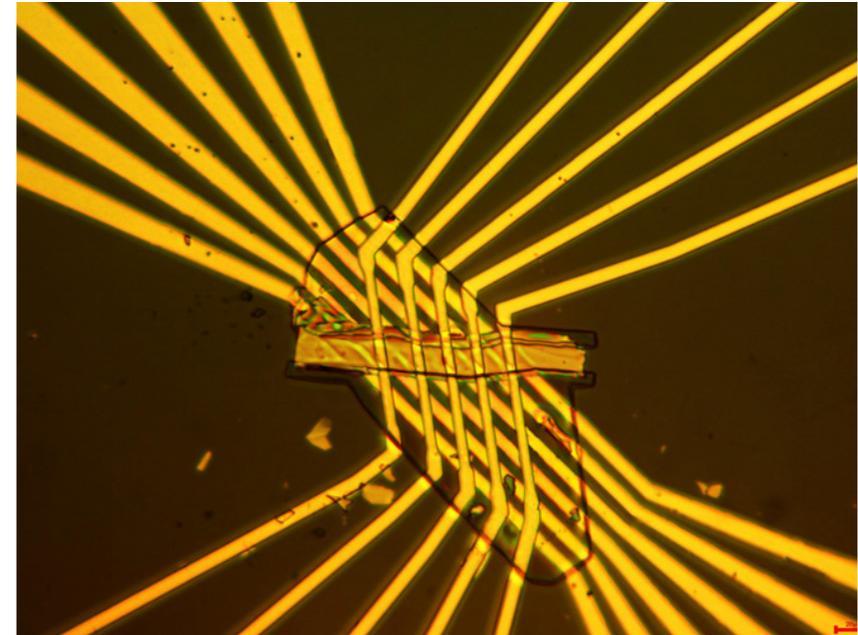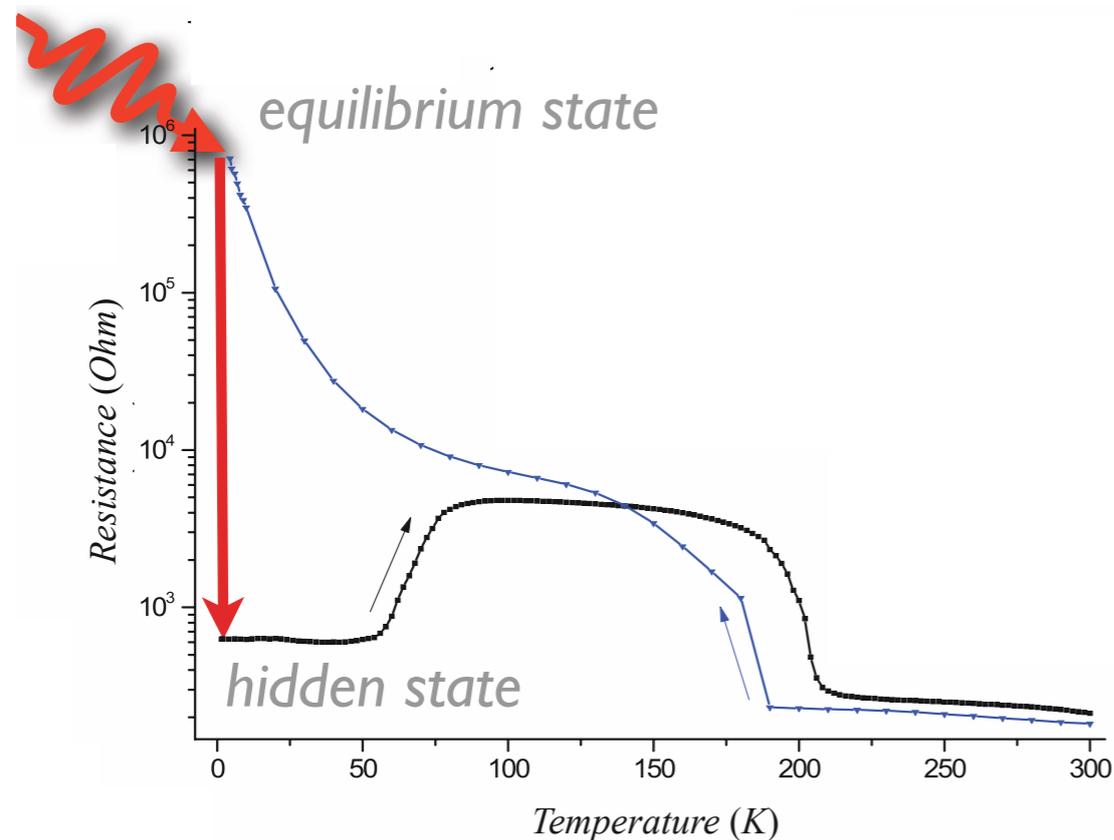

memory device with unprecedented speed and very low power consumption

Motivation

- **Challenge for theory/numerics** *Aoki et al. (2014)*
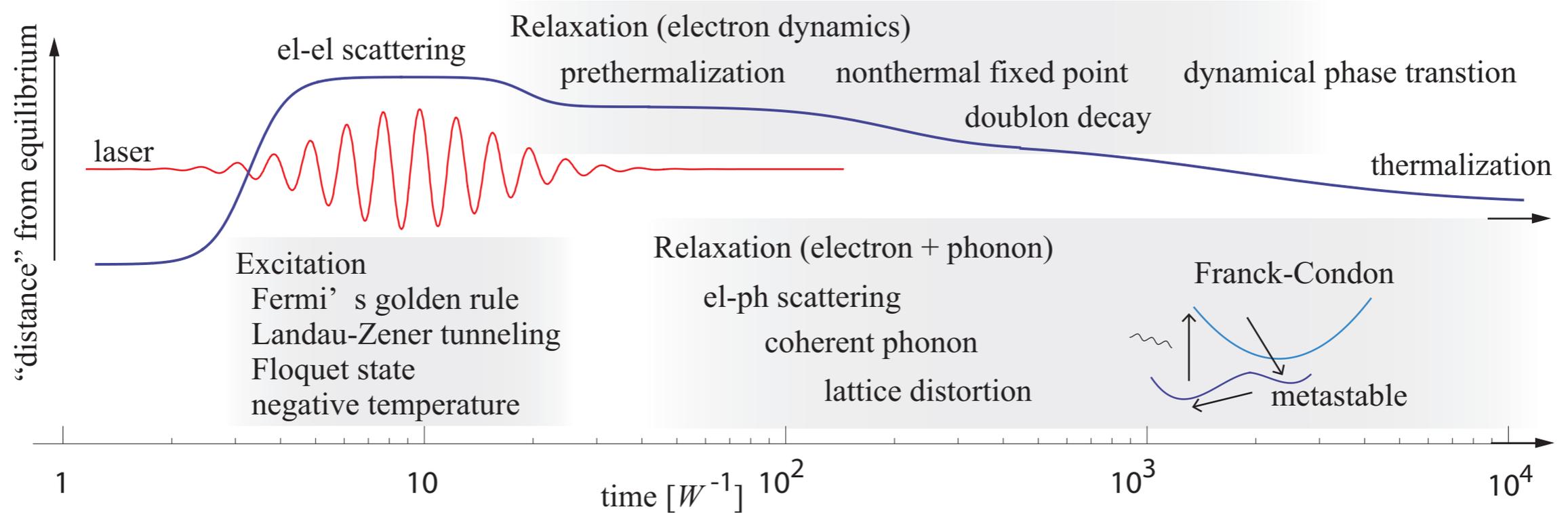
- Strongly interacting many-particle systems
- Strong perturbations
- Different relevant time scales

Overview

- *Dynamical mean field theory*

- *Cluster extension*

- *Nonequilibrium extension*

- *Nonequilibrium solvers and benchmarks*

- *Illustrations:*
  - *AC field quench - tuning of the interaction strength by external driving*
  - *Nonequilibrium phase transition - nonthermal fixed points*
  - *Cooling by photo-doping*

Model and method

- **Static mean field theory:** mapping to a single-site problem

  Weiss (1903)

lattice model $m_{\mathrm{latt}} \equiv m_{\mathrm{eff}}$ *single-site effective model*
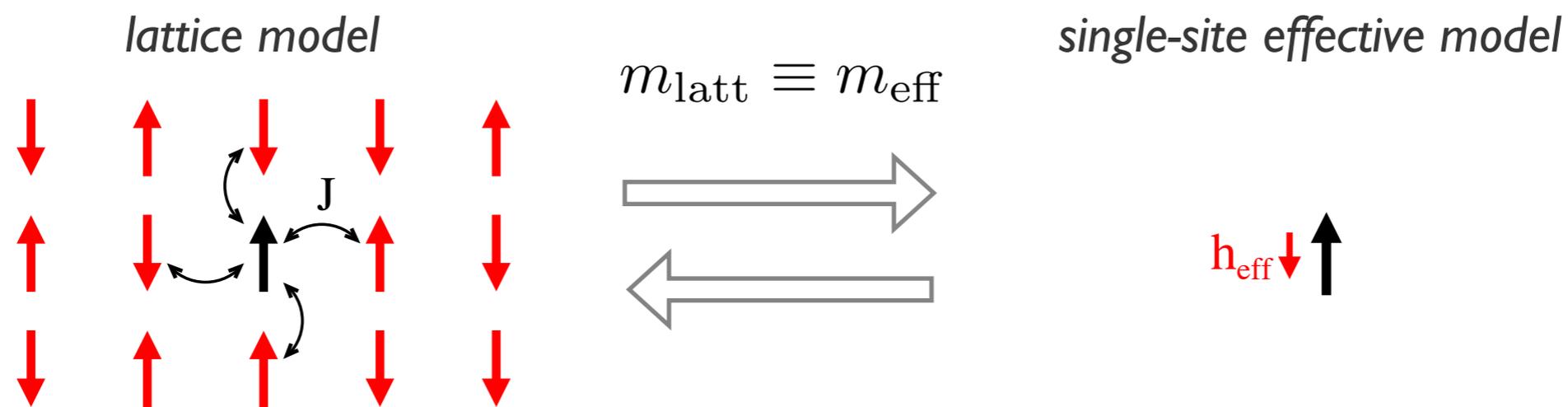
- **Effective model:** yields local observables (magnetization)

- **Parameter of the effective model ("mean field"):** optimized by requesting consistency between the lattice and single-site model

Model and method

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

  Georges & Kotliar (1992)

lattice model $G_{latt} \equiv G_{imp}$ *impurity model*

$\Sigma_{latt} \equiv \Sigma_{imp}$

- Impurity solver: computes the Green's function of the correlated site

- Bath parameters = "mean field": optimized in such a way that the bath mimics the lattice environment

Model and method

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

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Model and method

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lattice model

impurity model

DMFT self-consistency

$G_{\text{loc}}^{\text{latt}}(i\omega_n)$

$S_{\text{imp}}[\Delta(i\omega_n)]$

$G_{\text{loc}}^{\text{latt}} \equiv G_{\text{imp}}$

momentum average

impurity solver

$\Sigma_k^{\text{latt}} \equiv \Sigma_{\text{imp}}$

$$G_k^{\text{latt}} = \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma_k^{\text{latt}}}$$

$G_{\text{imp}}(i\omega_n), \Sigma_{\text{imp}}(i\omega_n)$

DMFT approximation

Model and method

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

Georges & Kotliar (1992)

lattice model

$G_{latt} \equiv G_{imp}$

$\Sigma_{latt} \equiv \Sigma_{imp}$

impurity model

t

t_k

- Single-site DMFT can treat two-sublattice order (e.g. AFM)

$$\text{Bath}_{B,\sigma}[G_{A,\sigma}], \quad \text{Bath}_{A,\sigma}[G_{B,\sigma}]$$

- Pure Neel order: $\text{Bath}_{B,\sigma} = \text{Bath}_{A,\bar{\sigma}} \quad \longrightarrow \quad \text{Bath}_{A,\bar{\sigma}}[G_{A,\sigma}]$

Model and method

- Equilibrium DMFT phase diagram (half-filling)

- Paramagnetic calculation: Metal - Mott insulator transition at low T

- Smooth crossover at high T
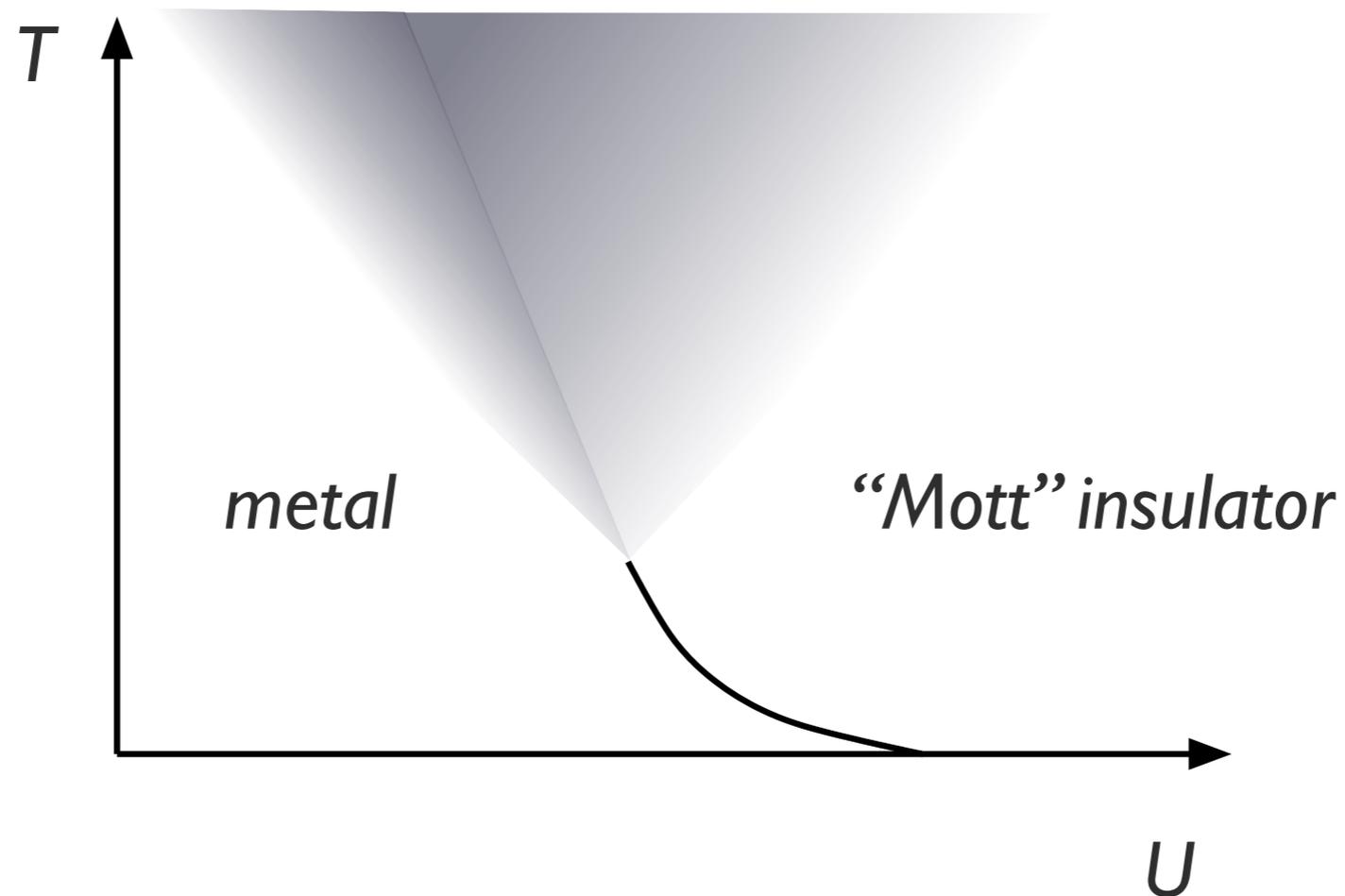
Model and method

- Equilibrium DMFT phase diagram (half-filling)

- With 2-sublattice order: Antiferromagnetic insulator at low T

- Smooth crossover at high T
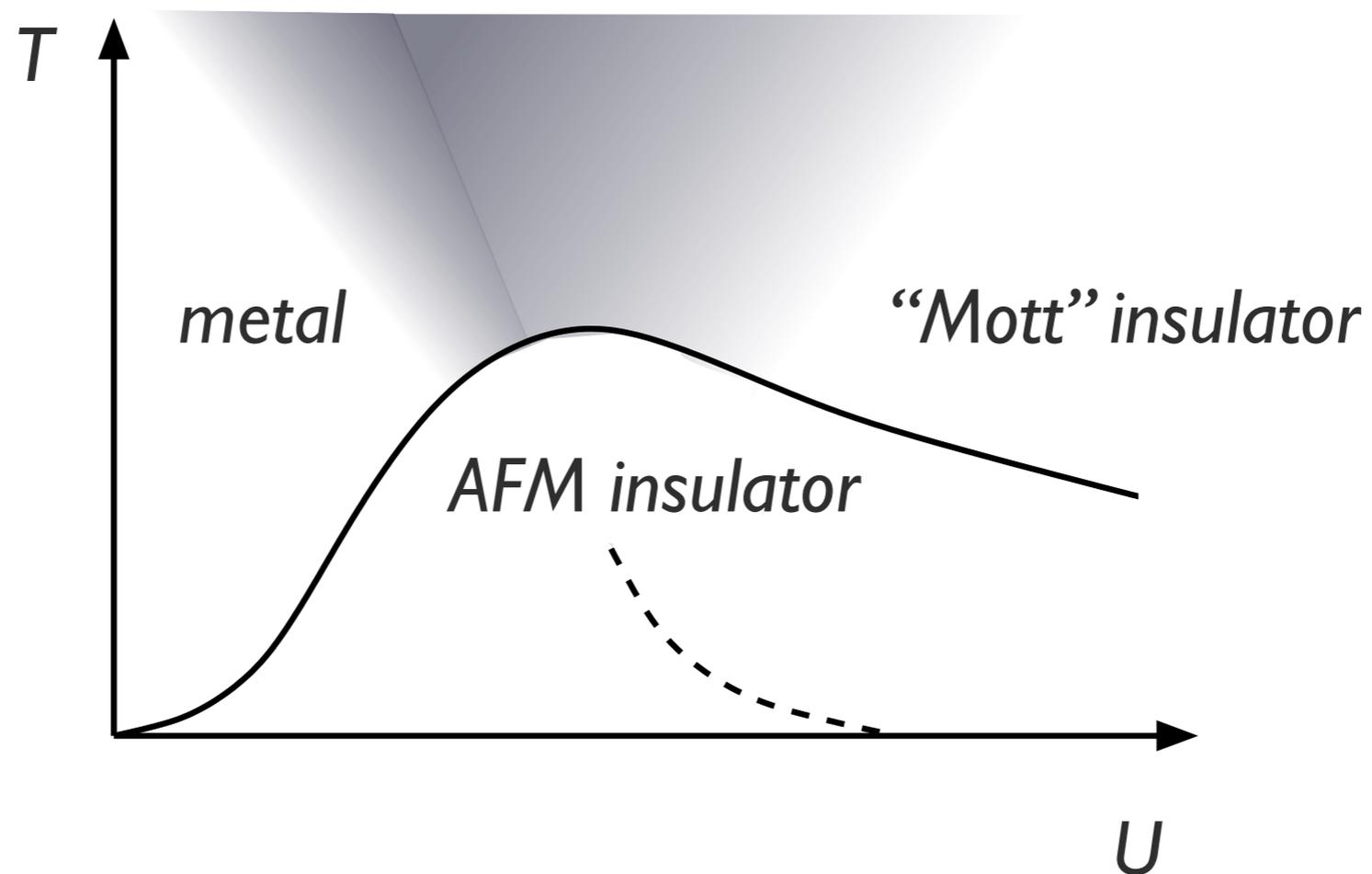
T

metal

"Mott" insulator

AFM insulator

U

Model and method

- Equilibrium DMFT phase diagram (half-filling)

- Transformation $c_{i\uparrow} \rightarrow c_{i\uparrow}^{\dagger} \quad (i \in A), \quad c_{i\uparrow} \rightarrow -c_{i\uparrow}^{\dagger} \quad (i \in B)$

  maps repulsive model onto attractive model

Model and method

- Equilibrium DMFT phase diagram

- Half-filling: transformation $c_{i\uparrow} \to c_{i\uparrow}^{\dagger}$ $(i \in A), \quad c_{i\uparrow} \to -c_{i\uparrow}^{\dagger}$ $(i \in B)$

  maps repulsive model onto attractive model

metal

superconductor

AFM insulator

"BEC"   *"BCS"*   *"Slater"*   *"Mott"*
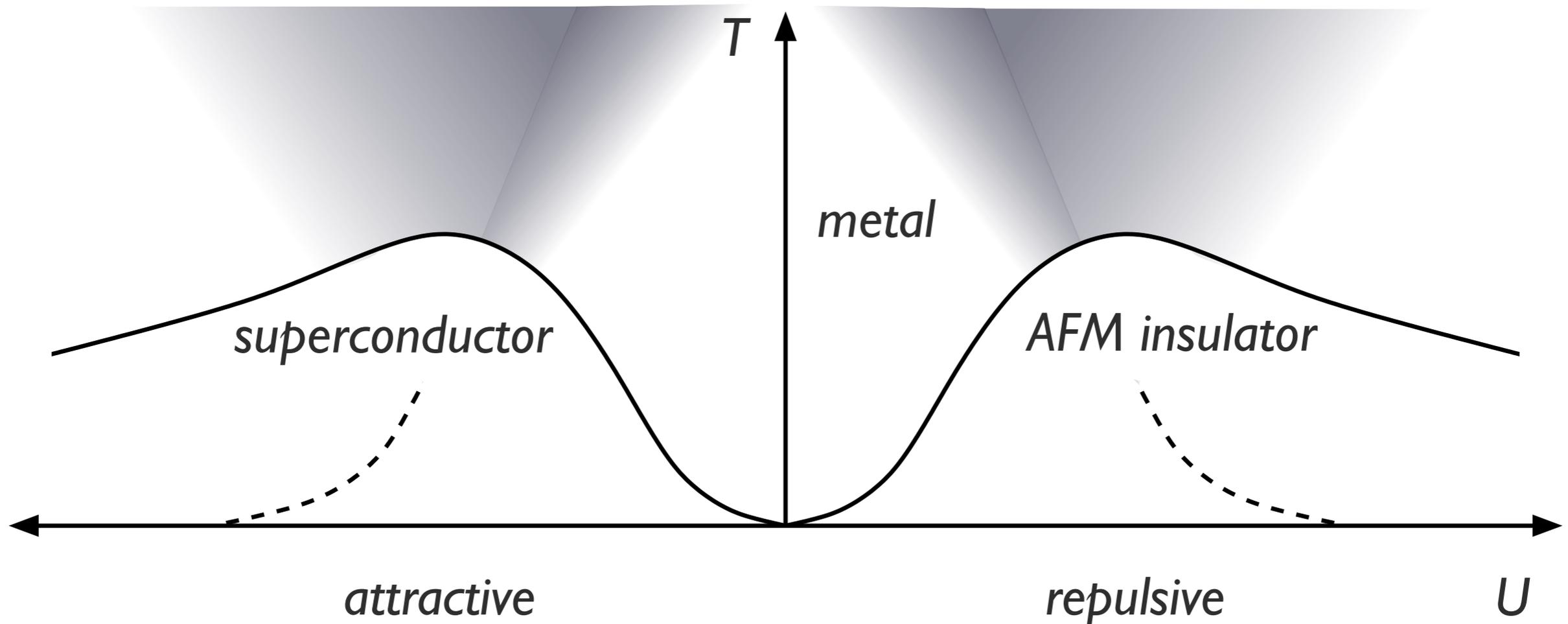
*attractive*   *repulsive* U
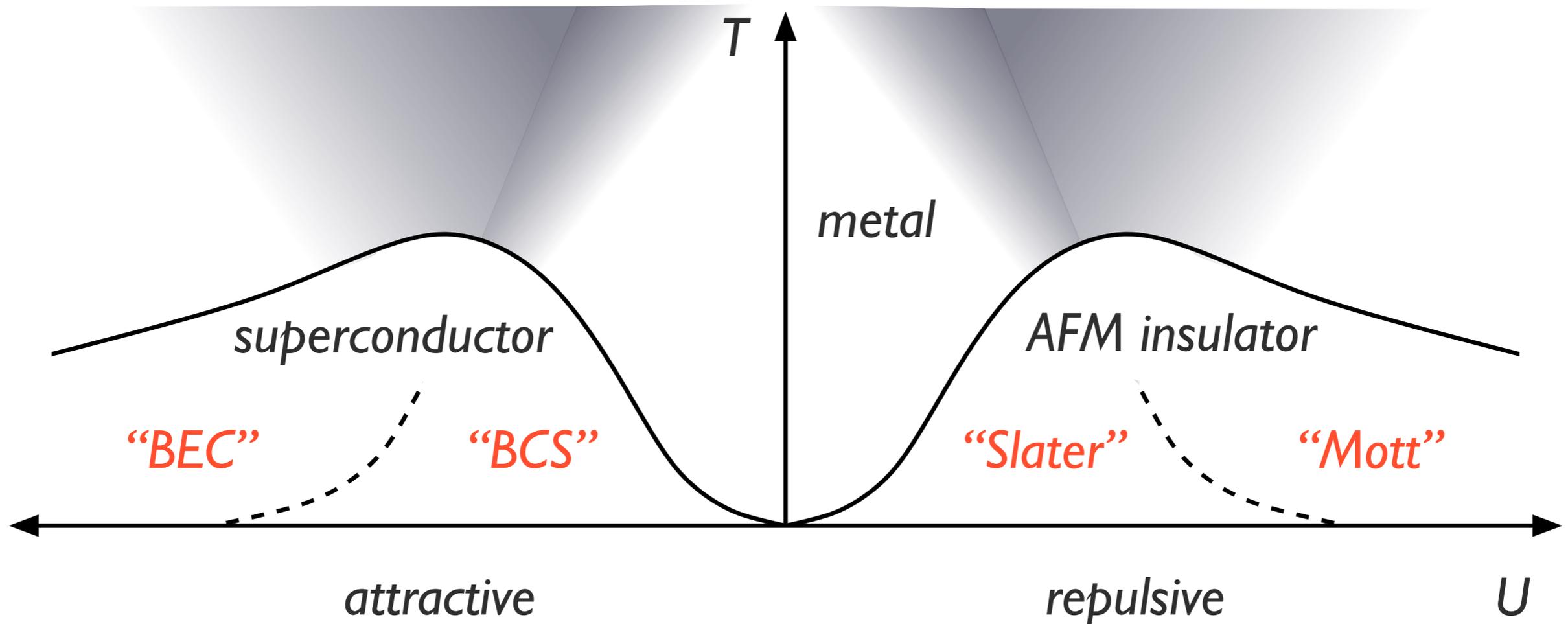
Cluster extension

