

# Dynamical mean field approach to correlated lattice systems in and out of equilibrium

Philipp Werner

University of Fribourg, Switzerland

# Overview

- *Dynamical mean field approximation applied to quantum field theory*  
*in collaboration with: O.Akerlund, P. de Forcrand, A. Georges*
- *Dynamical mean field theory for bosonic lattice systems*  
*in collaboration with: P.Anders, L. Pollet, M.Troyer*
- *Dynamical mean field theory for fermionic lattice systems*  
*in collaboration with: E. Gull, A. Millis*
- *Nonequilibrium extension of dynamical mean field theory*  
*in collaboration with: M. Eckstein, M. Kollar, N.Tsuji, T. Oka, H.Aoki*
- *Some applications: Hubbard model in strong electric fields*  
*in collaboration with: M. Eckstein