- Low-dimensional systems

- DMFT is exact in $d = \infty$ *Metzner & Vollhardt (1989)*

- Neglect of spatial fluctuations problematic in $d < 3$

- $d = 2$ Hubbard model is believed to describe the physics of high-*Tc* (cuprate) superconductors
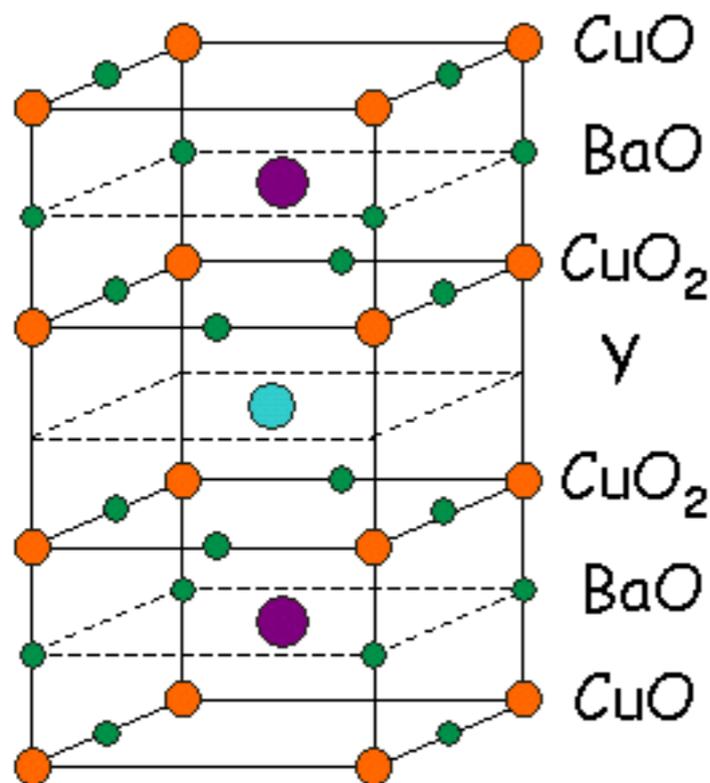
to describe the physics of the cuprates, we need a cluster extension of DMFT, with at least 4 sites
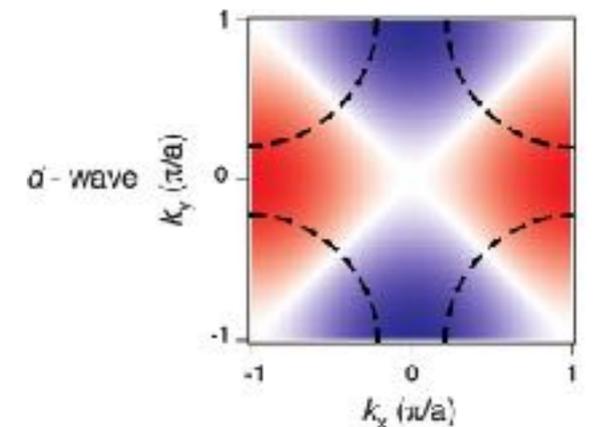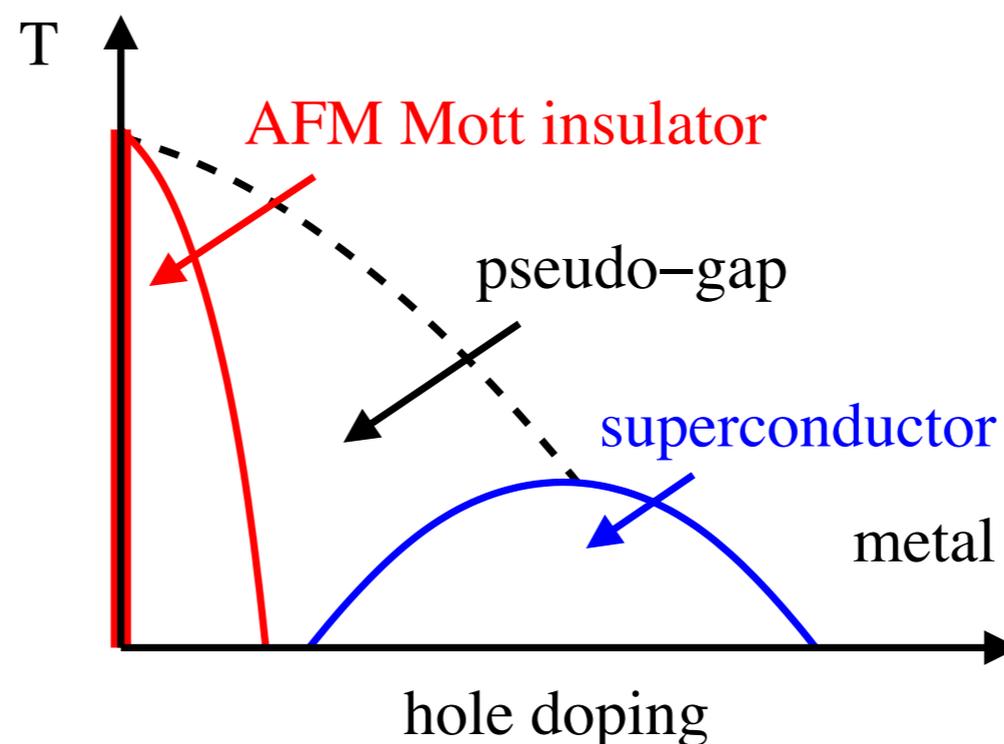
Cluster extension

- Low-dimensional systems

- Cluster DMFT self-consistently embeds a cluster of N_c sites into a fermionic bath *Hettler, Prushke, Krishnamurthy & Jarrell (1998)*

- If cluster is periodized: coarse-graining of the momentum-dependence

$$\Sigma(k, \omega) = \sum_a \phi_a(k) \Sigma_a(\omega)$$

- "Tiling" of the Brillouin zone
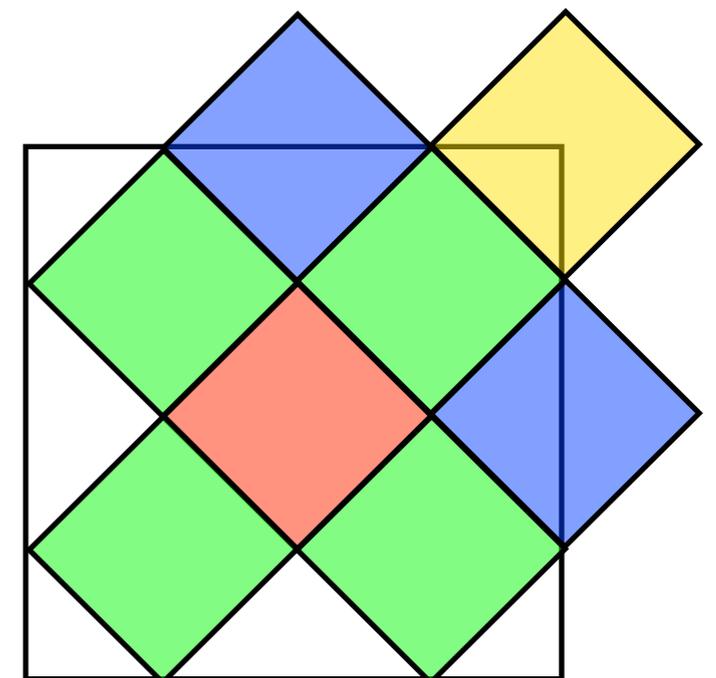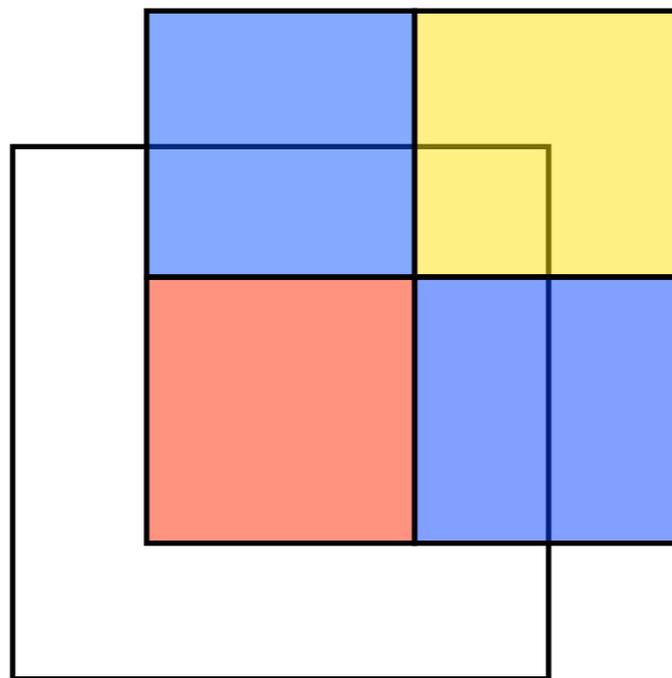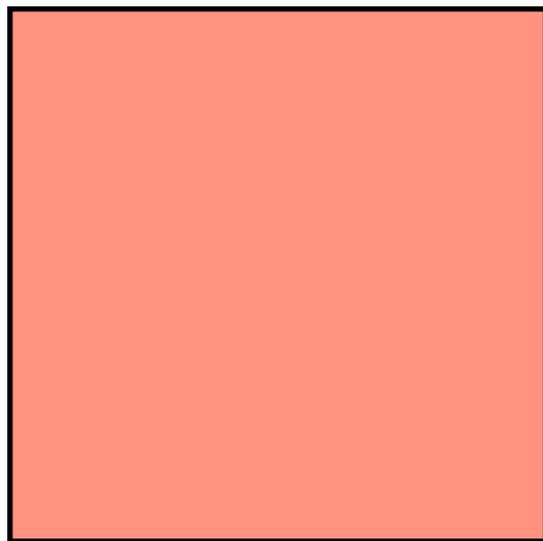
Cluster extension

- Dynamical cluster approach: mapping to an impurity cluster

  Hettler et al. (1998)
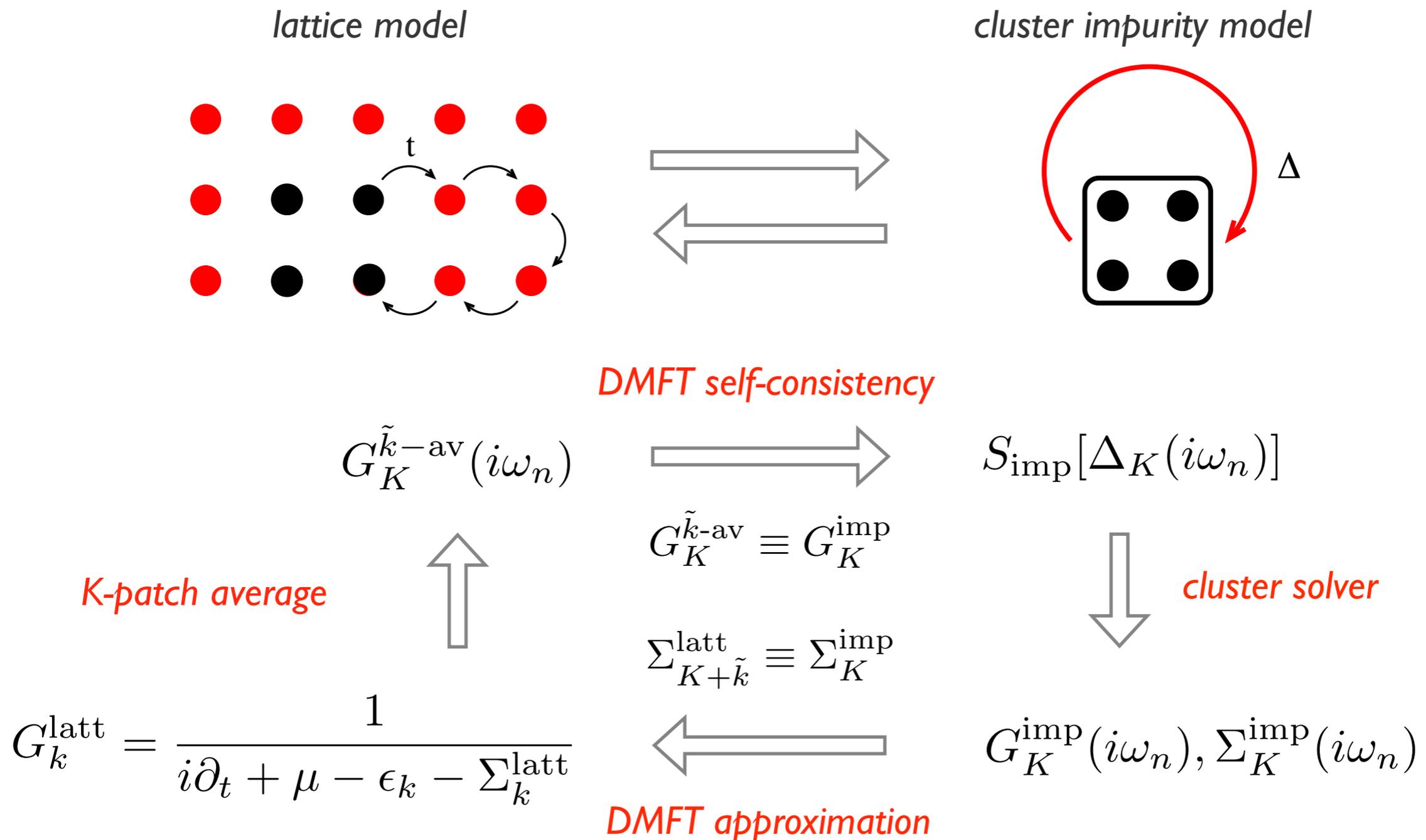
lattice model

cluster impurity model

t

Δ

DMFT self-consistency

$$G_K^{\tilde{k}-\mathrm{av}}(i\omega_n)$$

$$S_{\mathrm{imp}}[\Delta_K(i\omega_n)]$$

$$G_K^{\tilde{k}\text{-av}} \equiv G_K^{\mathrm{imp}}$$

K-patch average

cluster solver

$$\Sigma_{K+\tilde{k}}^{\mathrm{latt}} \equiv \Sigma_K^{\mathrm{imp}}$$

$$G_k^{\mathrm{latt}} = \frac{1}{i\partial_t + \mu - \epsilon_k - \Sigma_k^{\mathrm{latt}}}$$

$$G_K^{\mathrm{imp}}(i\omega_n), \Sigma_K^{\mathrm{imp}}(i\omega_n)$$

DMFT approximation
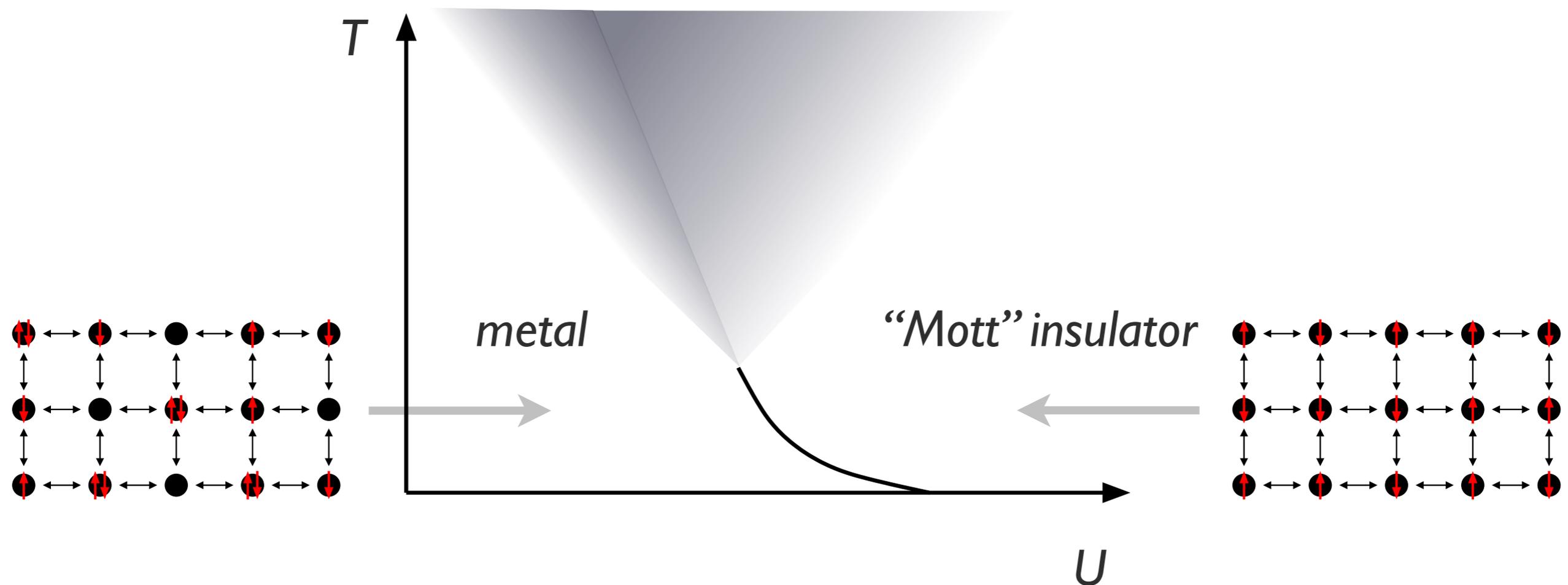
Cluster extension

- Equilibrium DMFT phase diagram (half-filling)

- Paramagnetic calculation: Metal - Mott insulator transition at low T

- Smooth crossover at high T

Cluster extension

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paramagnetic Mott insulator has large entropy:
metal-insulator transition upon increasing T

metal

"Mott" insulator

T

U
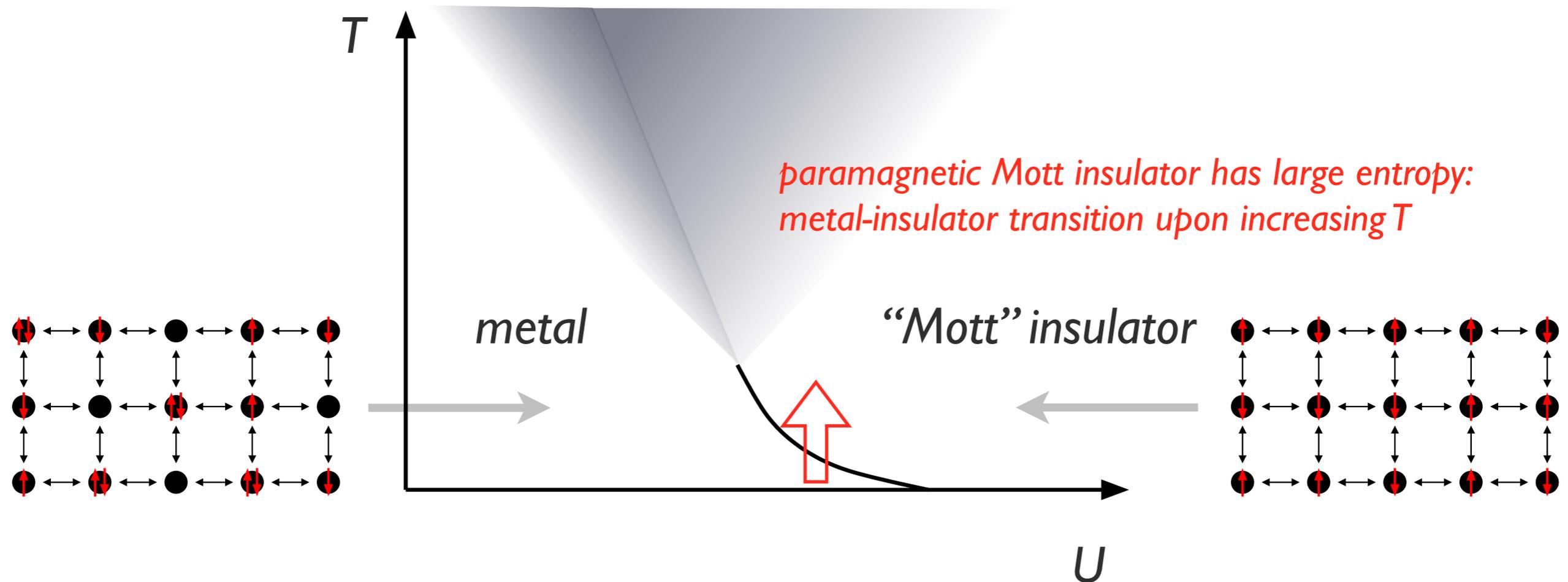
Cluster extension

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- Smooth crossover at high T

"plaquette singlet" state dominates low-T insulator

metal

"Mott" insulator

T

U

*curvature of the phase boundary changes if
short-range spatial correlations are taken into account*
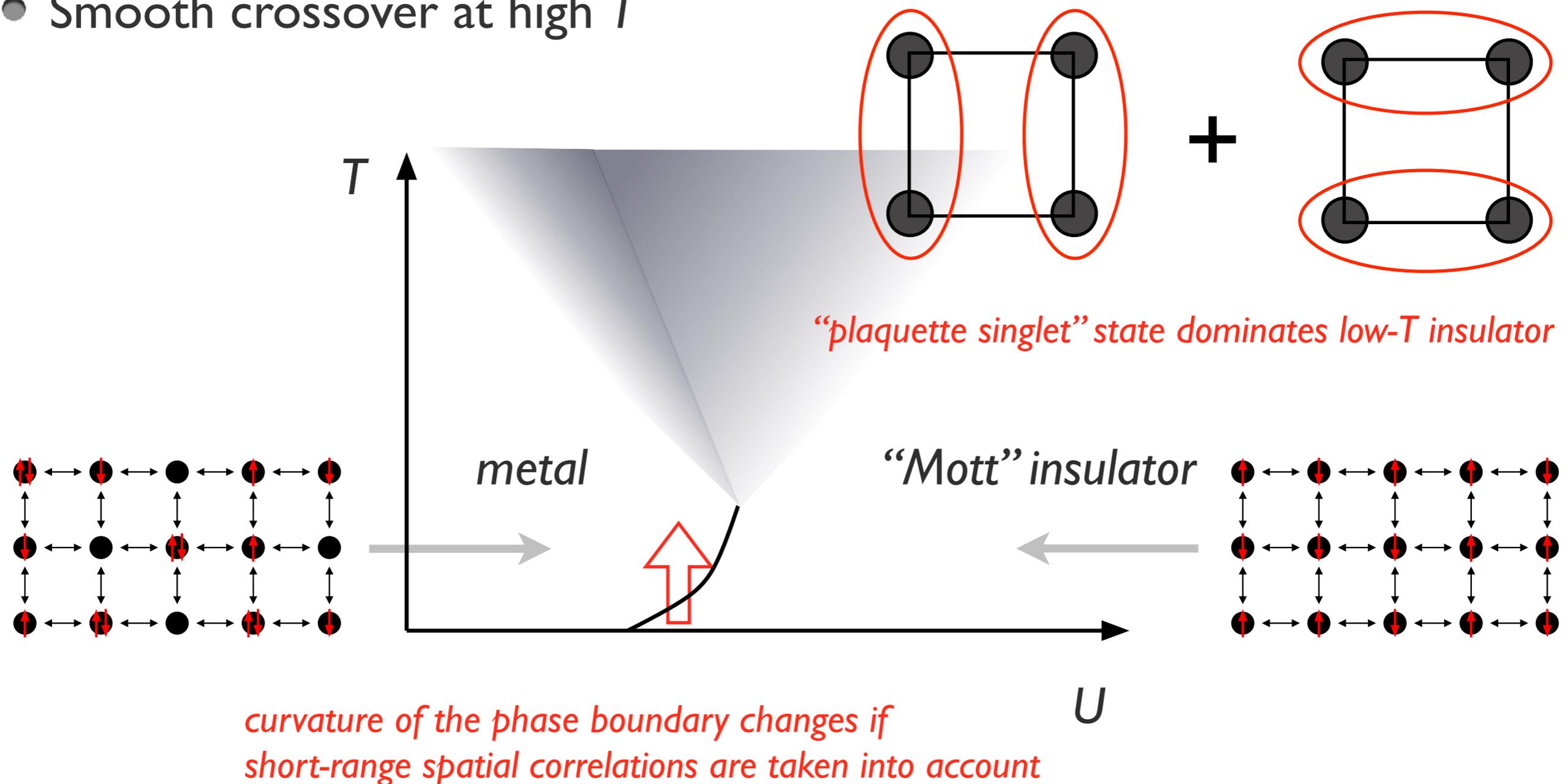
Nonequilibrium extension

- Kadanoff-Baym contour
- Initial state described by the density matrix $\rho(0) = \dfrac{1}{Z} e^{-\beta H(0)}$

- State at time t described by $\rho(t) = U(t,0)\,\rho(0)\,U(0,t)$

$$
U(t,t') \;=\; \begin{cases} \mathcal{T} \exp\left(-i \displaystyle\int_{t'}^{t} d\bar{t}\, H(\bar{t})\right) & t > t' \\[2em] \tilde{\mathcal{T}} \exp\left(-i \displaystyle\int_{t'}^{t} d\bar{t}\, H(\bar{t})\right) & t < t' \end{cases}
$$

- Time dependent expectation value of observable $\mathcal{O}$

$$
\langle \mathcal{O}(t) \rangle = \mathrm{Tr}\left[\rho(t)\mathcal{O}\right] = \mathrm{Tr}\left[U(t,0)\rho(0)U(0,t)\mathcal{O}\right]
$$

Nonequilibrium extension

- Kadanoff-Baym contour
- Express $\rho(0)$ as time-propagation along an imaginary time branch

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

$$= \mathrm{Tr}\left[\frac{1}{Z} \left(\mathcal{T}_\tau e^{-\int_0^\beta d\tau H(\tau)} \right) \left(\tilde{\mathcal{T}} e^{i \int_0^t ds H(s)} \right) \mathcal{O} \left(\mathcal{T} e^{-i \int_0^t ds H(s)} \right) \right]$$
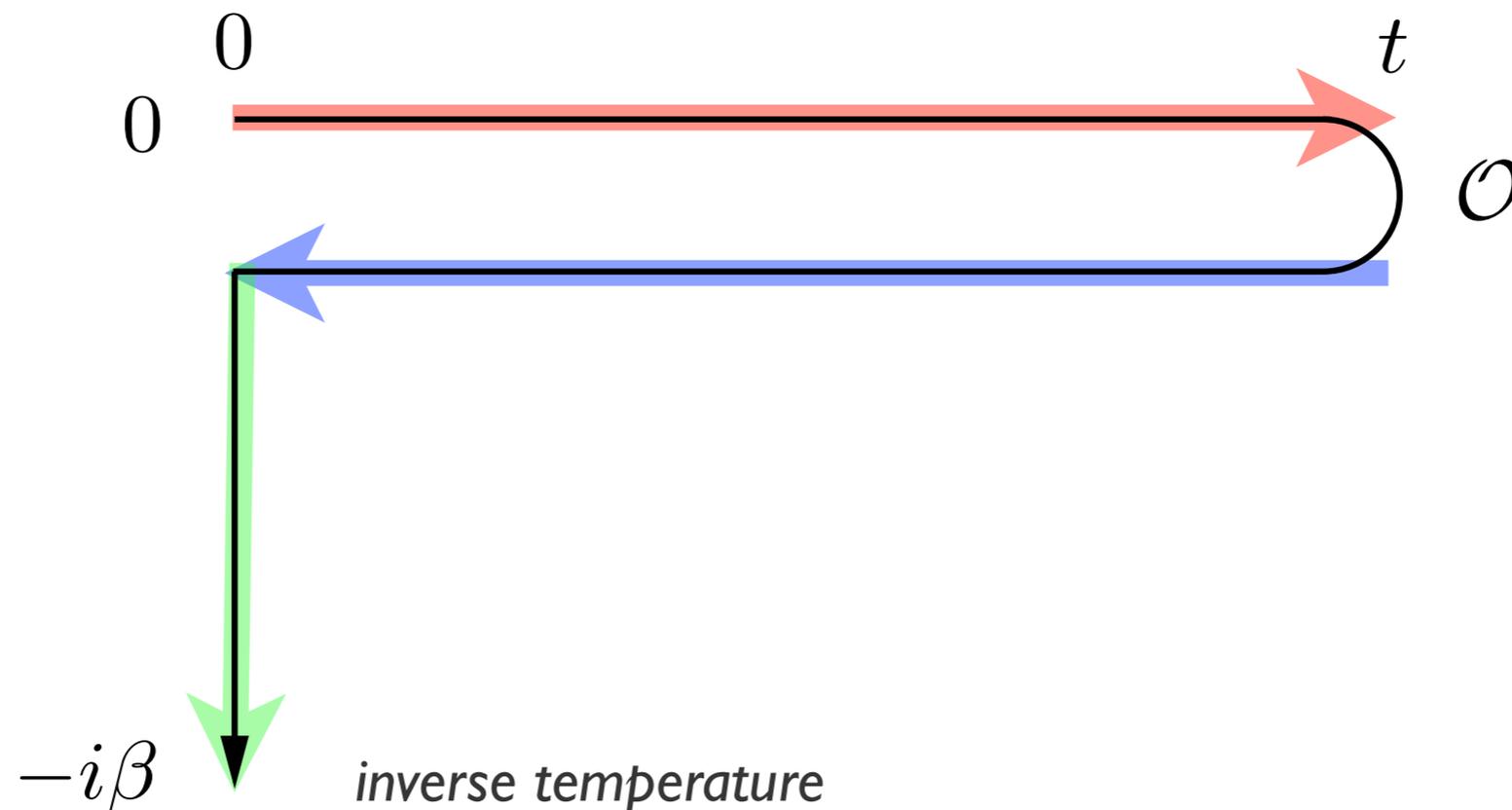
0

0

t

$\mathcal{O}$

$-i\beta$ *inverse temperature*

Nonequilibrium extension

- Kadanoff-Baym contour
- Define contour ordering $\mathcal{T}_\mathcal{C}$ on the contour $\mathcal{C}: 0 \to t \to 0 \to -i\beta$

$$\langle \mathcal{O}(t) \rangle = \frac{1}{Z} \text{Tr} \left[\mathcal{T}_\mathcal{C} \, e^{-i \int_\mathcal{C} ds \, H(s)} \mathcal{O}(t) \right]$$
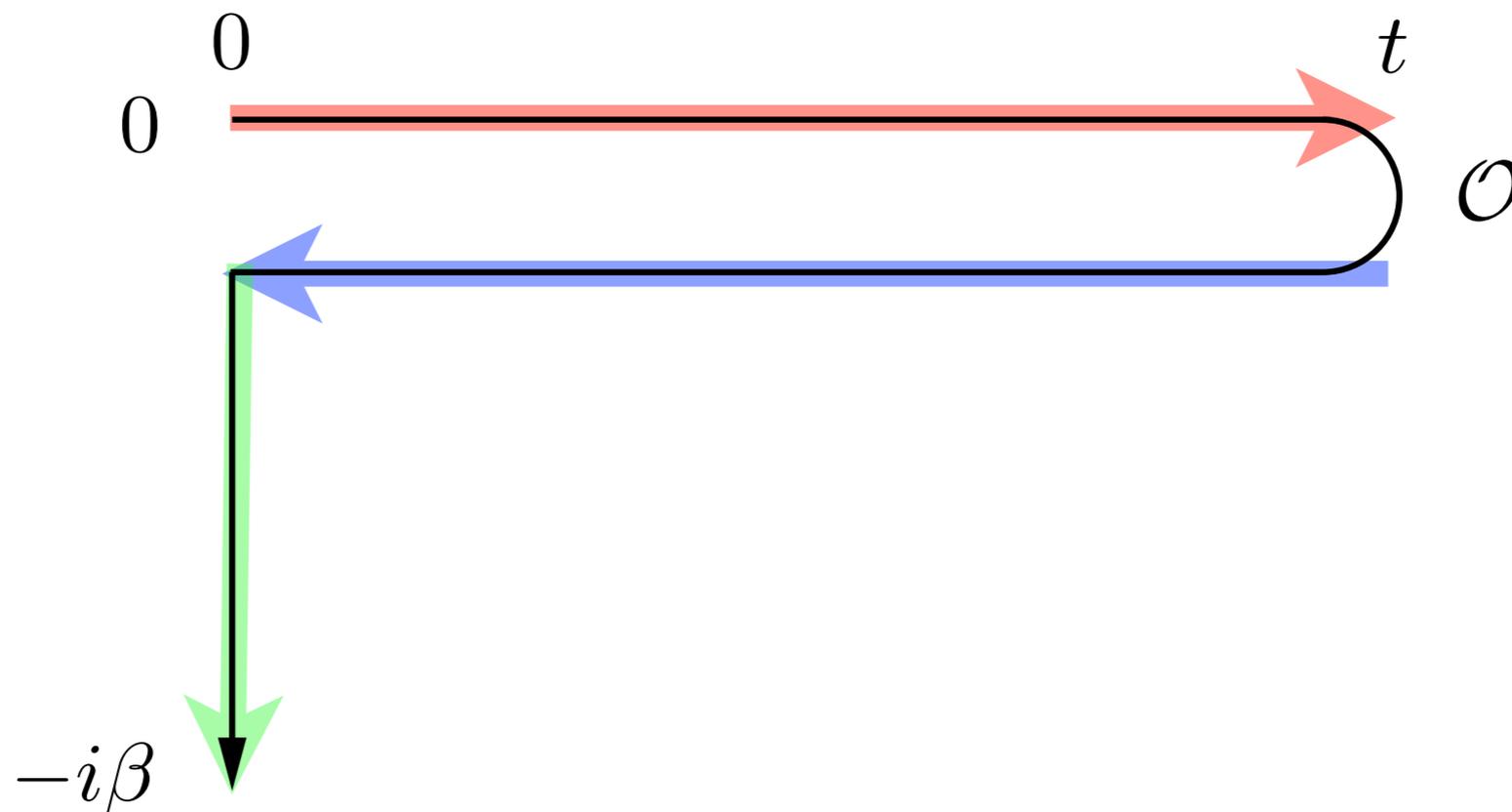
Nonequilibrium extension

- Kadanoff-Baym contour

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- Contour-ordered formalism can also be applied to 2-point functions

$$\langle \mathcal{T}_\mathcal{C} \, \mathcal{A}(t) \mathcal{B}(t') \rangle \equiv \frac{1}{Z} \mathrm{Tr} \left[\mathcal{T}_\mathcal{C} \, e^{-i \int_\mathcal{C} ds \, H(s)} \mathcal{A}(t) \mathcal{B}(t') \right]$$

- Particularly relevant: Green's function

$$G(t, t') \quad \equiv -i \langle \mathcal{T}_\mathcal{C} \, d(t) \, d^\dagger(t') \rangle$$

Nonequilibrium extension
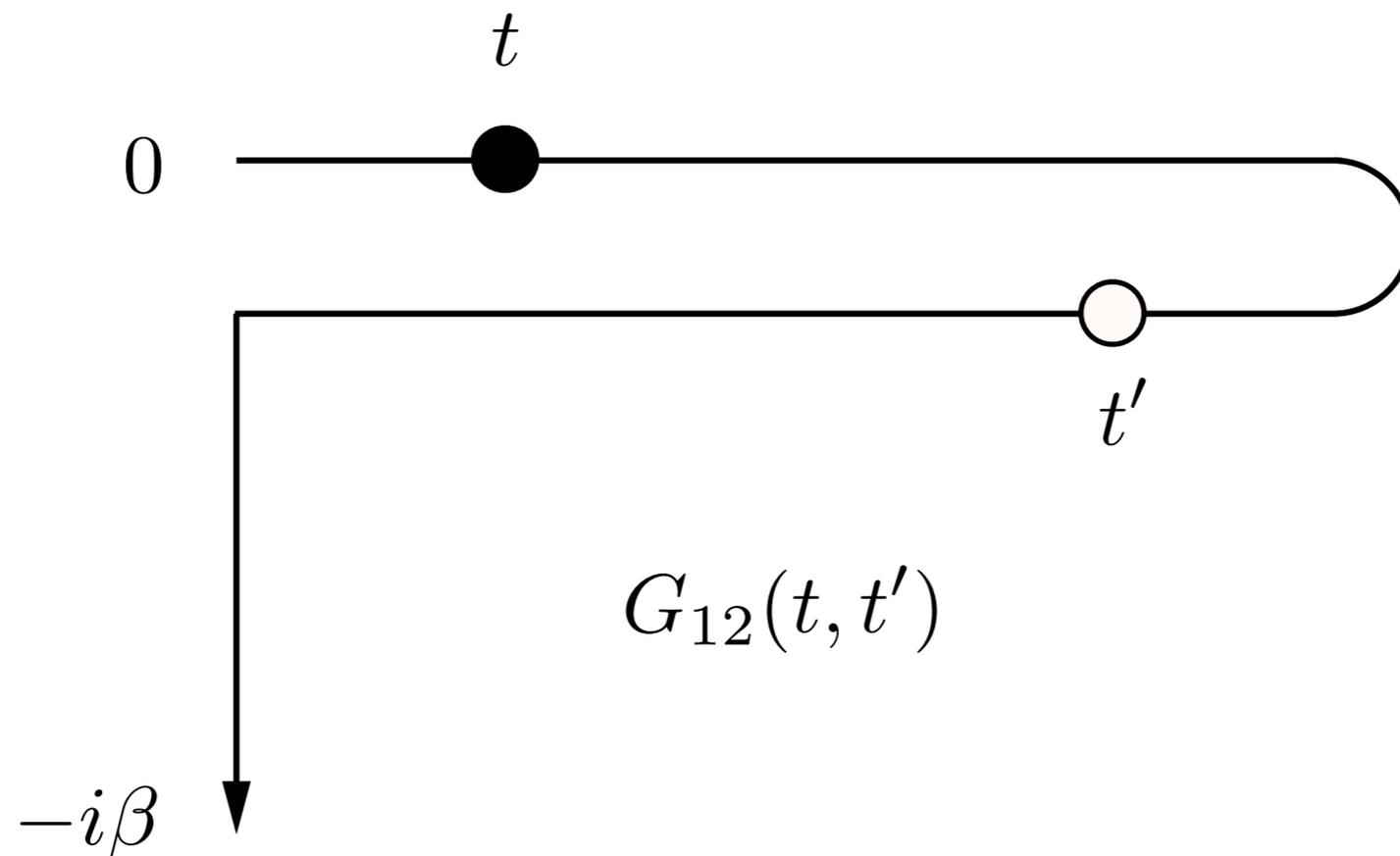
- Kadanoff-Baym contour
- Due to the 3 branches, the Green's function has 9 components

$$G(t,t') \equiv G_{ij}(t,t'), \quad t \in \mathcal{C}_i, t' \in \mathcal{C}_j, \quad i,j = 1,2,3$$

Nonequilibrium extension

- Kadanoff-Baym contour
- Due to the 3 branches, the Green's function has 9 components

$$G(t, t') \equiv G_{ij}(t, t'), \quad t \in \mathcal{C}_i, t' \in \mathcal{C}_j, \quad i, j = 1, 2, 3$$

t'

0

t

$G_{21}(t, t')$

$-i\beta$
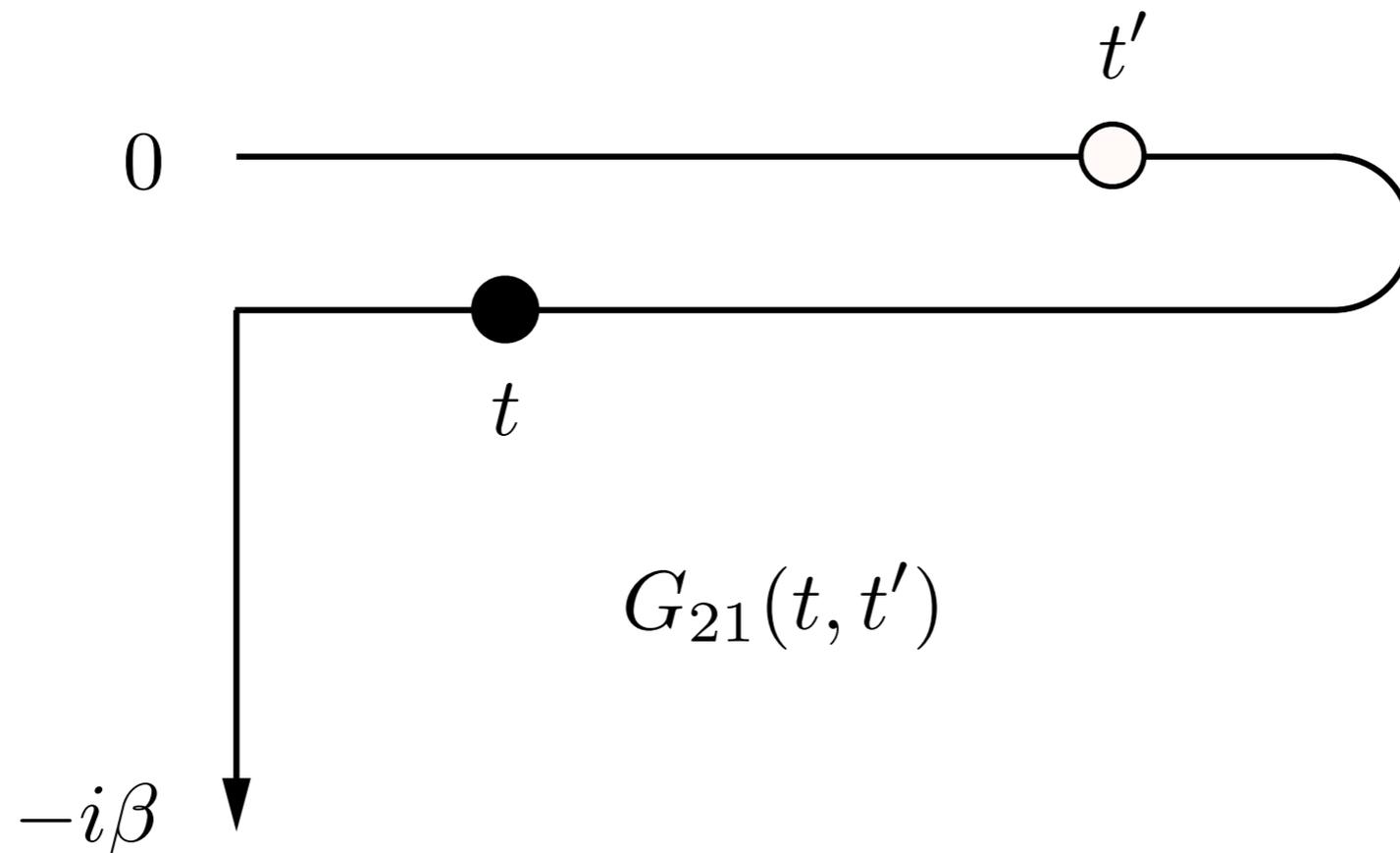
Nonequilibrium extension

- Nonequilibrium DMFT: Solve DMFT equations on the Kadanoff-Baym contour $\mathcal{C}$ *Freericks et al. (2006)*
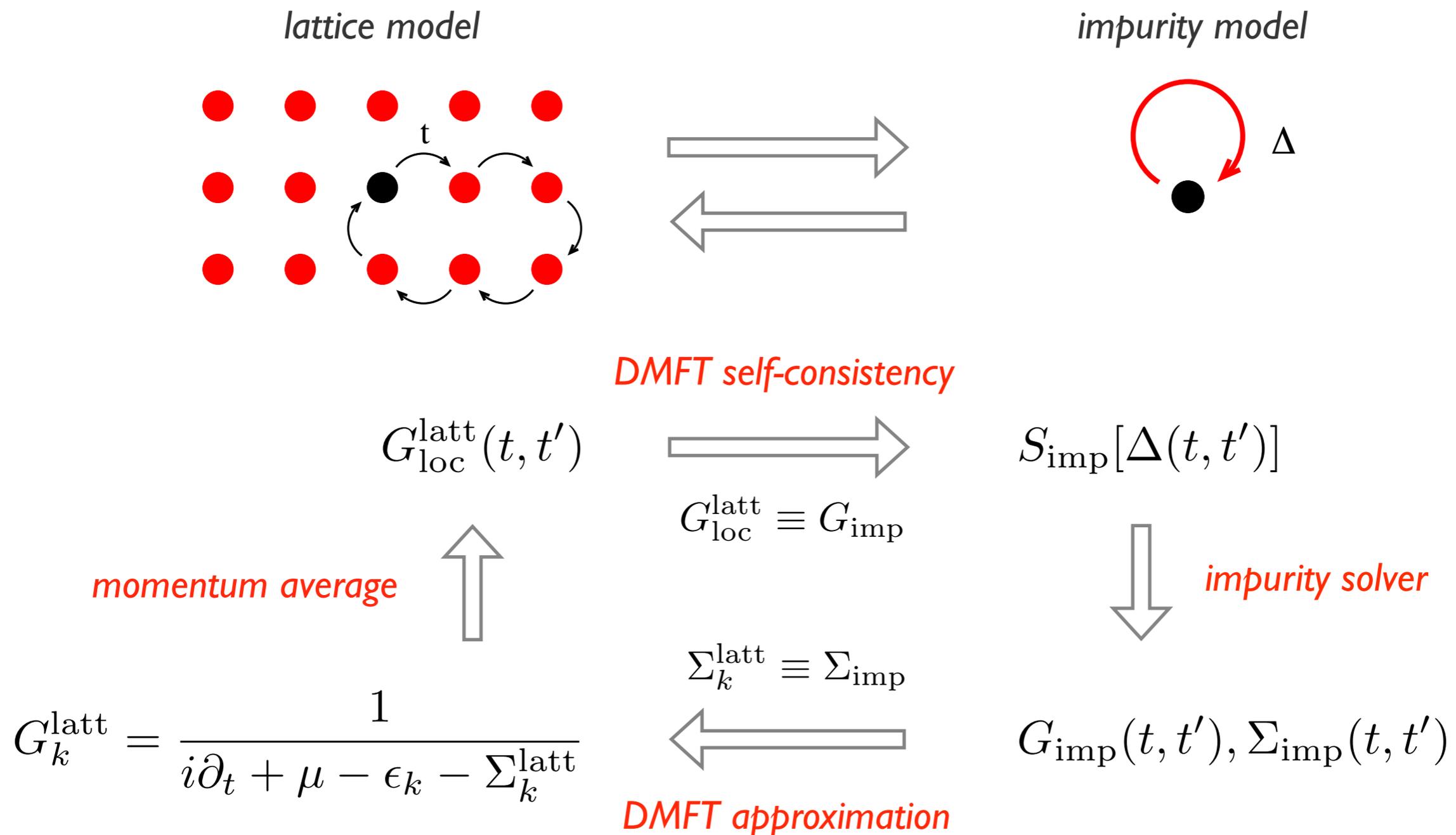
lattice model

impurity model

DMFT self-consistency

$$G_{\text{loc}}^{\text{latt}}(t, t')$$

$$G_{\text{loc}}^{\text{latt}} \equiv G_{\text{imp}}$$

$$S_{\text{imp}}[\Delta(t, t')]$$

momentum average

impurity solver

$$\Sigma_k^{\text{latt}} \equiv \Sigma_{\text{imp}}$$

$$G_k^{\text{latt}} = \frac{1}{i\partial_t + \mu - \epsilon_k - \Sigma_k^{\text{latt}}}$$

$$G_{\text{imp}}(t, t'), \Sigma_{\text{imp}}(t, t')$$

DMFT approximation

Nonequilibrium extension

- Nonequilibrium DMFT: Solve DMFT equations on the Kadanoff-Baym contour $\mathcal{C}$ *Tsuji et al. (2014)*

lattice model

cluster impurity model

DMFT self-consistency

$$G_K^{\tilde{k}\text{-av}}(t, t')$$

$$S_{\text{imp}}[\Delta_K(t, t')]$$

$$G_K^{\tilde{k}\text{-av}} \equiv G_K^{\text{imp}}$$

K-patch average

cluster solver

$$\Sigma_{K+\tilde{k}}^{\text{latt}} \equiv \Sigma_K^{\text{imp}}$$

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DMFT approximation
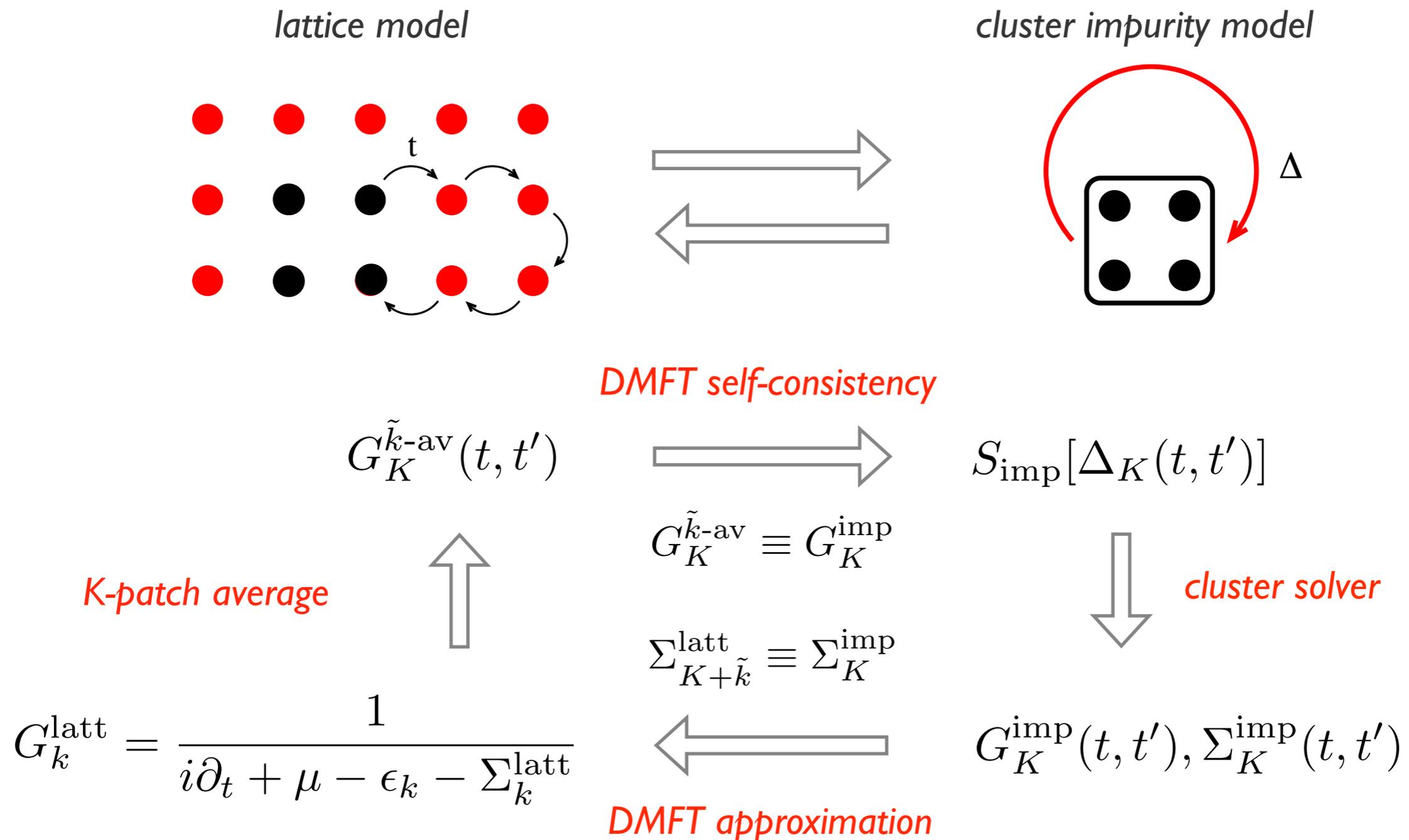
Nonequilibrium extension

- **Nonequilibrium DMFT:** Solve DMFT equations on the Kadanoff-Baym contour $\mathcal{C}$

- Nonequilibrium Anderson impurity model

$$S_{\mathrm{imp}} = -i \int_{\mathcal{C}} dt\, H_{\mathrm{loc}}(t) - i \sum_{\sigma} \int_{\mathcal{C}} dt\, dt'\, d_{\sigma}^{\dagger}(t) \Delta(t, t') d_{\sigma}(t')$$

⇑ *interaction and chemical potential terms*

⇑ *contour hybridization function*

- Hybridization function is equivalent to "Weiss" Green's function

$$\mathcal{G}_0(t, t') = (i\partial_t + \mu(t))\delta_{\mathcal{C}}(t, t') - \Delta(t, t')$$

Nonequilibrium extension

- **Nonequilibrium DMFT:** Solve DMFT equations on the Kadanoff-Baym contour $\mathcal{C}$

- Nonequilibrium Anderson impurity model

$$S_{\mathrm{imp}} = -i \int_{\mathcal{C}} dt\, H_{\mathrm{loc}}(t) - i \sum_{\sigma} \int_{\mathcal{C}} dt\, dt'\, d_{\sigma}^{\dagger}(t) \Delta(t, t') d_{\sigma}(t')$$

⇑

interaction and chemical potential terms

⇑

contour hybridization function

- Impurity Green's function

$$G_{\mathrm{imp}}(t, t') = -i \langle \mathcal{T}_{\mathcal{C}}\, d(t) d^{\dagger}(t') \rangle_{S_{\mathrm{imp}}}$$

$$\langle \cdots \rangle_{S_{\mathrm{imp}}} = \frac{\mathrm{Tr}[\mathcal{T}_{\mathcal{C}}\, \exp(S_{\mathrm{imp}}) \cdots]}{\mathrm{Tr}[\mathcal{T}_{\mathcal{C}}\, \exp(S_{\mathrm{imp}})]}$$

Nonequilibrium extension

- Impurity solver: weak-coupling continuous-time QMC *Werner et al. (2009)*

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

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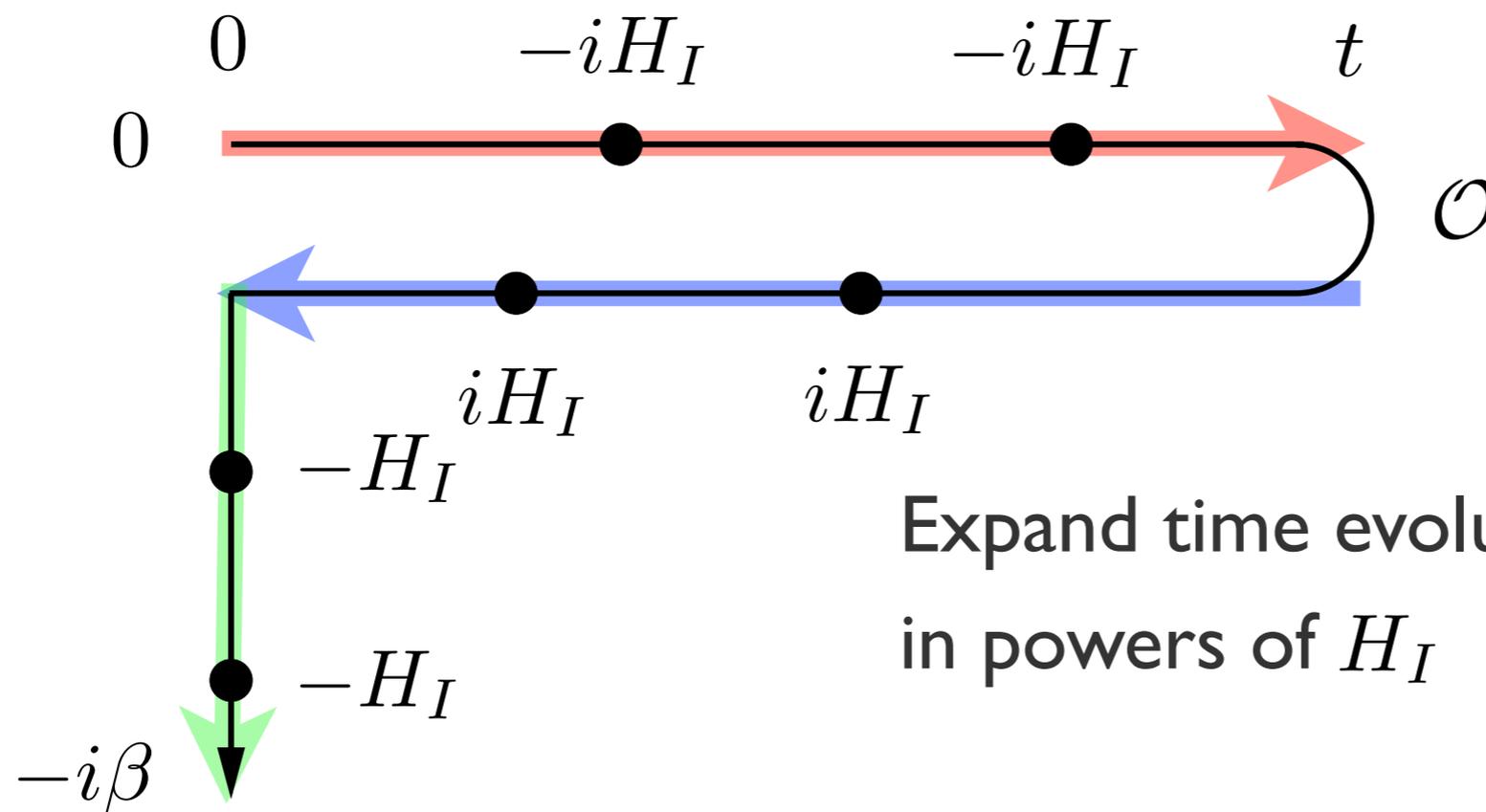
Expand time evolution operators in powers of H_I

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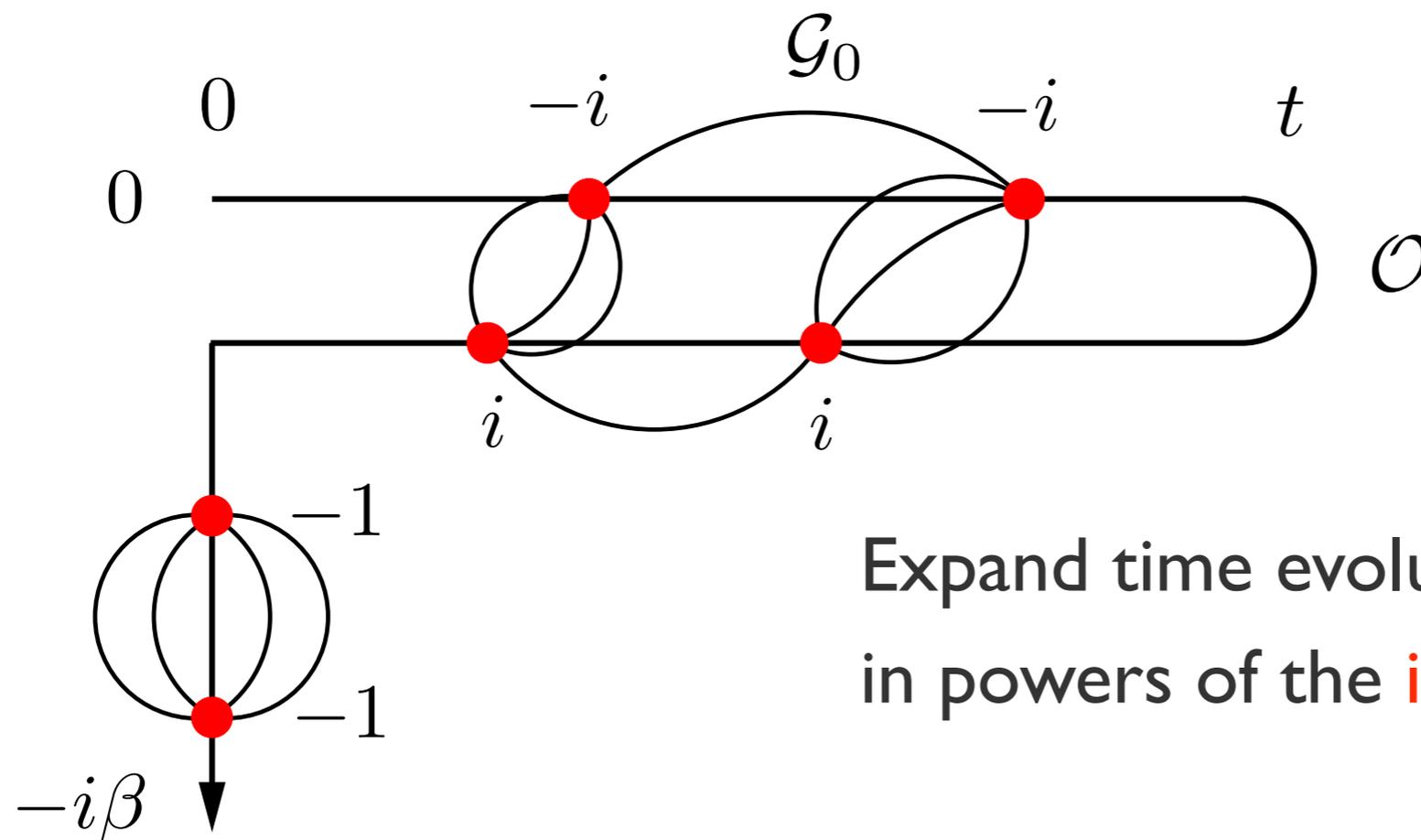
Expand time evolution operators in powers of the interaction term

Nonequilibrium extension

- **Impurity solver:** weak-coupling continuous-time QMC *Werner et al. (2009)*

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

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

- Time evolution of double occupation after a quench from *U*=0
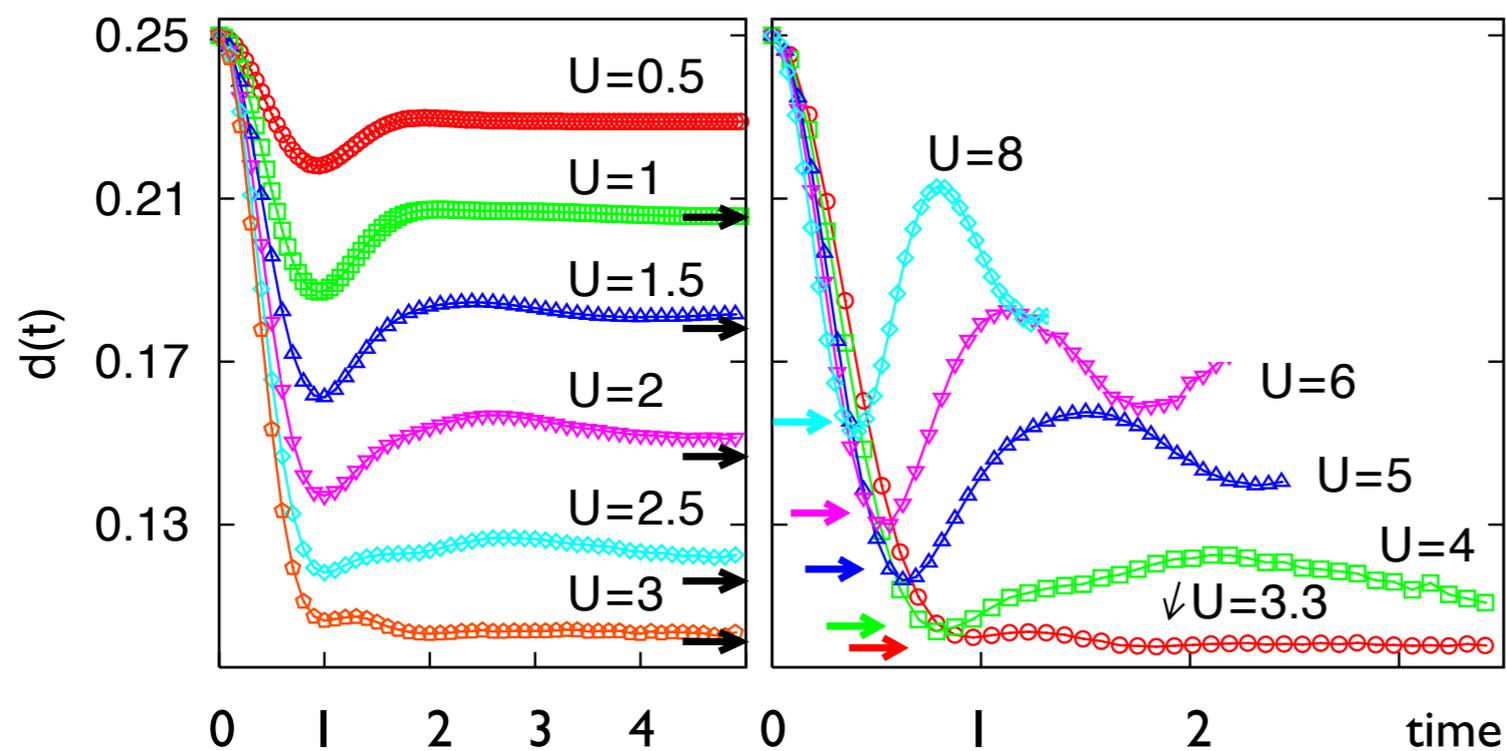
intermediate/strong correlation regime:

can reach a few inverse hopping times

Eckstein et al. (2009)

Nonequilibrium extension

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

$$\Sigma_{\text{imp}} = \overset{\displaystyle U}{\underset{t \quad t'}{}}$$

$$G_{\text{imp}} = \mathcal{G}_0 + \mathcal{G}_0 \star \Sigma_{\text{imp}} \star G_{\text{imp}}$$

$$G_{\text{imp}} = \overset{\displaystyle \mathcal{G}_0}{\longrightarrow}$$

$$+$$

$$+ \cdots$$

Nonequilibrium extension

- **Impurity solver:** weak-coupling perturbation theory
- Generate a subset of all weak-coupling diagrams by approximating the self-energy
- Boldified expansion: conserving, but not accurate

$$\Sigma_{\mathrm{imp}} = \quad U$$

$$G_{\mathrm{imp}} = \mathcal{G}_0 + \mathcal{G}_0 \star \Sigma_{\mathrm{imp}} \star G_{\mathrm{imp}}$$

$$G_{\mathrm{imp}} = \quad \mathcal{G}_0$$

Nonequilibrium extension

- Impurity solver: weak-coupling perturbation theory
- Generate a subset of all weak-coupling diagrams by approximating the self-energy
- Boldified expansion: conserving, but not accurate *Eckstein et al. (2009)*
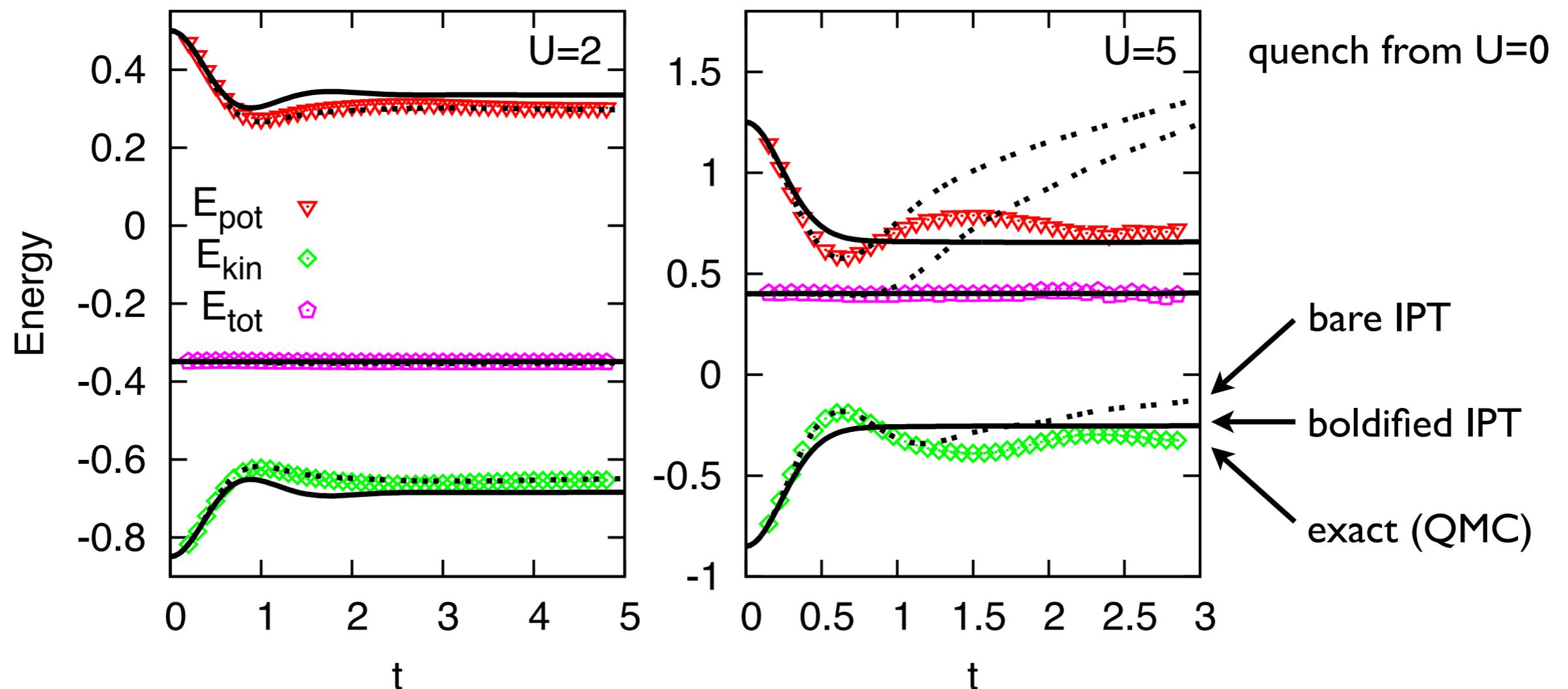
Nonequilibrium extension

- Impurity solver: Strong-coupling perturbation theory

- Introduce pseudo-particle propagators G_α for local states $\{0, \uparrow, \downarrow, \uparrow\downarrow\}$

- Approximate pseudo-particle self-energy
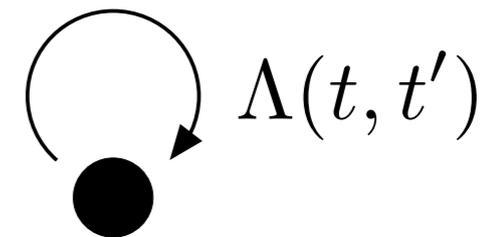
Non-crossing approximation (NCA)

Keiter & Kimball (2009)

Nonequilibrium extension

- **Impurity solver:** Strong-coupling perturbation theory

- Introduce pseudo-particle propagators G_α for local states $\{0, \uparrow, \downarrow, \uparrow\downarrow\}$

- Approximate pseudo-particle self-energy

$$\Sigma_\alpha = \underset{t \;\; G_\beta \;\; t'}{\overset{\Lambda}{\cdots\cdots}} + \cdots\cdots + \cdots$$

$$\Lambda(t, t')$$

$$G_\alpha = \overset{G_{0,\alpha}}{\longrightarrow}$$

One-crossing approximation (OCA)

Pruschke & Grewe (1989)

$$+ \quad \longrightarrow\!\!\!\frown\!\!\!\longrightarrow$$

$$+ \quad \longrightarrow\!\!\frown\!\!\frown\!\!\longrightarrow \qquad + \quad \longrightarrow\!\!\frown\!\!\!\frown\!\!\longrightarrow$$

Nonequilibrium extension

- Impurity solver: Strong-coupling perturbation theory

- Introduce pseudo-particle propagators G_α for local states $\{0, \uparrow, \downarrow, \uparrow\downarrow\}$

- Approximate pseudo-particle self-energy
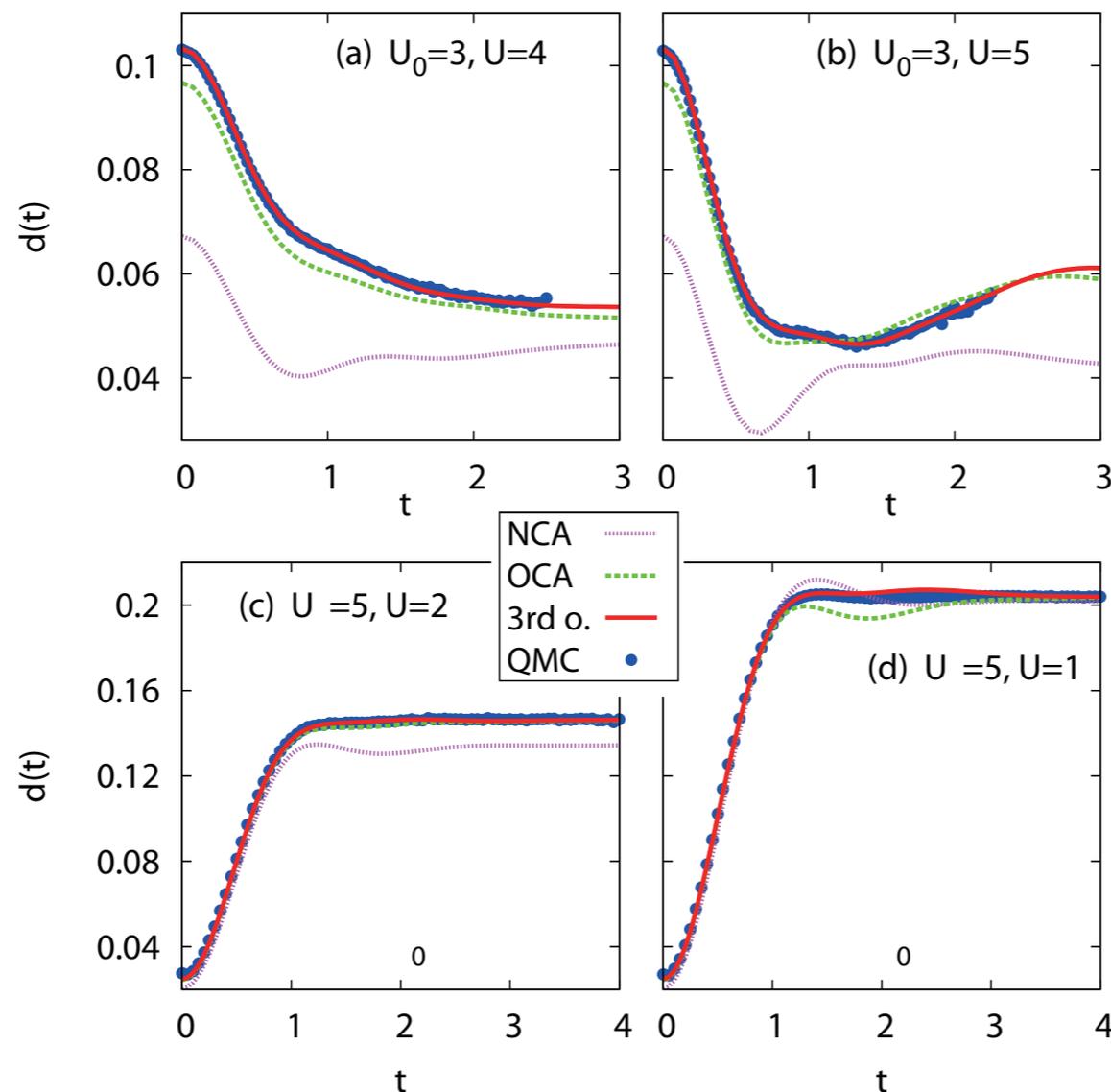
conserving approximation

systematically converging to the exact result

accurate in the strong-coupling regime

Eckstein & Werner (2010)

Nonequilibrium extension

- Calculation of the lattice Green's function

- Noninteracting lattice:

$$H_0(t) = \sum_k [\epsilon_k(t) - \mu(t)] d_k^\dagger d_k$$

$$G_{0,k}(t,t') = -i\langle \mathcal{T}_\mathcal{C} d_k(t) d_k^\dagger(t') \rangle_0$$

- Green's function satisfies:

$$\big[i\partial_t + \mu(t) - \epsilon_k(t)\big] G_{0,k}(t,t') = \delta_\mathcal{C}(t,t')$$

$$G_{0,k}(t,t')\big[-i\overleftarrow{\partial_{t'}} + \mu(t') - \epsilon_k(t')\big] = \delta_\mathcal{C}(t,t')$$

- Inverse lattice Green's function:

$$G_{0,k}^{-1}(t,t') = \delta_\mathcal{C}(t,t')[i\partial_t + \mu(t) - \epsilon_k(t)]$$

$$G_{0,k}^{-1} \star G_{0,k} = G_{0,k} \star G_{0,k}^{-1} = \delta_\mathcal{C}$$

Nonequilibrium extension

- Calculation of the lattice Green's function

- Interacting lattice Green's function satisfies Dyson equation:

$$
\begin{aligned}
G_k &= G_{0,k} + G_{0,k} \star \Sigma \star G_k \\
&= G_{0,k} + G_k \star \Sigma \star G_{0,k}
\end{aligned}
$$

integral form

⇑

impurity self-energy (DMFT)

$$[G_{0,k}^{-1} - \Sigma] \star G_k = G_k \star [G_{0,k}^{-1} - \Sigma] = \delta_{\mathcal{C}}$$ *differential form*

- Imaginary-time branch: boundary-value problem ⟶ solve by FT

$$G_k(i\omega_n) = \frac{1}{G_{0,k}^{-1}(i\omega_n) - \Sigma(i\omega_n)} = \frac{1}{i\omega_n + \mu(0) - \epsilon_k(0) - \Sigma(i\omega_n)}$$

- Usual equilibrium DMFT calculation for the initial equilibrium state

Nonequilibrium extension

- Calculation of the lattice Green's function

- Interacting lattice Green's function satisfies Dyson equation:

$$G_k \;=\; G_{0,k} + G_{0,k} \star \Sigma \star G_k$$
$$ \;=\; G_{0,k} + G_k \star \Sigma \star G_{0,k}$$

integral form

$\Uparrow$

impurity self-energy (DMFT)

$$[G_{0,k}^{-1} - \Sigma] \star G_k = G_k \star [G_{0,k}^{-1} - \Sigma] = \delta_{\mathcal{C}}$$

differential form

- Real-time branches: initial-value problem

$$[i\partial_t + \mu(t) - \epsilon_k(t)]G_k(t,t') - \int_{\mathcal{C}} d\bar{t}\, \Sigma(t,\bar{t})G_k(\bar{t},t') = \delta_{\mathcal{C}}(t,t')$$

- Defines time-propagation scheme for *G* in which the self-energy plays the role of a memory-kernel

Nonequilibrium extension

- Calculation of the lattice Green's function

0 t

0

$-i\beta$

vertical branch:
initial equilibrium
state

*propagate and converge the DMFT
solution step by step along the
real-time axis*

- Real-time branches: initial-value problem

$$[i\partial_t + \mu(t) - \epsilon_k(t)]G_k(t,t') - \int_{\mathcal{C}} d\bar{t}\, \Sigma(t,\bar{t})G_k(\bar{t},t') = \delta_{\mathcal{C}}(t,t')$$

- Defines time-propagation scheme for G in which the self-energy plays the role of a memory-kernel

Nonequilibrium extension

- Calculation of the lattice Green's function

- Open source library:

nessi.tuxfamily.org

Nonequilibrium extension

- Electric fields

- Vector potential $A(r,t)$, scalar potential $\Phi(r,t)$: $E = -\nabla \Phi - \partial_t A$

$$v_{ij}(t) = v_{ij} \exp\left(-ie \int_{R_i}^{R_j} dr\, A(r,t)\right)$$

$$\Downarrow$$
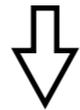
$$
\begin{aligned}
H(t) \quad = \quad & -\sum_{\langle ij \rangle \sigma} v_{ij}(t)(d_{i\sigma}^\dagger d_{j\sigma} + d_{j\sigma}^\dagger d_{i\sigma}) \\
& +U(t) \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_{i\sigma} \mu(t) n_{i\sigma}
\end{aligned}
$$

$$\Uparrow$$

$$\mu(t) = \mu + e\Phi(R_i, t)$$

- Convenient choice: gauge with pure vector potential:

$$\Phi \equiv 0, \quad E = -\partial_t A$$

Nonequilibrium extension

- **Electric fields**

- Neglecting the *r*-dependence of *A* (assumption: field varies slowly on the atomic scale):

$$v_{ij}(t) = v_{ij} \exp\left(-ie \int_{R_i}^{R_j} dr \, A(t)\right) \qquad A(t) = -\int_0^t ds E(s)$$

⇩ *Fourier transformation*

$$\epsilon_k(t) = \epsilon_{k-eA(t)}$$

- Electric field enters in the lattice Dyson equation in the form of a time-dependent dispersion:

$$[i\partial_t + \mu(t) - \epsilon_k(t)]G_k(t,t') - \int_{\mathcal{C}} d\bar{t} \, \Sigma(t,\bar{t})G_k(\bar{t},t') = \delta_{\mathcal{C}}(t,t')$$

Spectroscopy

- "Physical" Green's functions

- The 9 elements of the 3x3 Green's function matrix

$$\hat{G} \;=\; \begin{pmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{pmatrix}$$

are not independent:

$$G_{21}(t, t')$$

Spectroscopy

- "Physical" Green's functions
- The 9 elements of the 3x3 Green's function matrix

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are not independent:
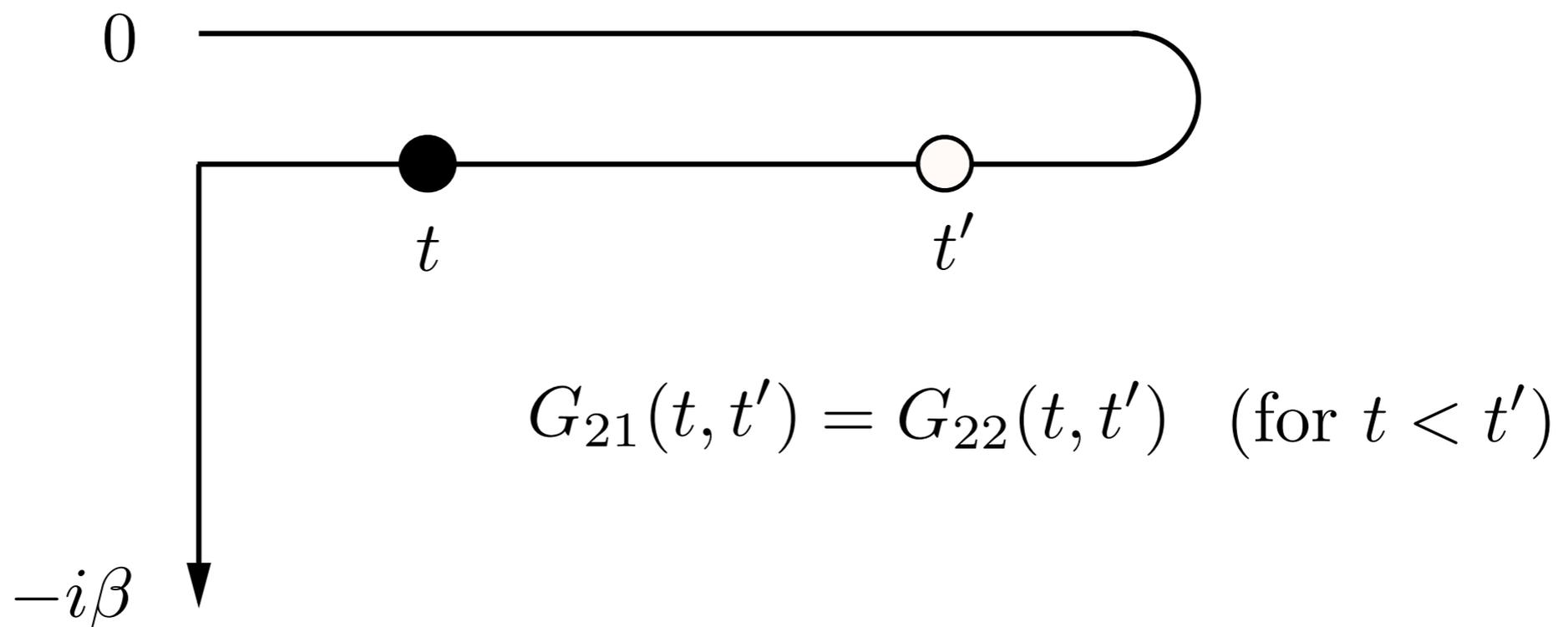
$$G_{21}(t, t') = G_{22}(t, t') \quad (\text{for } t < t')$$

Spectroscopy

- "Physical" Green's functions
- We have the following redundancies

$$
\begin{aligned}
G_{11}(t, t') &= G_{12}(t, t') && \text{(for } t \leq t') \\
G_{11}(t, t') &= G_{21}(t, t') && \text{(for } t > t') \\
G_{22}(t, t') &= G_{21}(t, t') && \text{(for } t < t') \\
G_{22}(t, t') &= G_{12}(t, t') && \text{(for } t \geq t') \\
G_{13}(t, \tau') &= G_{23}(t, \tau') \\
G_{31}(\tau, t') &= G_{32}(\tau, t')
\end{aligned}
$$

which allow to eliminate 3 of the 9 components
→ define 6 "physical" Green's functions

$$
G^R, G^A, G^K, \ldots
$$

Spectroscopy

- "Physical" Green's functions
- Relevant for the following discussion: Retarded Green's function

$$G^R(t, t') = \tfrac{1}{2}(G_{11} - G_{12} + G_{21} - G_{22}) = -i\theta(t - t')\langle\{d(t), d^\dagger(t')\}\rangle$$

and lesser Green's functions

$$G^<(t, t') = G_{12} = i\langle d^\dagger(t')d(t)\rangle$$

- In equilibrium:

  - Spectral function: $A(\omega) = -\tfrac{1}{\pi}\operatorname{Im} G^R(\omega)$

  - Occupation: $N(\omega) = \tfrac{1}{2\pi}\operatorname{Im} G^<(\omega)$

  - Distribution function: $N(\omega)/A(\omega) = f(\omega)$ *Fermi function*

Spectroscopy

- "Physical" Green's functions
- Relevant for the following discussion: Retarded Green's function

$$G^R(t, t') = \tfrac{1}{2}(G_{11} - G_{12} + G_{21} - G_{22}) = -i\theta(t - t')\langle\{d(t), d^\dagger(t')\}\rangle$$

  and lesser Green's functions

$$G^<(t, t') = G_{12} = i\langle d^\dagger(t')d(t)\rangle$$

- Out of equilibrium: $t_{\text{av}} = (t + t')/2, t_{\text{rel}} = t - t'$

  - Spectral function: $A(\omega, t_{\text{av}}) = -\tfrac{1}{\pi}\text{Im} \int dt_{\text{rel}} e^{i\omega t_{\text{rel}}} G^R(t, t')$

  - Occupation: $N(\omega, t_{\text{av}}) = \tfrac{1}{2\pi}\text{Im} \int dt_{\text{rel}} e^{i\omega t_{\text{rel}}} G^<(t, t')$

  - "Distribution function": $N(\omega, t_{\text{av}})/A(\omega, t_{\text{av}})$

Spectroscopy

- Time-resolved photoemission spectrum *Freericks et al. (2009)*

$$\cos[\Omega(t - t_p + \phi)]S(t - t_p)$$

probe envelope
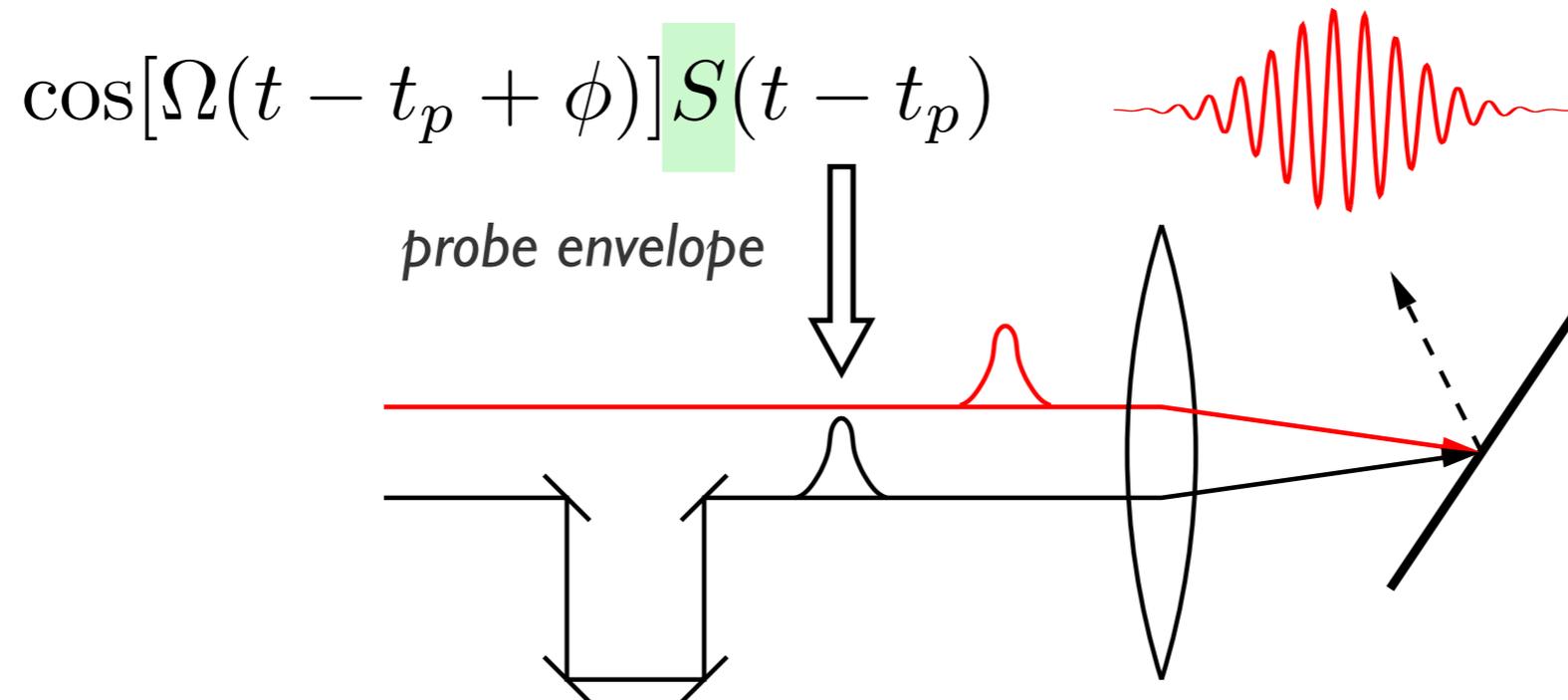
$$I(k_f, E; t_p) \propto \sum_k \delta_{k_\parallel + q_\parallel, k_{f\parallel}} I_k(E - \hbar\Omega_q - W; t_p),$$

$$I_k(\omega; t_p) = -i \int dt dt' S(t)S(t') e^{i\omega(t' - t)} G_k^<(t + t_p, t' + t_p)$$

probe time

Spectroscopy

- Time-resolved photoemission spectrum   *Freericks et al. (2009)*
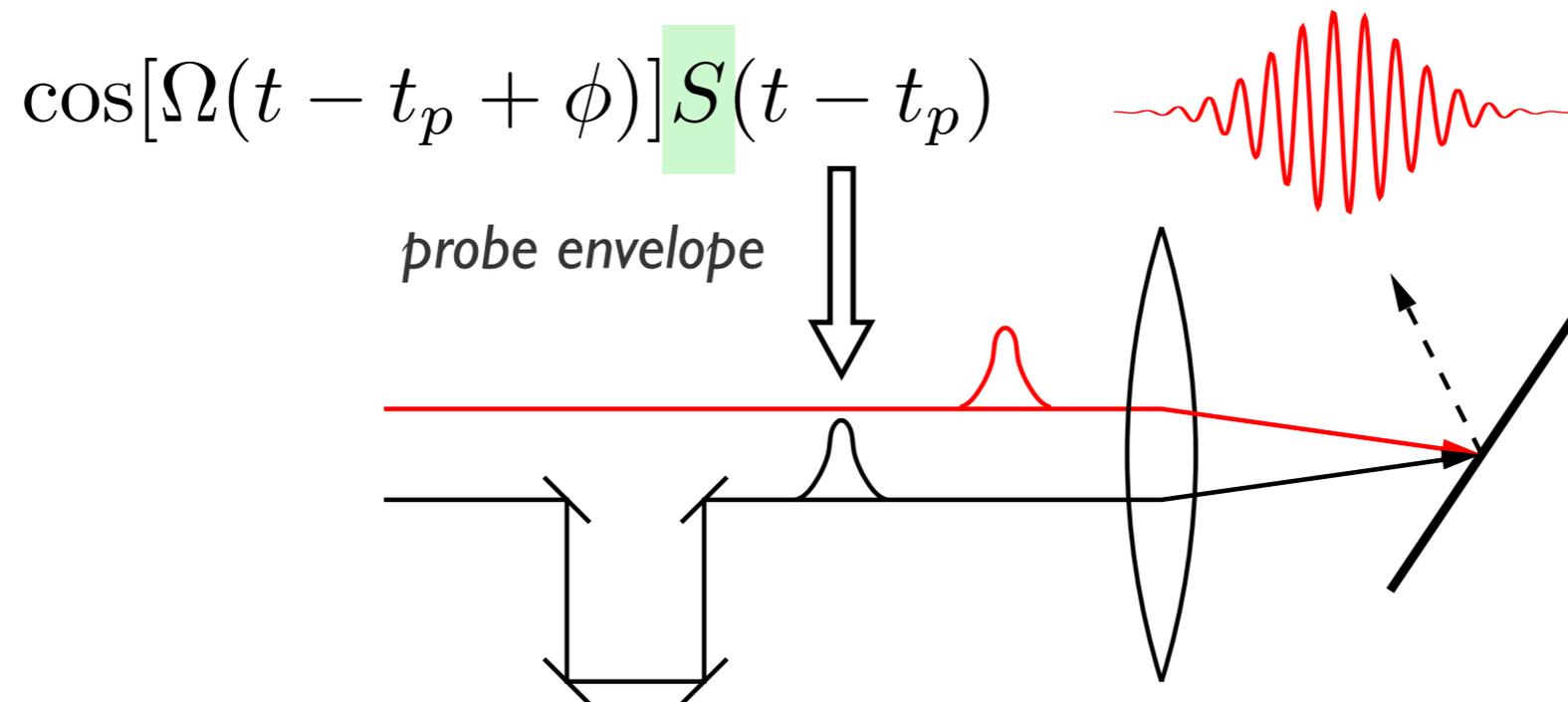
$$\cos[\Omega(t - t_p + \phi)]S(t - t_p)$$

probe envelope

$$I(k_f, E; t_p) \propto \sum_k \delta_{k_\parallel + q_\parallel, k_{f\parallel}} I_k(E - \hbar\Omega_q - W; t_p),$$

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- Formula contains time-energy uncertainty

Spectroscopy

- Time-resolved photoemission spectrum *Freericks et al. (2009)*

$$\cos[\Omega(t - t_p + \phi)]S(t - t_p)$$

probe envelope
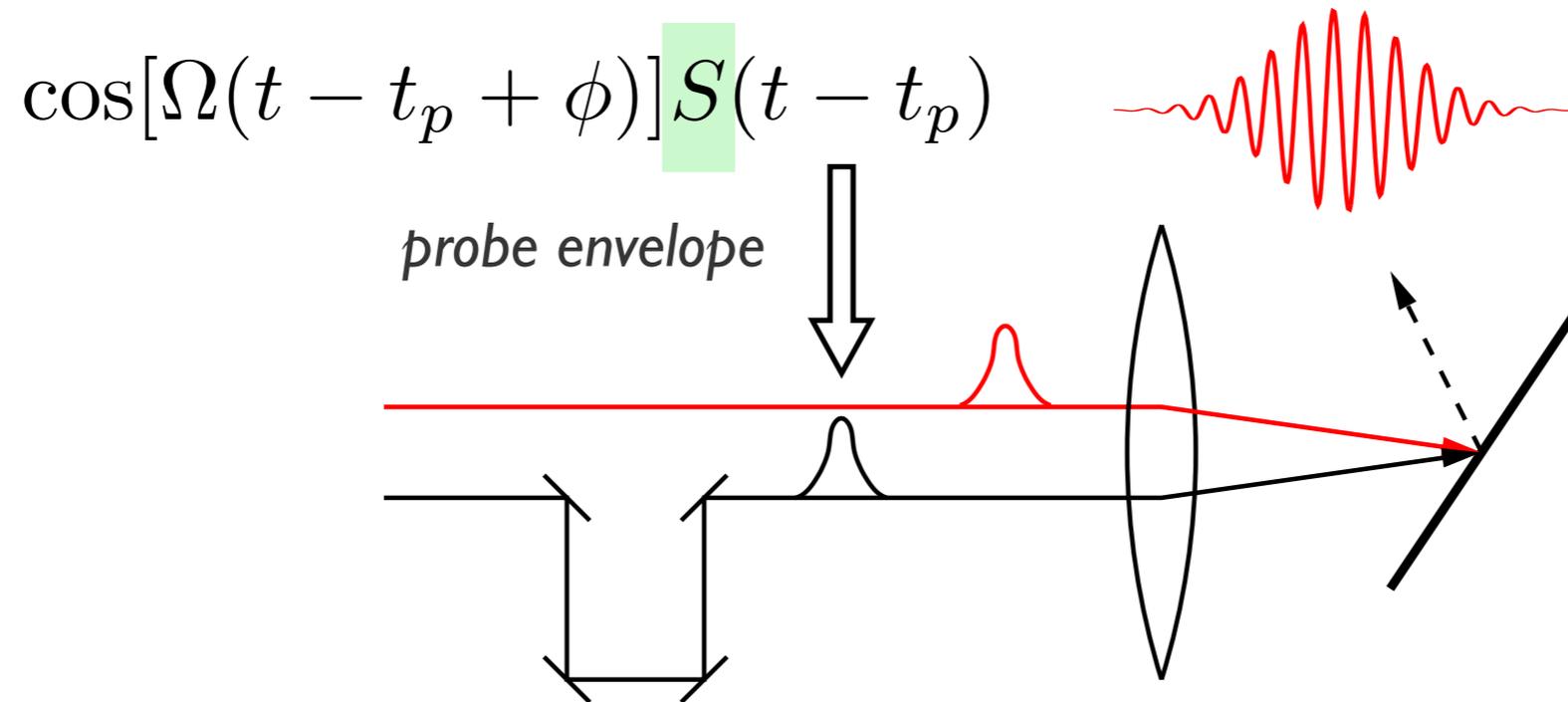
$S(t) \sim \delta(t - t_p) :$ measure occupation $n_k(t_p)$

$S(t) \sim \mathrm{const} :$ measure spectral function $A_k(\omega, t_p)$

$$I_k(\omega; t_p) = -i \int dt\, dt'\, S(t) S(t') e^{i\omega(t' - t)} G_k^<(t + t_p, t' + t_p)$$

- Formula contains time-energy uncertainty

Accuracy of nonequilibrium DMFT

- Benchmark against DMRG for 1D Hubbard model
  - Quench from *U=0* to *U=1*

Tsuji, Barmettler, Aoki & Werner (2014)
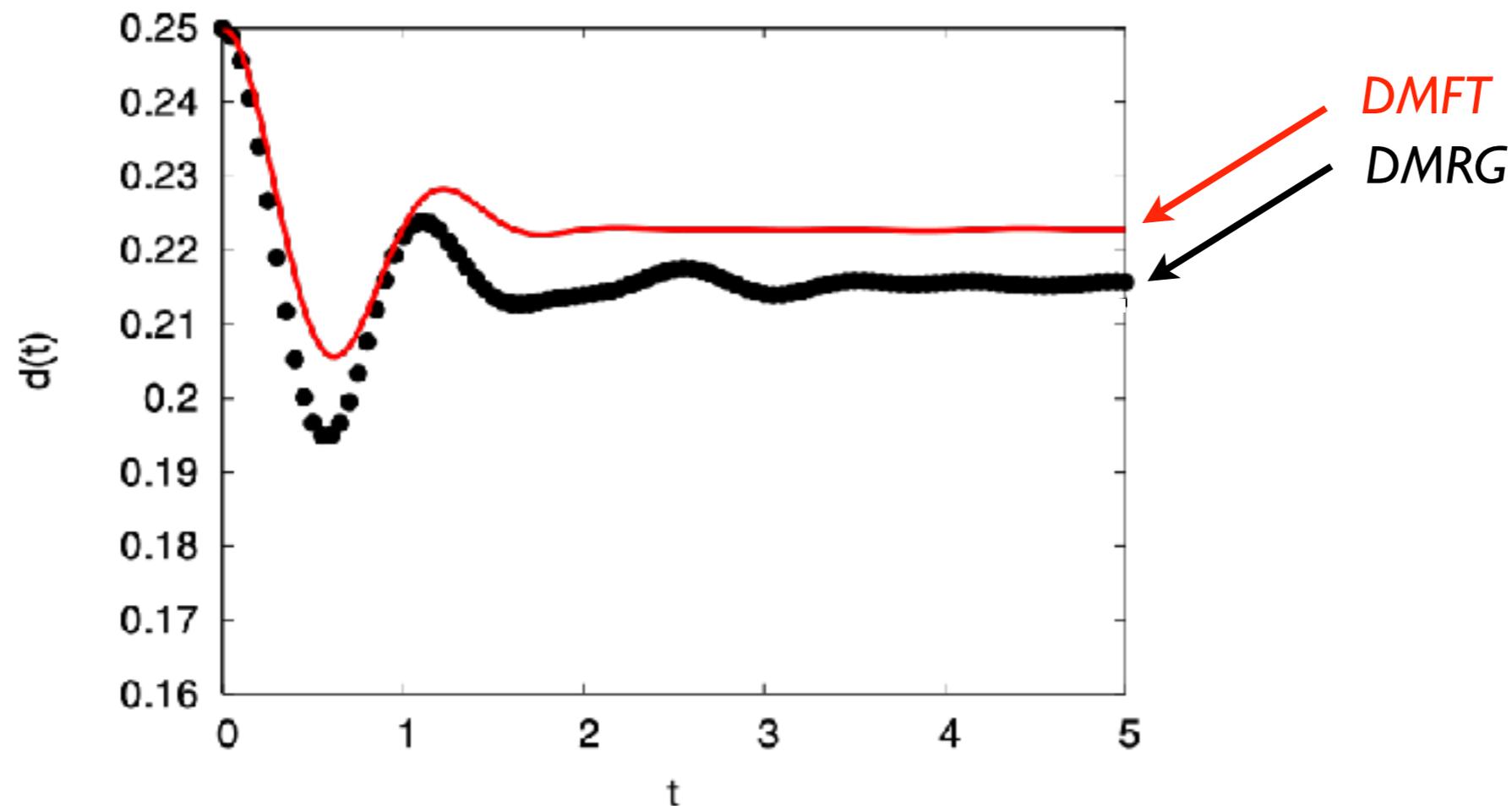
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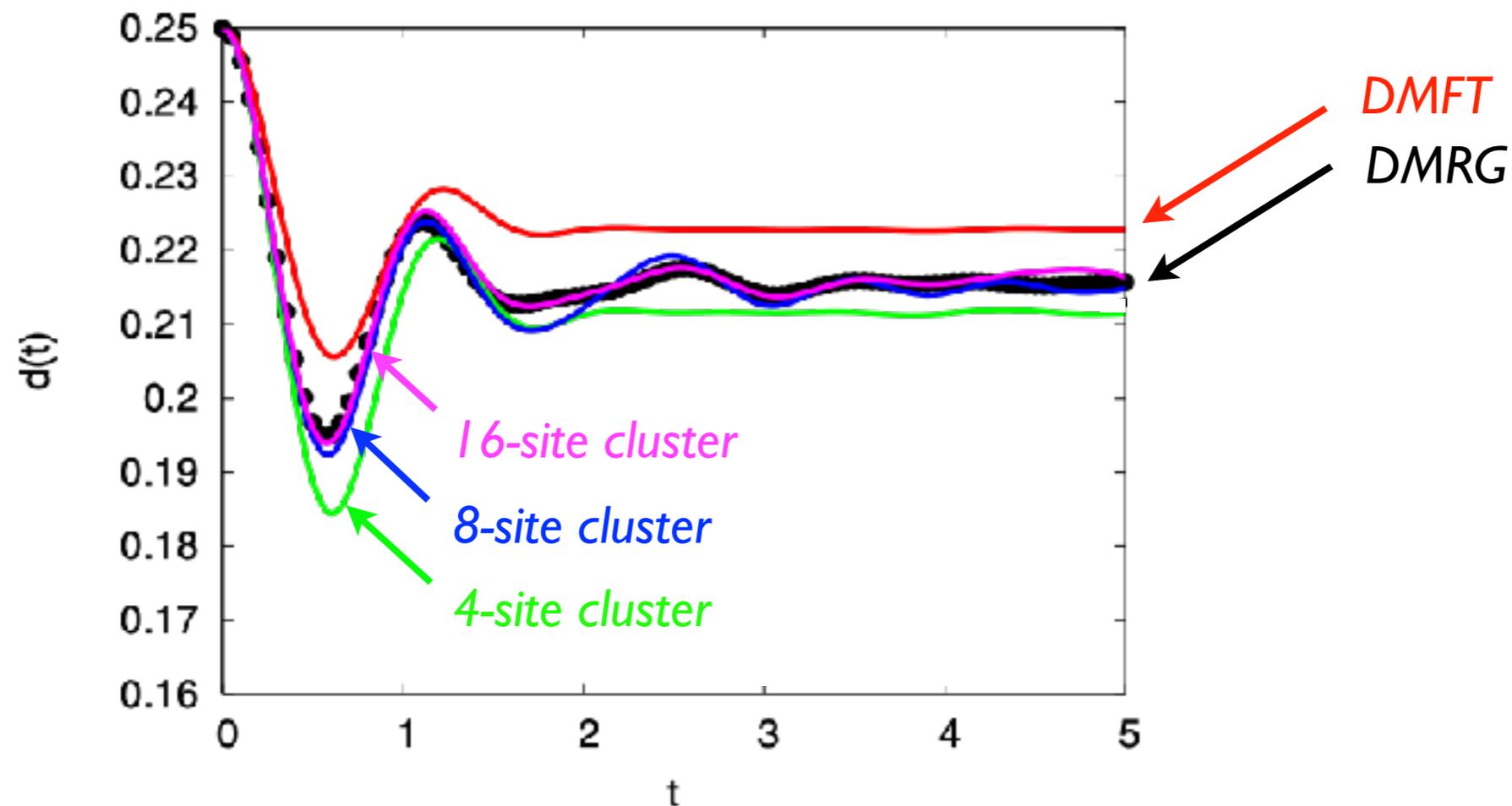
- Cluster extensions of DMFT capture short-range correlations

  Tsuji et al. (2014); Eckstein & Werner (2016); Bittner et al. (2019)

Accuracy of nonequilibrium DMFT

- **Benchmark against cold atom simulator** *Sandholzer et al. (2019)*
  - Resonant excitation ($\Omega = U$) of Mott insulating Hubbard model
  - linear ramp of pulse amplitude K_0
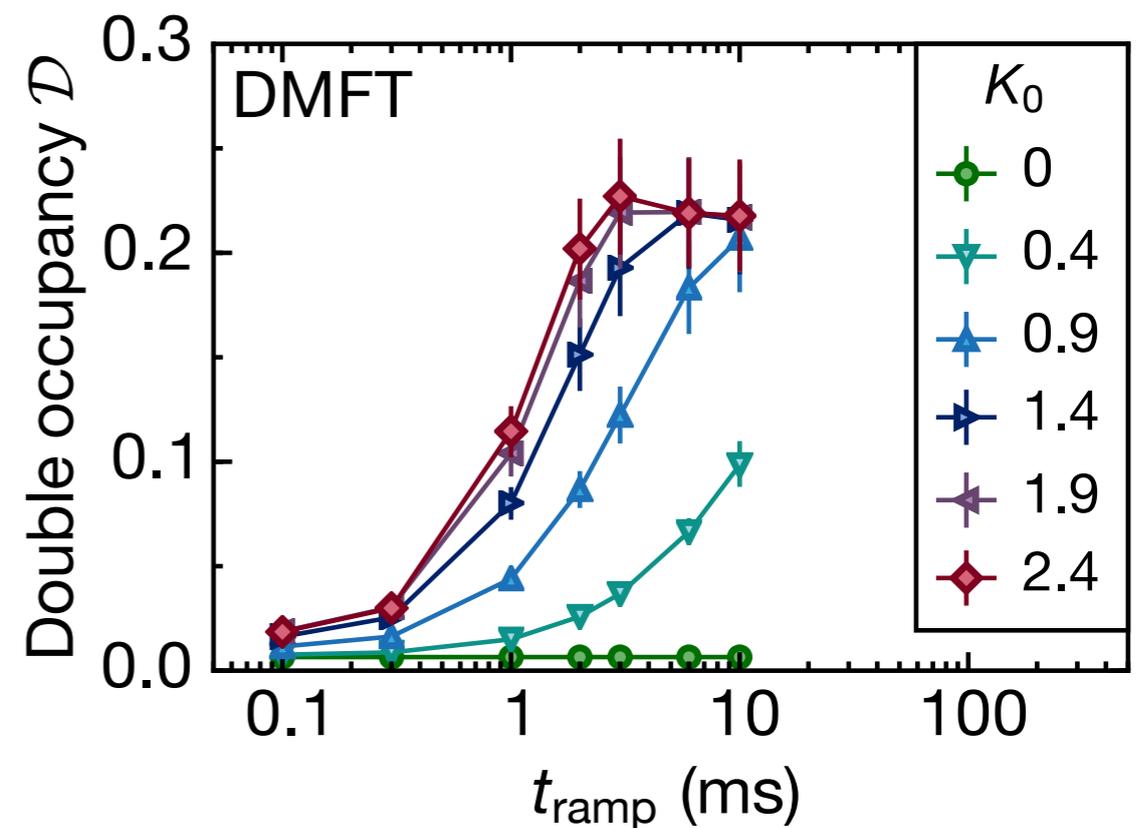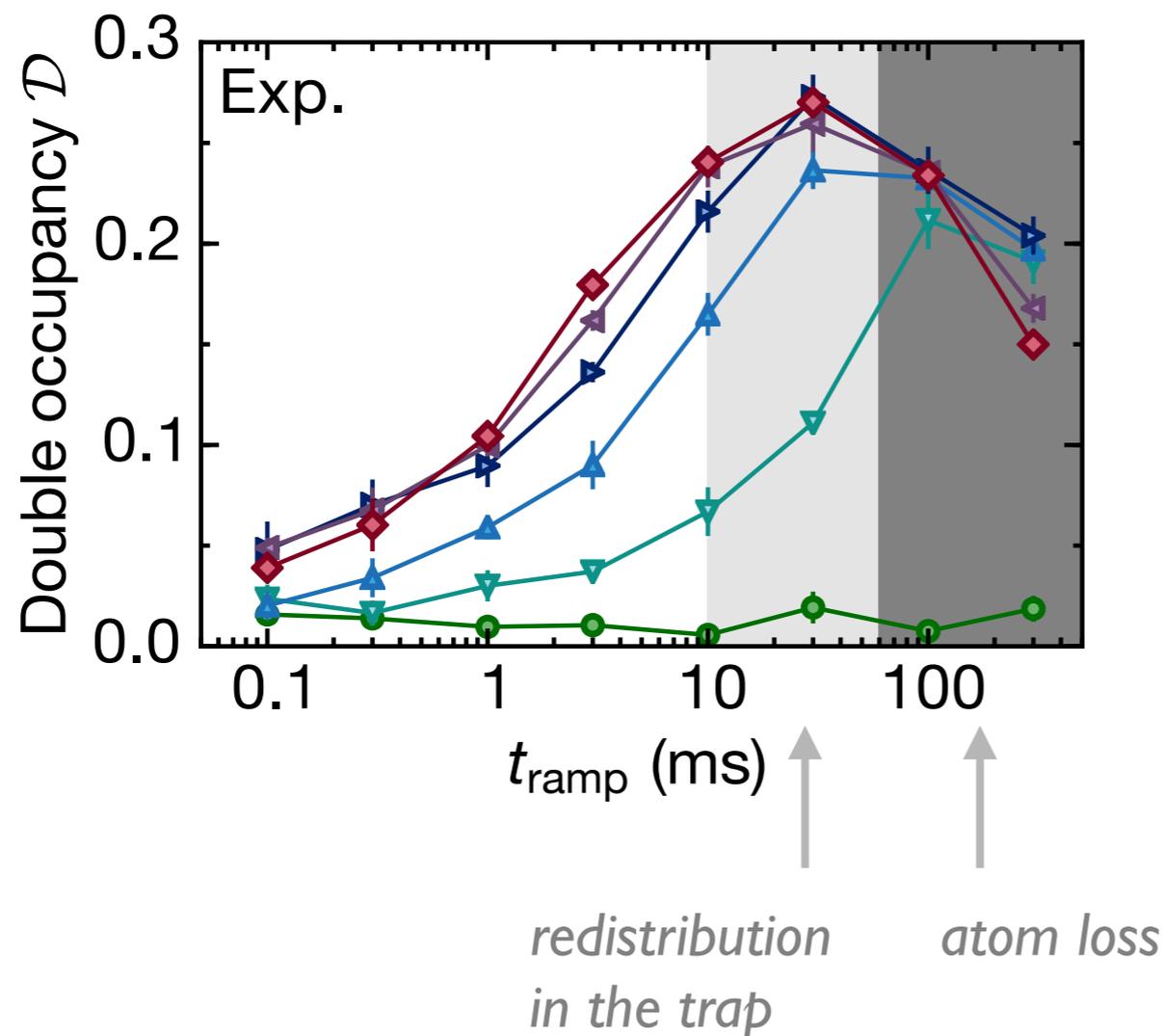
redistribution in the trap

atom loss

1. Periodic electric fields

- AC-field quench in the Hubbard model (metal phase)

Tsuji, Oka, Werner and Aoki (2011)

Electric field (amplitude E, frequency Ω) applied at $t=0$
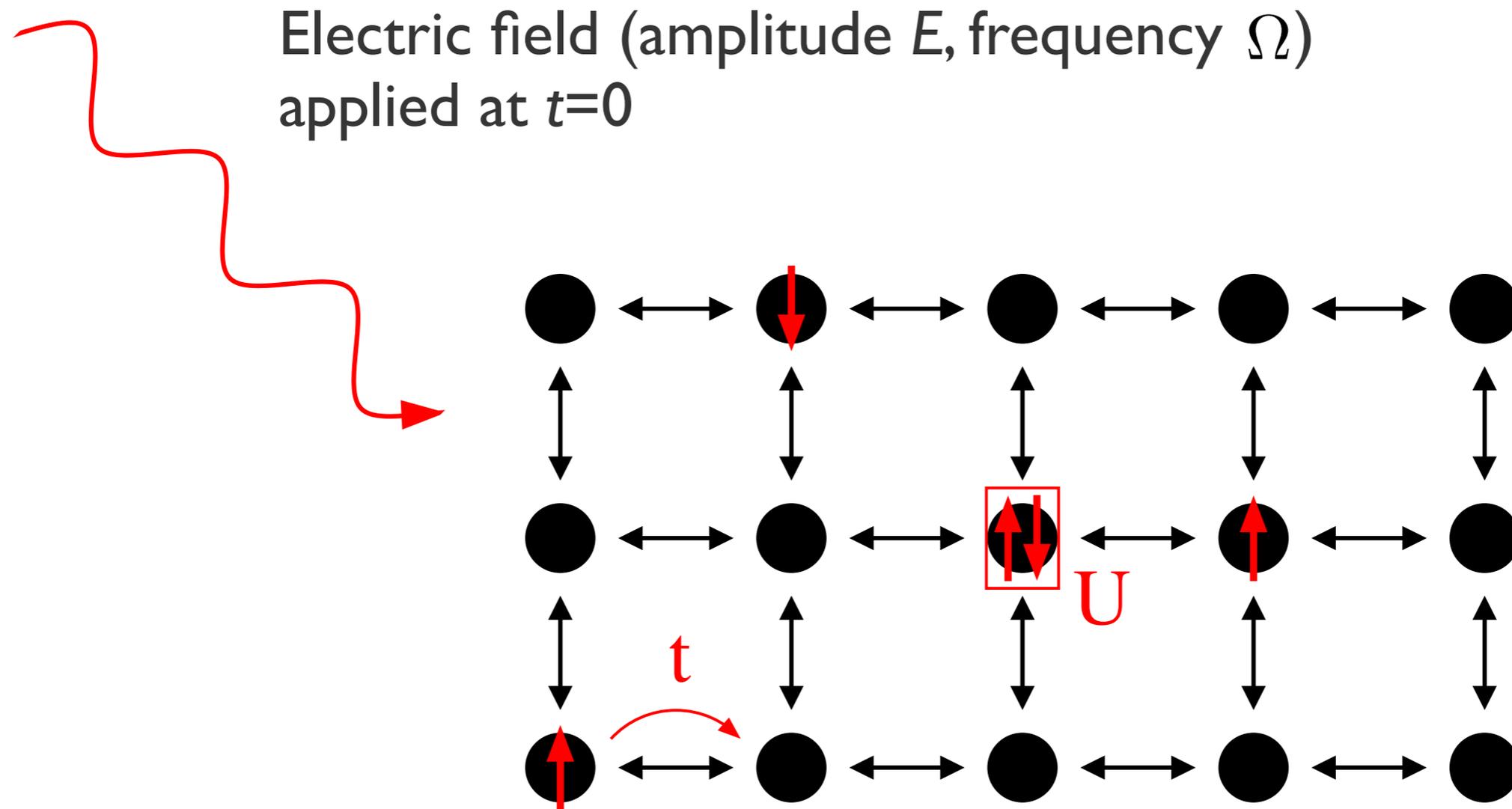
1. Periodic electric fields

AC-field quench in the Hubbard model (metal phase)

Tsuji, Oka, Werner and Aoki (2011)
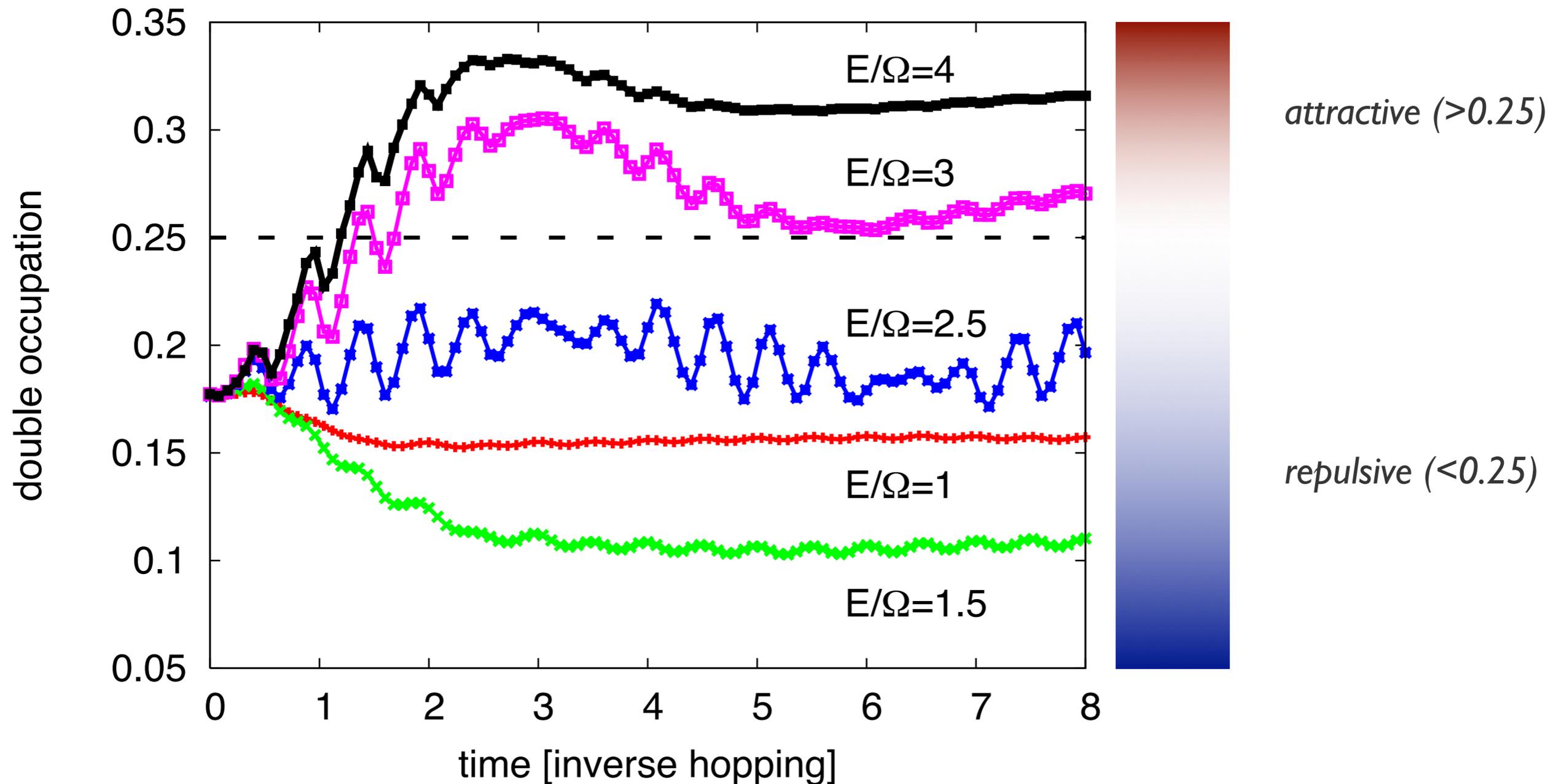
1. Periodic electric fields

- AC-field quench in the Hubbard model (metal phase)
  - Sign inversion of the interaction: repulsive ⟷ attractive
  - *Dynamically generated* high-Tc superconductivity?
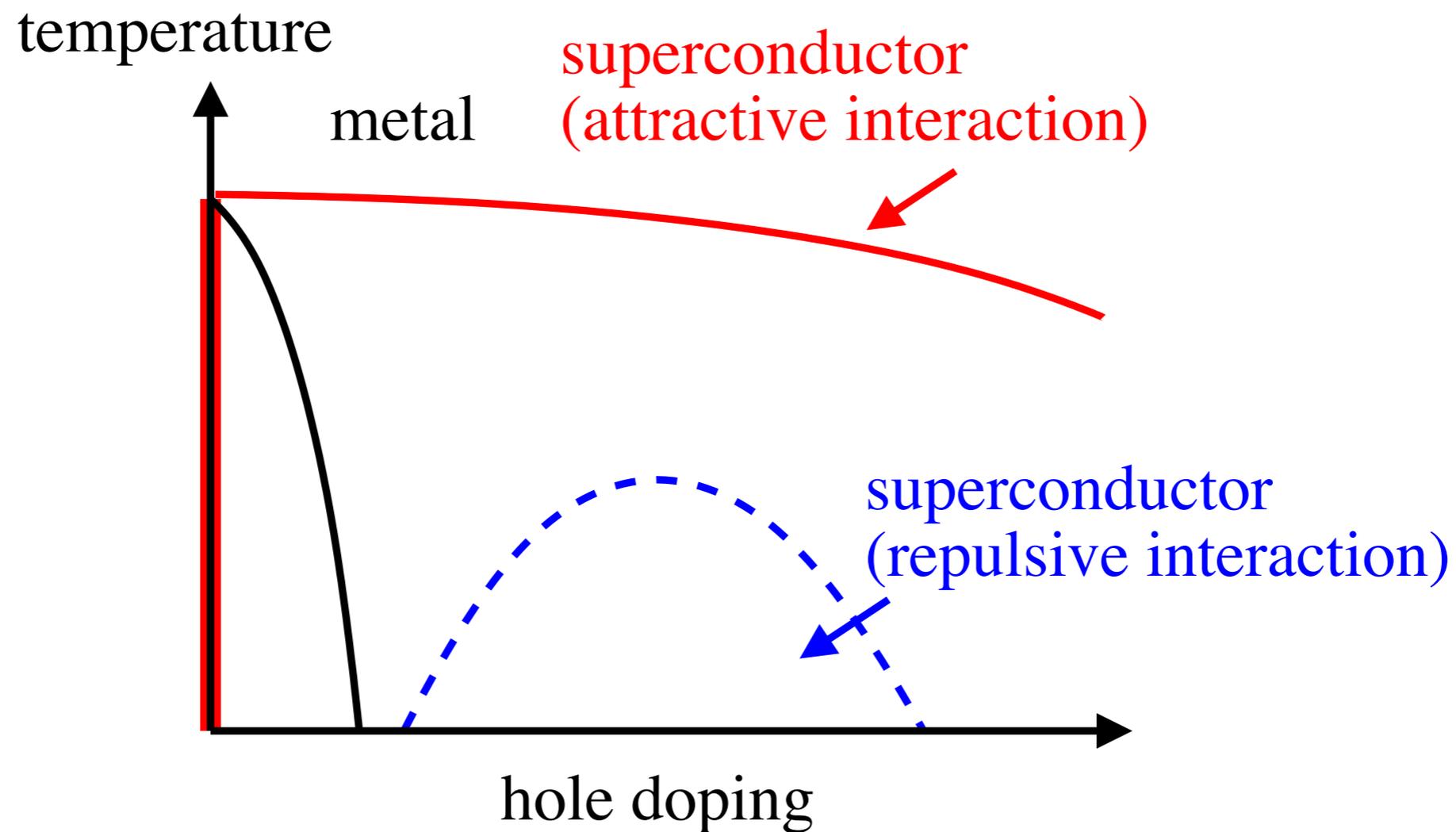
1. Origin of the attractive interaction

- **Periodic E-field leads to a population inversion**

$$E(t)$$

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

- Renormalized dispersion

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

- Periodic E-field leads to a population inversion

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

- Renormalized dispersion

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

- Periodic E-field leads to a population inversion

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

- Renormalized dispersion

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

- Periodic E-field leads to a population inversion

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

- Renormalized dispersion

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

- Periodic E-field leads to a population inversion

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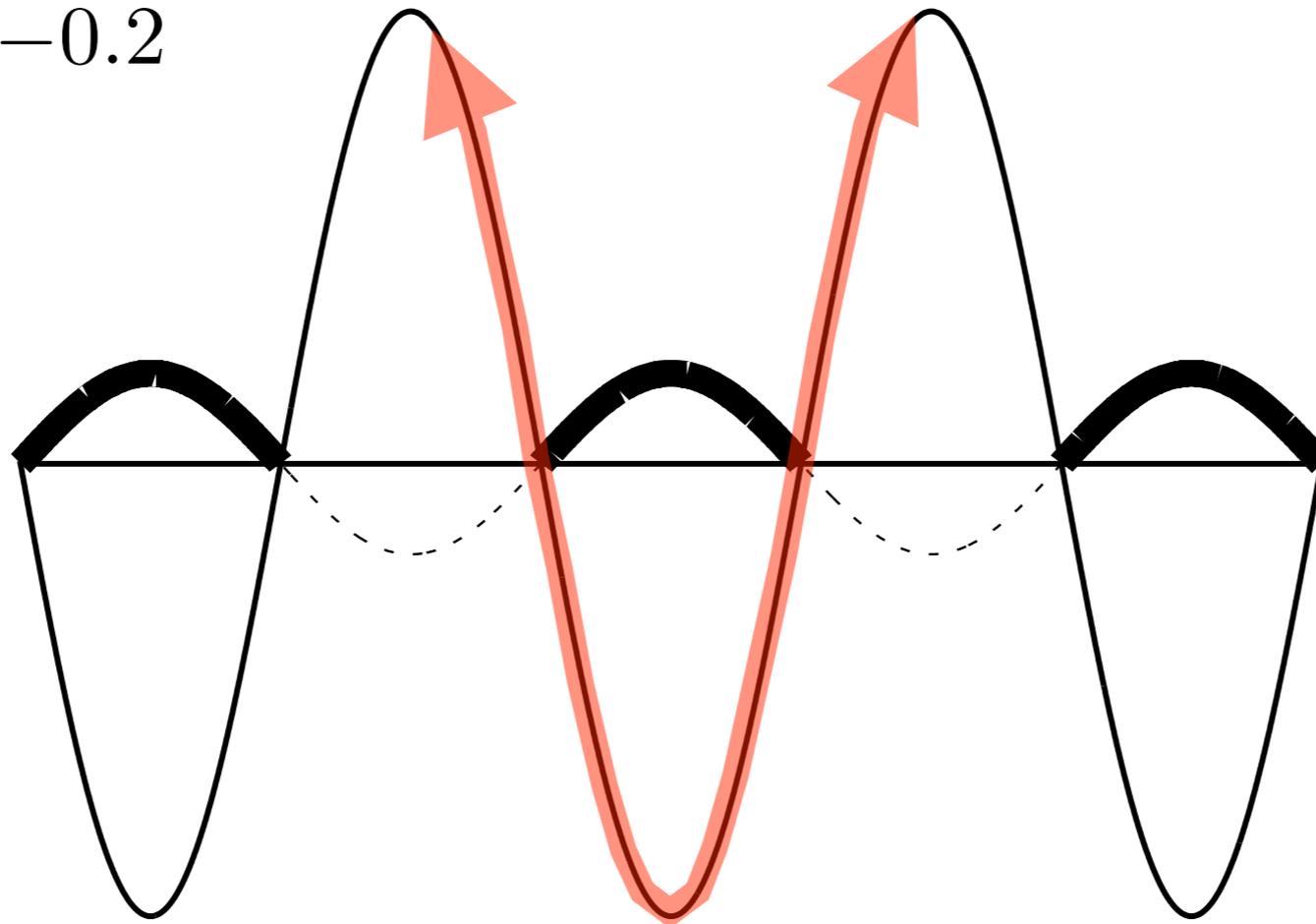
- Renormalized dispersion

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

1. 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

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

1. Effect on superconductivity

- AC-field quench from $U = 1$ to $U_{\text{eff}} = -2.5$ (NCA solver)

reduced pair susceptibility due to "heating"
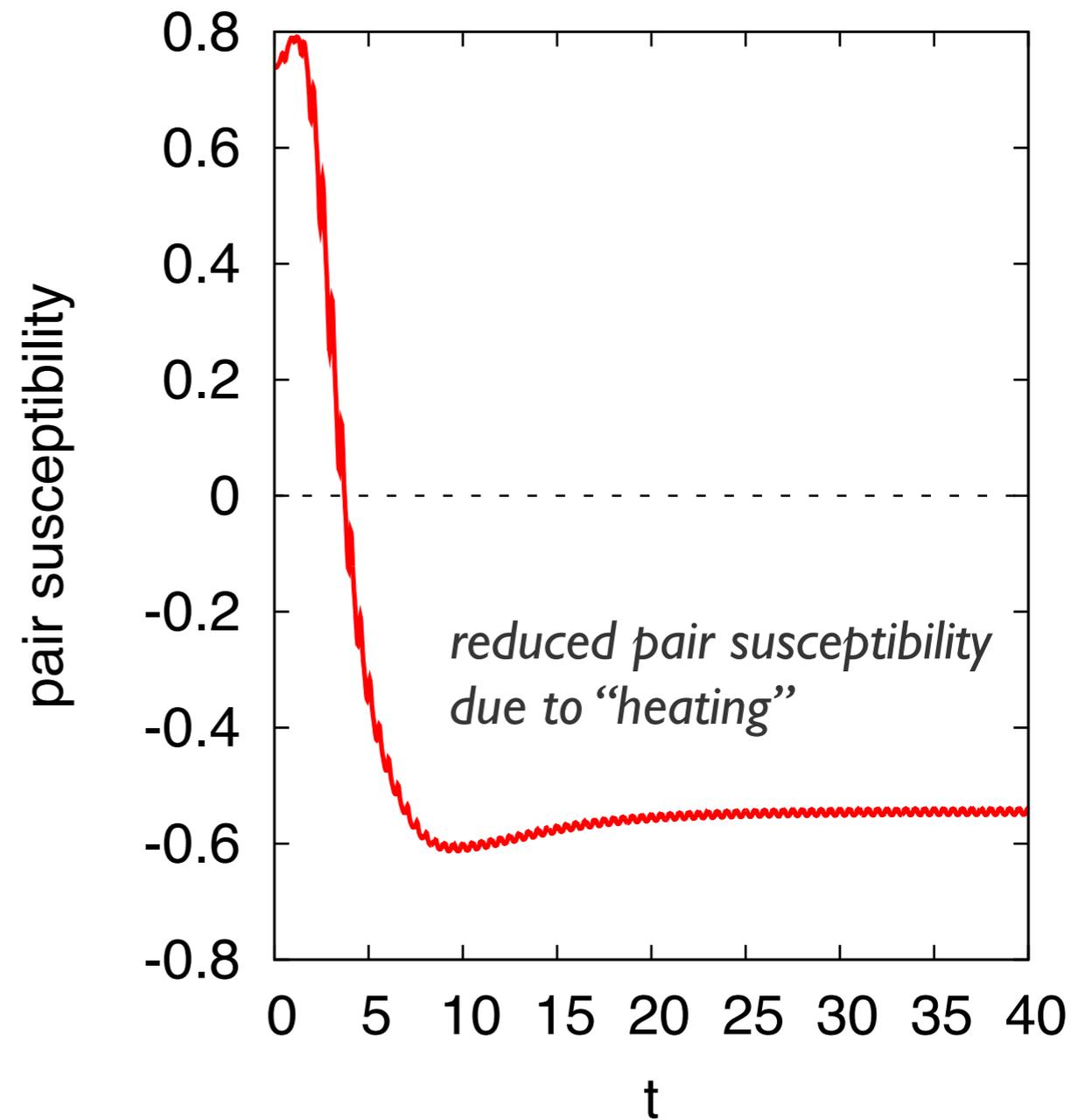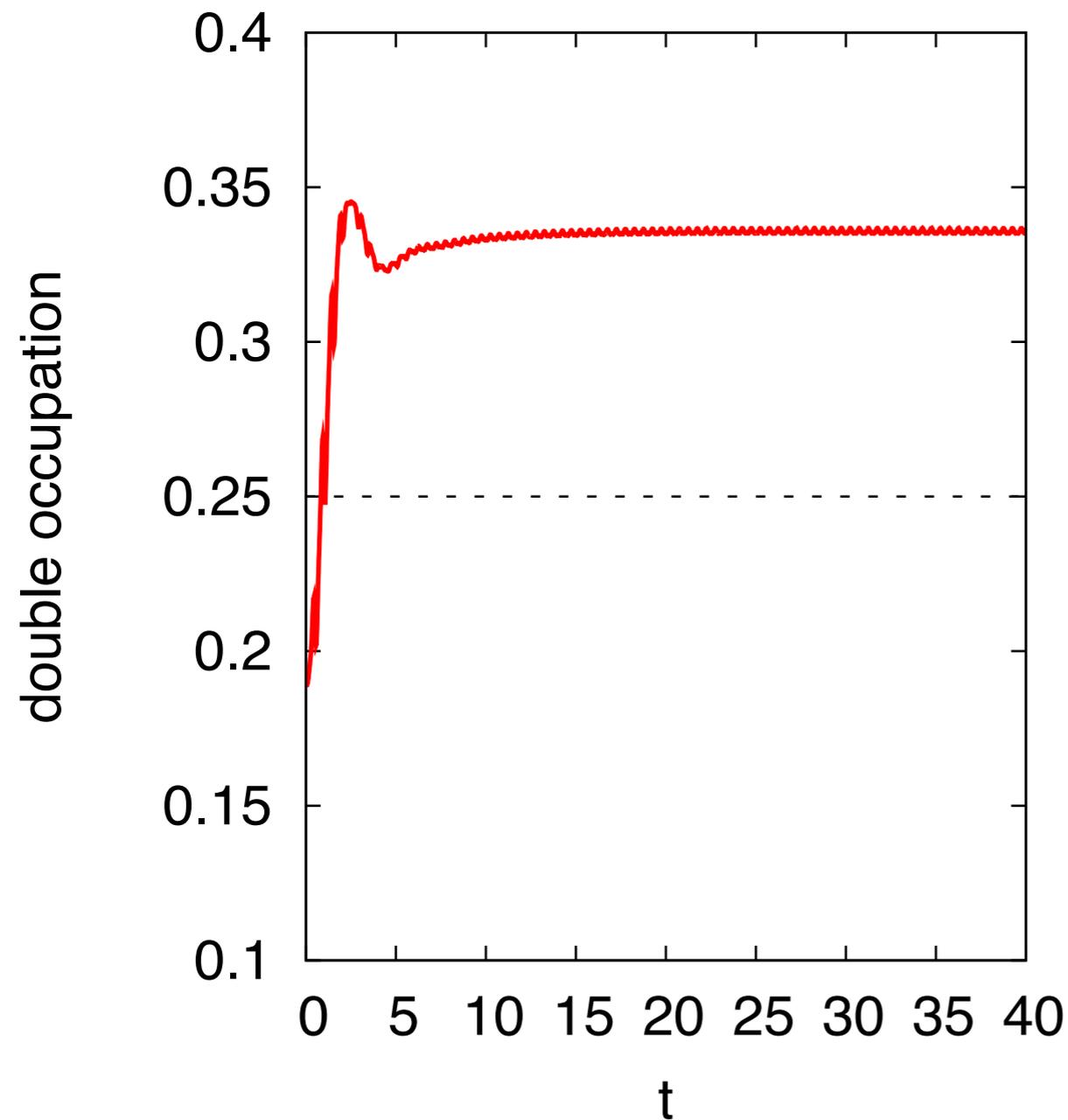
- Equilibrium DMFT phase diagram (half-filling)

- Half-filling: transformation $c_{i\uparrow} \to c_{i\uparrow}^{\dagger}$ $(i \in A)$, $c_{i\uparrow} \to -c_{i\uparrow}^{\dagger}$ $(i \in B)$

  maps repulsive model onto attractive model

T

metal

superconductor

AFM insulator

"BEC"   "BCS"   "Slater"   "Mott"

attractive   repulsive   U
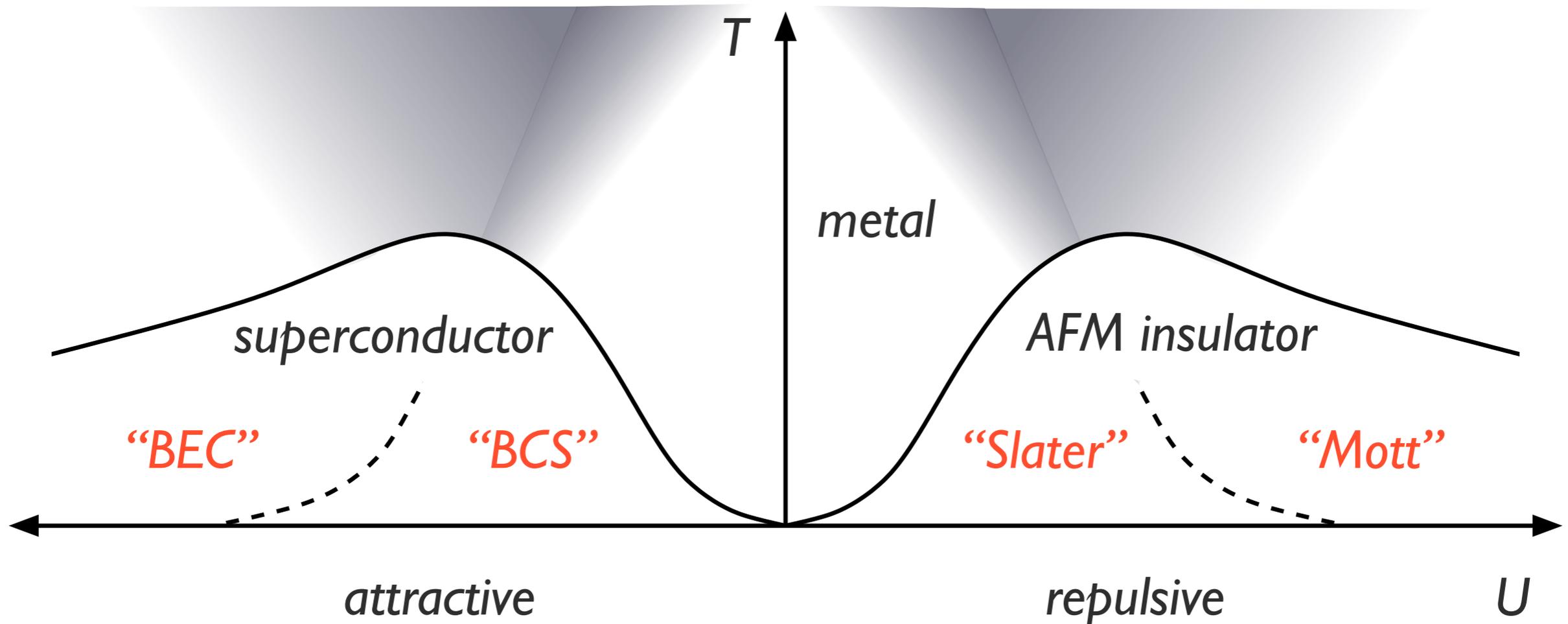
- Weak-coupling regime

  Tsuji, Eckstein & Werner (2012)

- Slow ramp from (Slater-)Antiferromagnet to Paramagnet
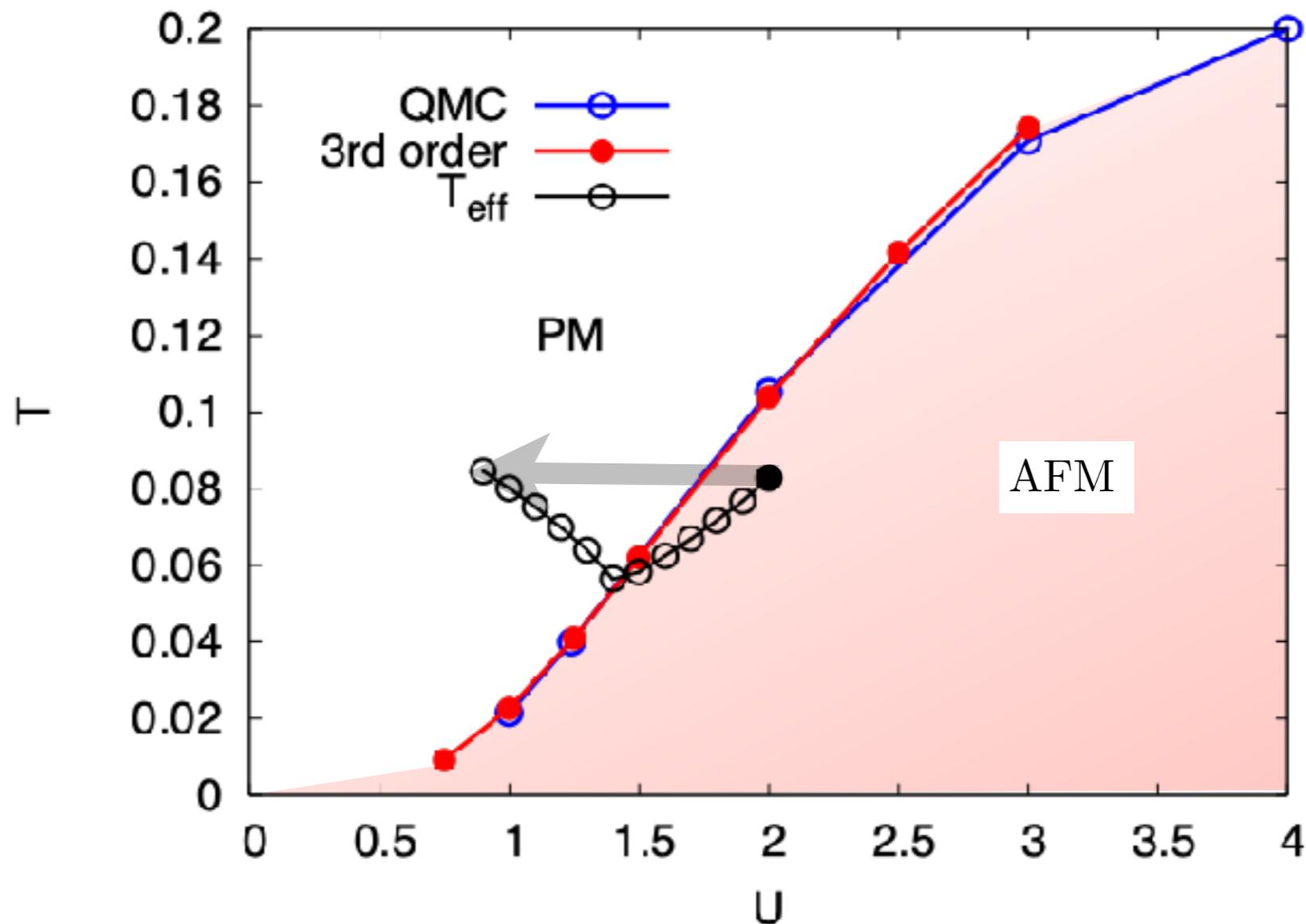
- **Weak-coupling regime**

  Tsuji, Eckstein & Werner (2012)

- Time-evolution of the magnetization for different final U
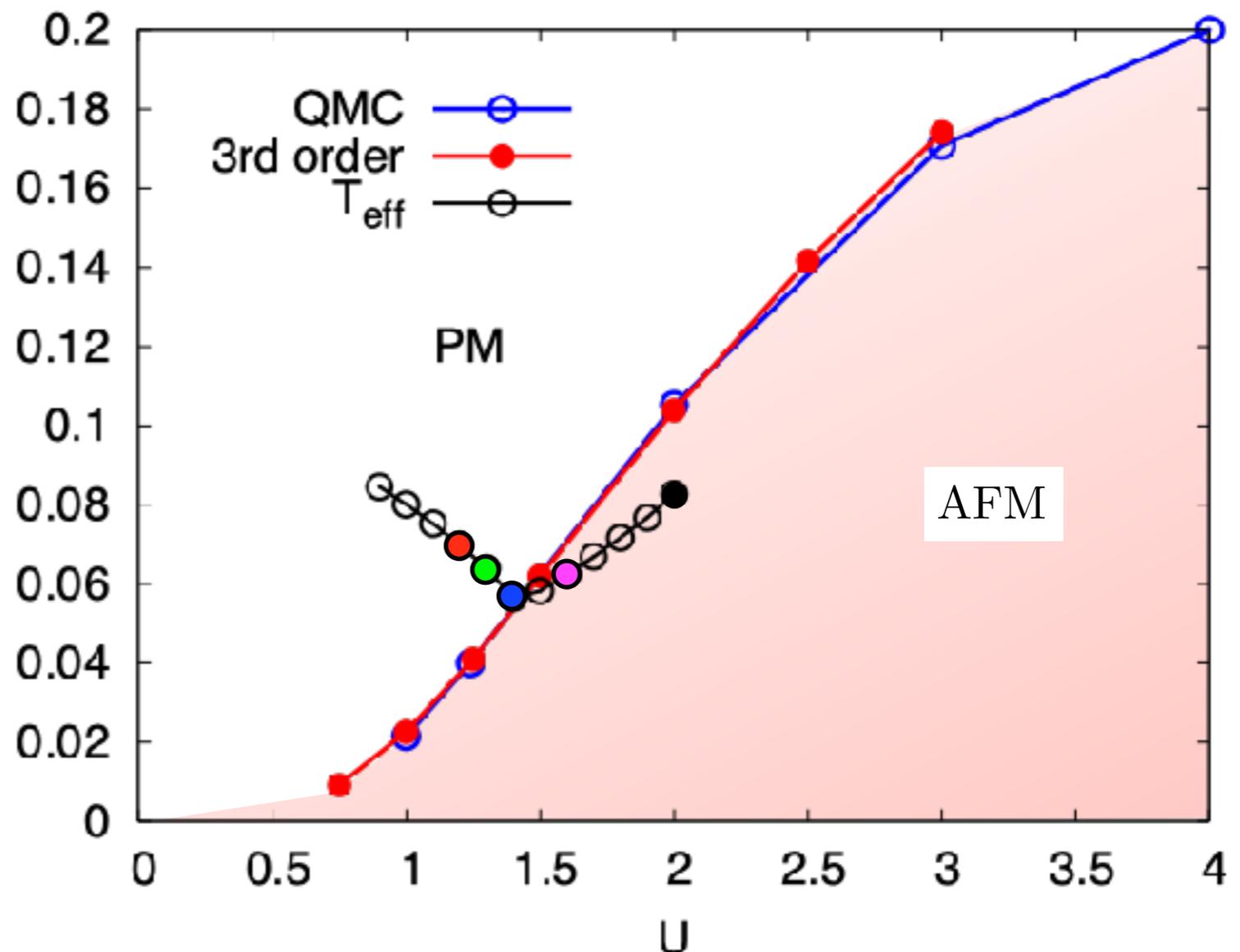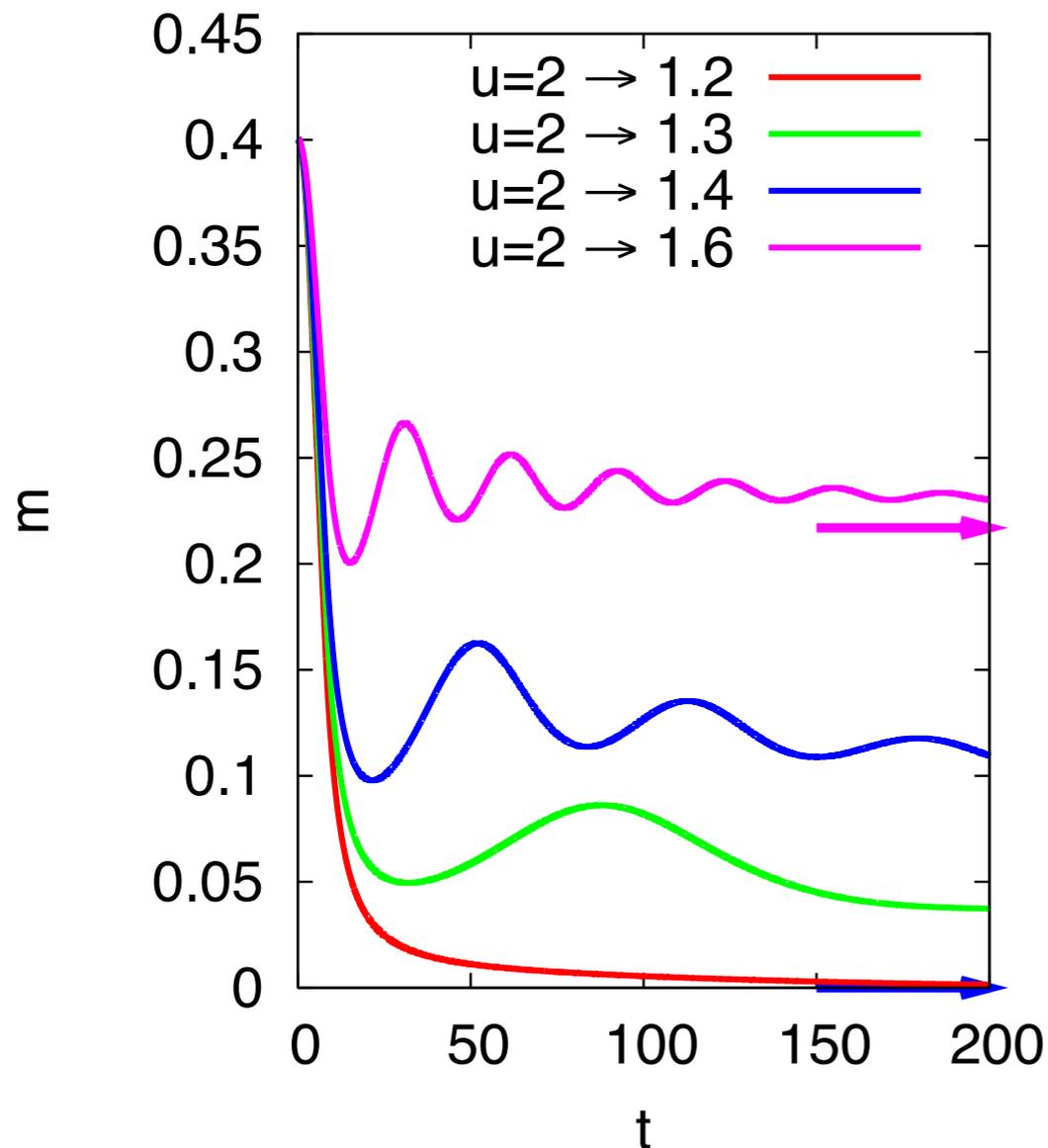
II. Nonthermal symmetry-broken states

- **Weak-coupling regime**

  Tsuji, Eckstein & Werner (2012)

- Time-evolution of the magnetization for different final U (Hartree)

- **Weak-coupling regime**

  Tsuji, Eckstein & Werner (2012)

- Time-evolution of the magnetization for different final U

II. Nonthermal symmetry-broken states

- **Weak-coupling regime**

  Tsuji, Eckstein & Werner (2012)

- Evidence for a nonthermal critical point

II. Nonthermal symmetry-broken states

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  Tsuji, Eckstein & Werner (2012)

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- **Weak-coupling regime**

  Tsuji, Eckstein & Werner (2012)

- Evidence for a **nonthermal critical point**

"RG flow" after quench

AFM fixed point

PM fixed point

τ^{-1} (inv. dephasing time)
ω (amplitude mode)

nonthermal critical point

$U_{c,thermal}$

U_{final}

II. Nonthermal symmetry-broken states

- **Weak-coupling regime**

  Tsuji, Eckstein & Werner (2012)

- Evidence for a **nonthermal critical point**

Berges et al. (2004)

nonthermal fixed point

"RG flow" after quench

AFM fixed point

PM fixed point

τ^{-1} (inv. dephasing time)

ω (amplitude mode)

nonthermal critical point

$U_{c,thermal}$

U_{final}

III. Cooling by photo-doping

- **Photo-doping from core levels** *Werner, Eckstein, Mueller & Refael (2019)*
  - Dipolar excitations with appropriate frequency Ω transfer electrons from core to system and **cool down the system**

*core DOS
(completely filled)*

*system DOS
(partially filled)*

- **Photo-doping from core levels** *Werner, Eckstein, Mueller & Refael (2019)*
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III. Cooling by photo-doping
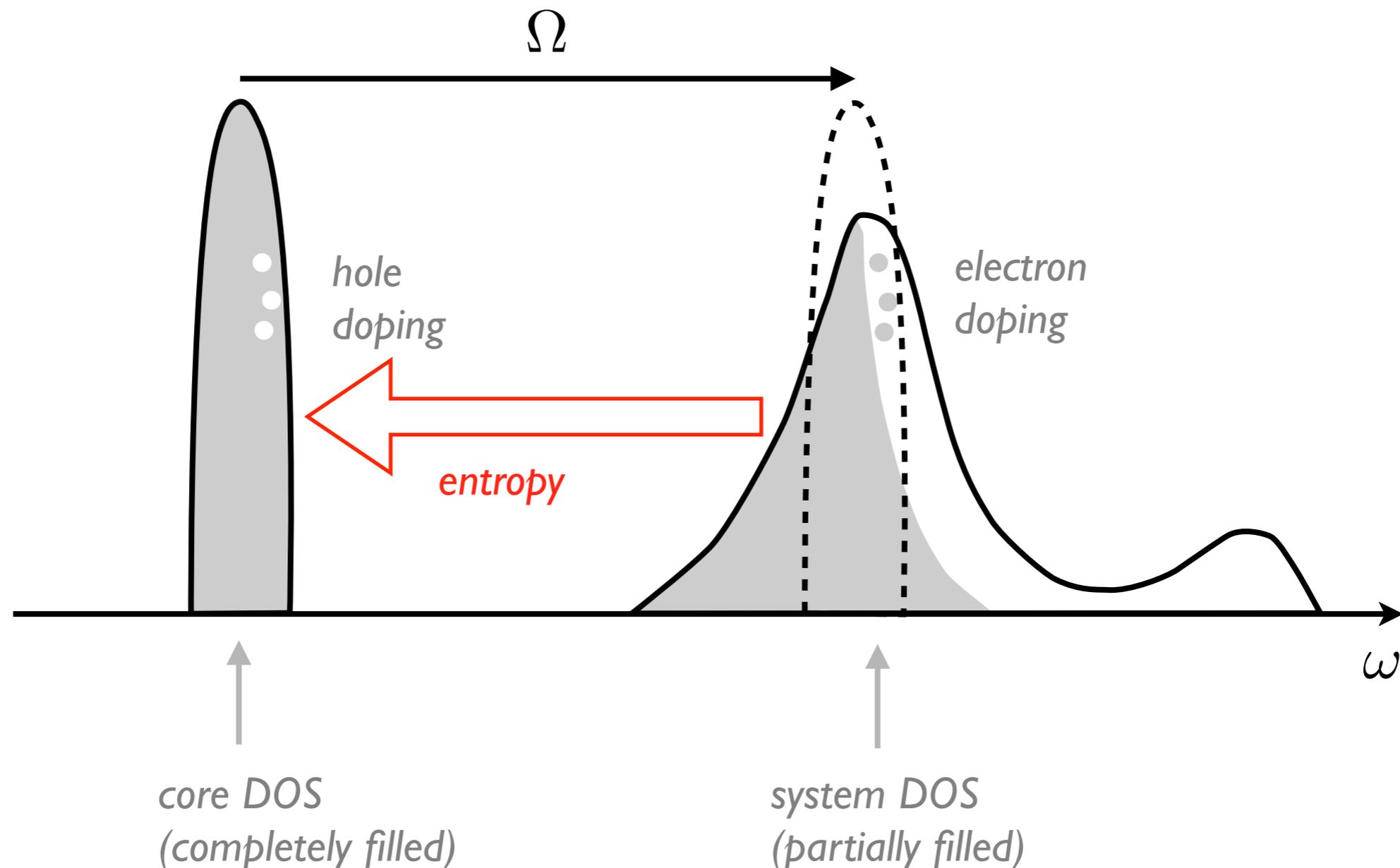
- **Photo-doping from core levels** *Werner, Eckstein, Mueller & Refael (2019)*

  - Entropy of the core band in the narrow band (atomic) limit:

  $$S_{\mathrm{core}} = -2n_\sigma \ln(n_\sigma) - 2(1 - n_\sigma) \ln(1 - n_\sigma)$$


rapid increase of entropy of the core upon hole doping
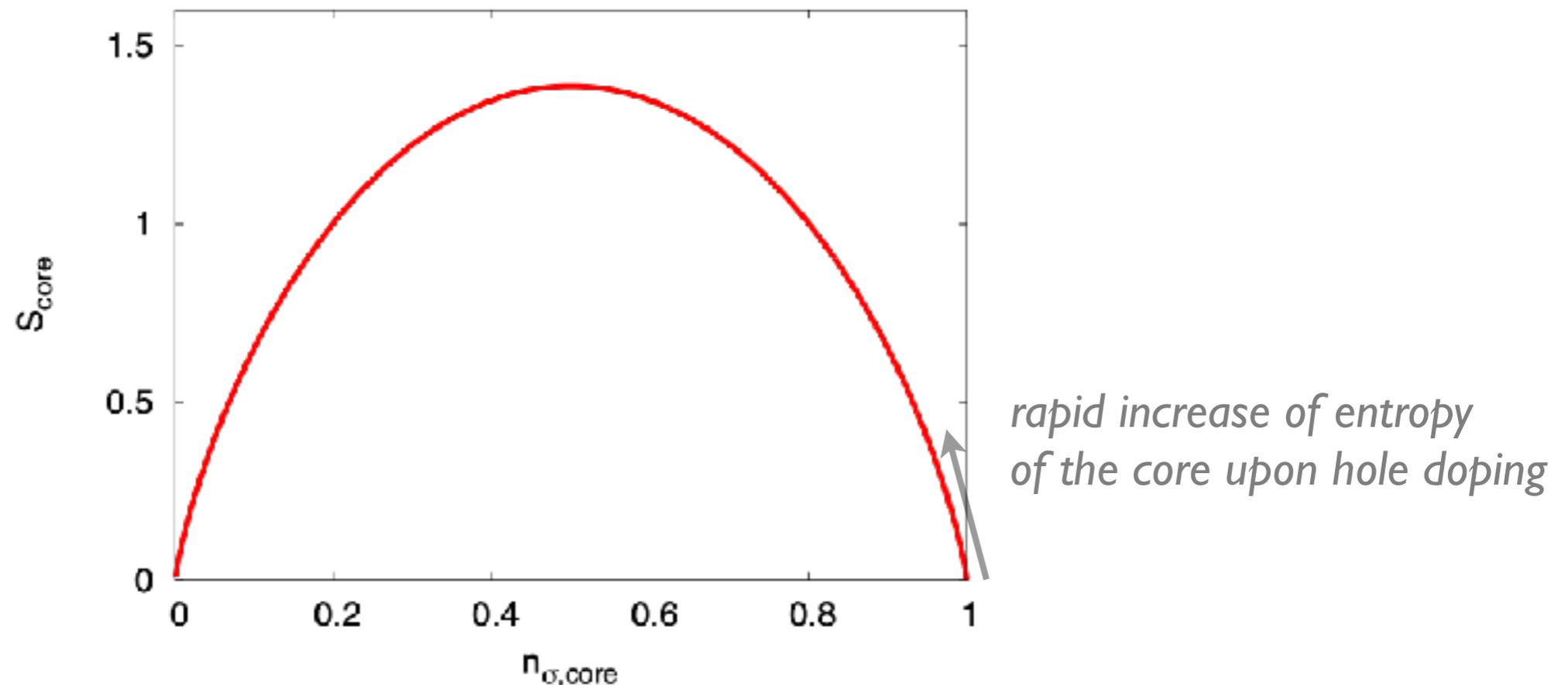
  - In case of isentropic doping process:

  $$\Delta S_{\mathrm{core}} \nearrow \;\; \Rightarrow \;\; \Delta S_{\mathrm{system}} \searrow$$

cooling of system due to entropy reshuffling

- **Photo-doping from core levels**   *Werner, Eckstein, Mueller & Refael (2019)*
 - Constant entropy contours in the filling-temperature plane

system

S=0.8
S=0.7
S=0.6
S=0.5
...

$\Delta S_{system}=0$
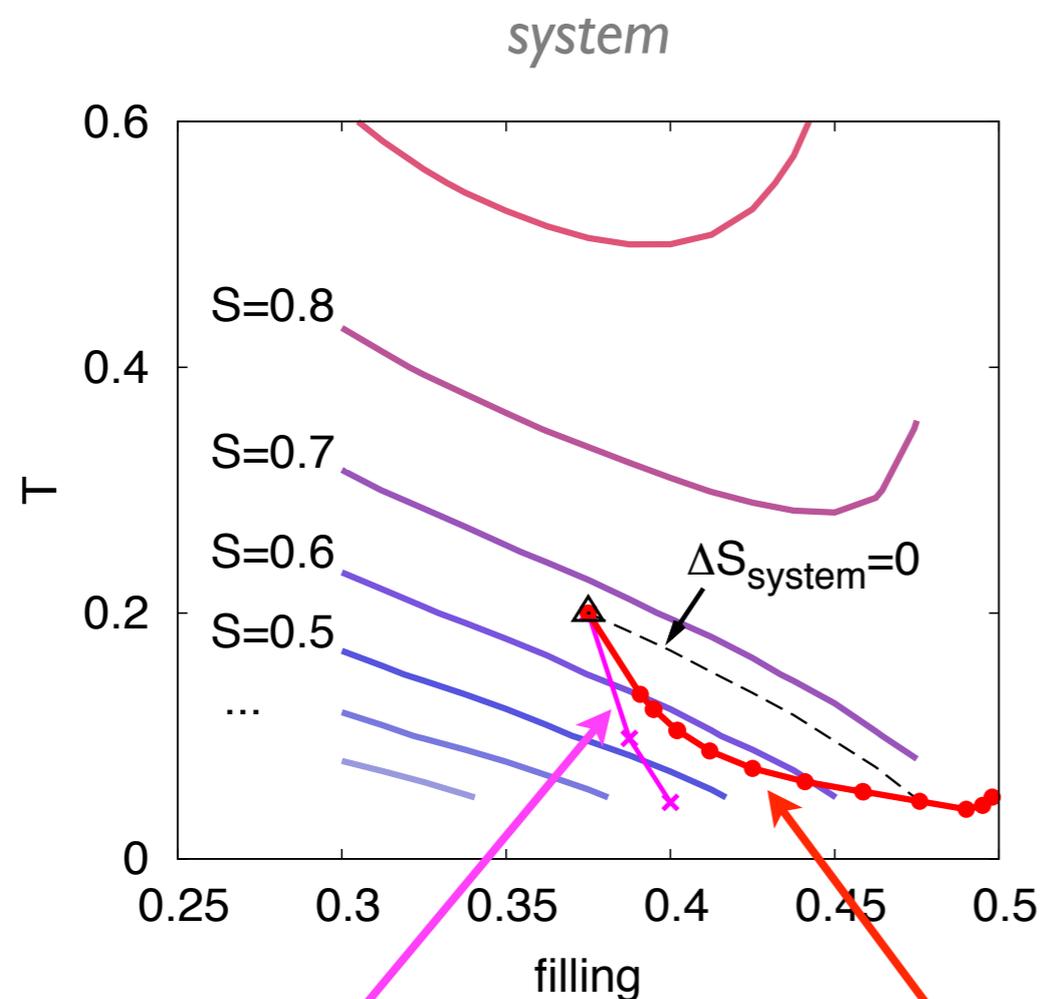
isentropic case

quasi-particle temperature and fillings realized by chirped pulses

- **Photo-doping from core levels**   *Werner, Eckstein, Mueller & Refael (2019)*
  - Constant entropy contours in the filling-temperature plane
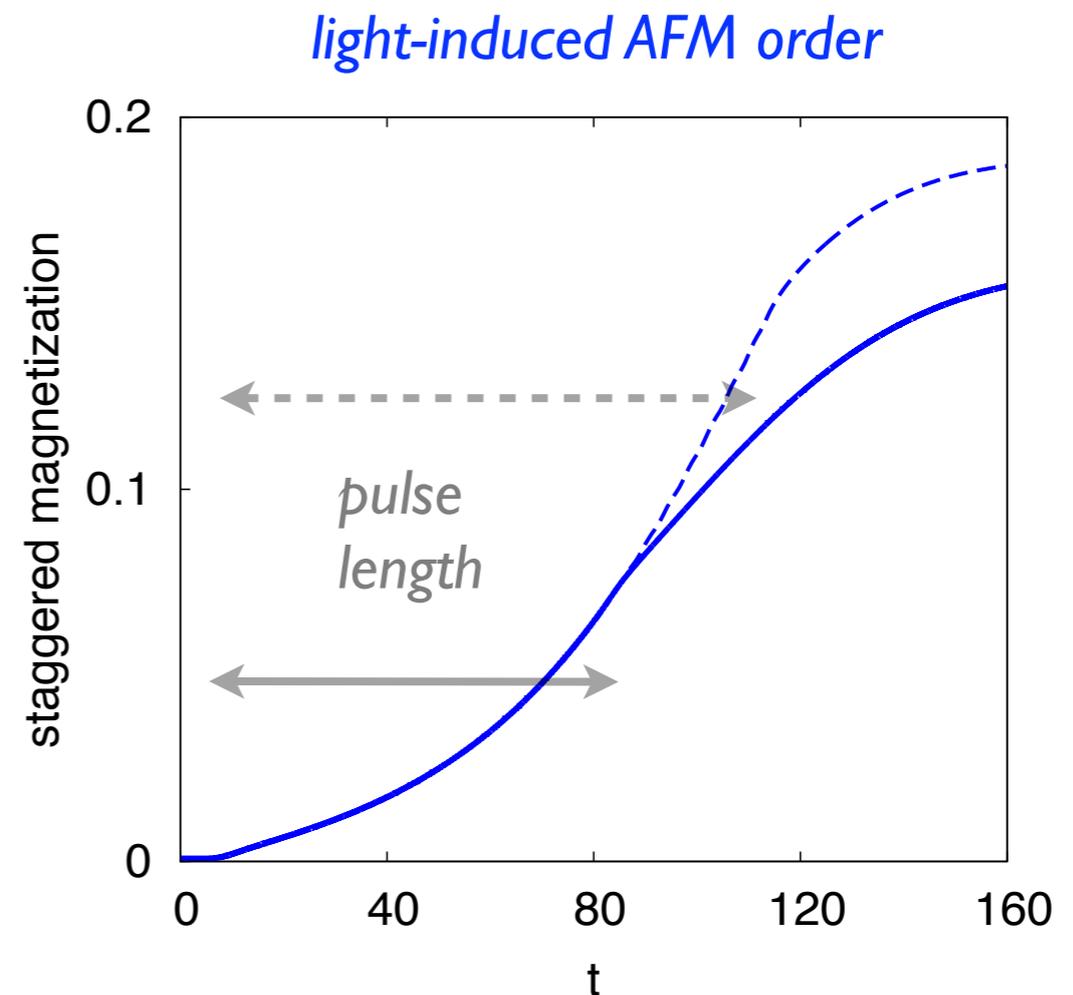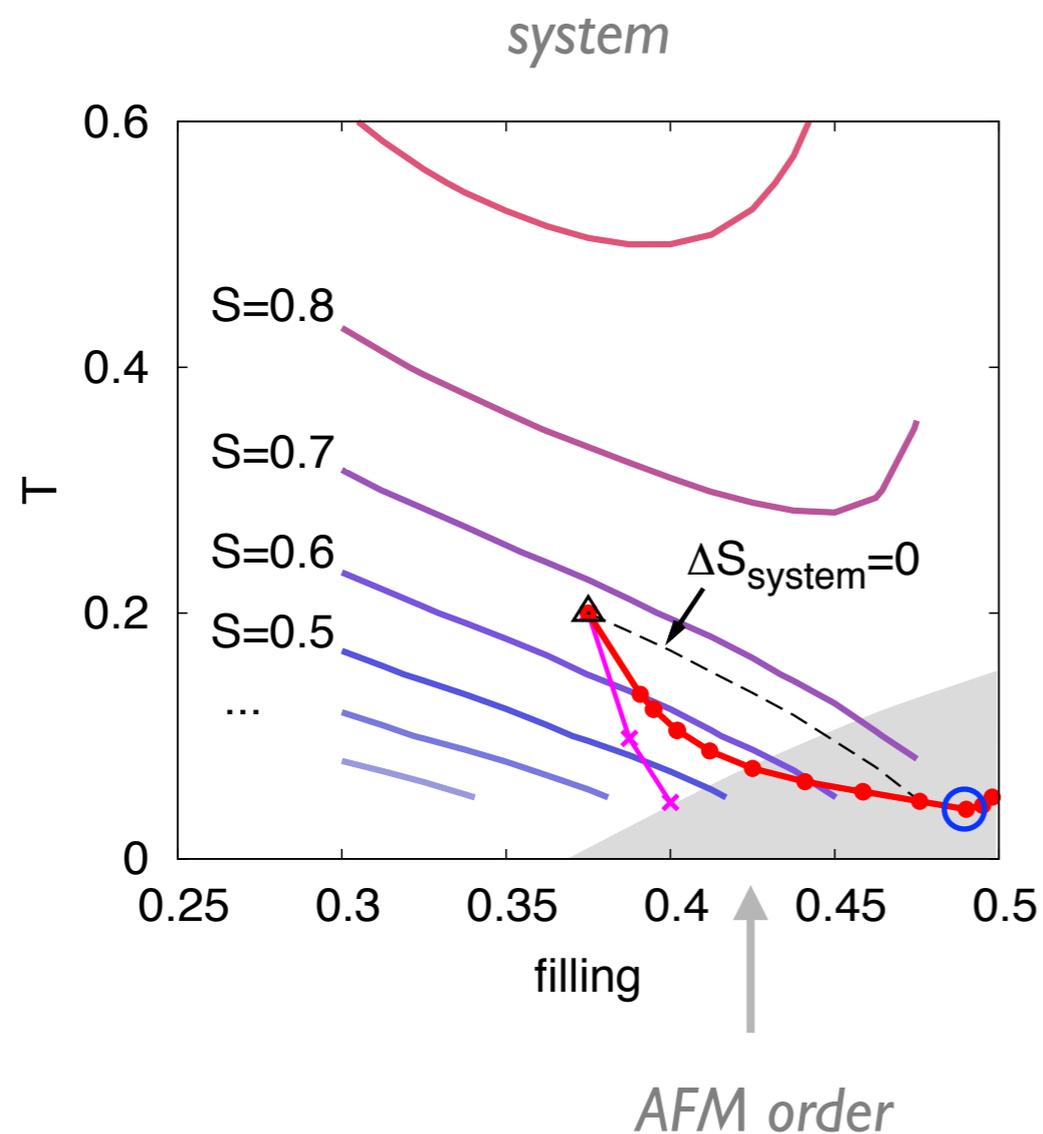
III. Cooling by photo-doping

- Related example of a nonthermal superconducting state
  - η-pairing in a repulsive Hubbard model with inverted population
   *Rosch, Rasch, Binz & Vojta (2008); Kaneko et al. (2019); Werner, Li, Golez & Eckstein (2019)*
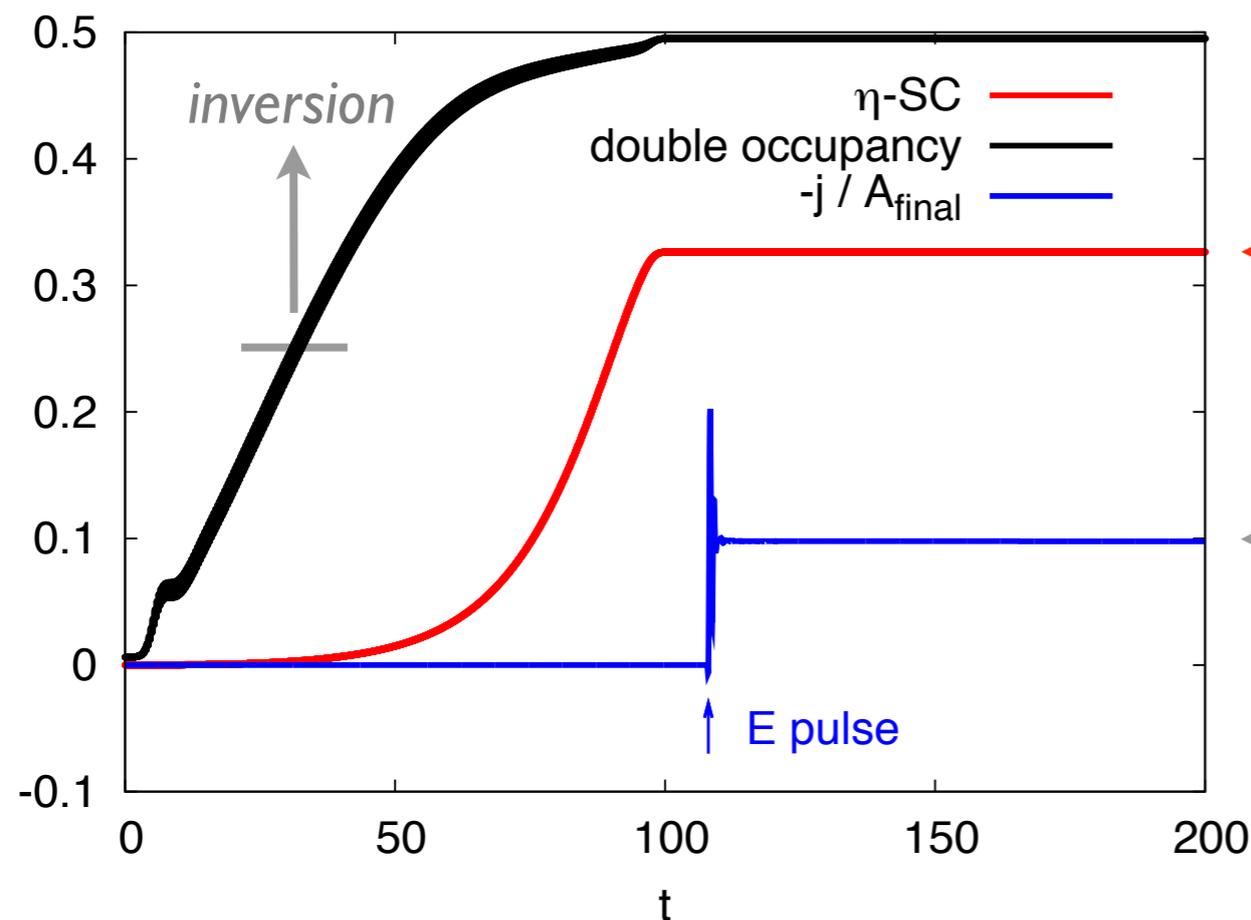
light-induced η-pairing

non-decaying current consistent with superconductivity

uniform pairing

staggered η-pairing
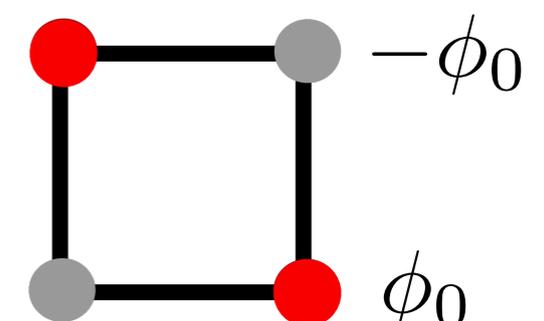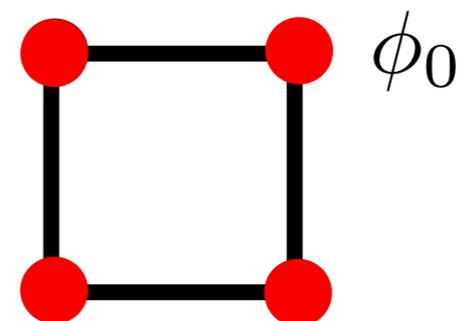
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- Acknowledments: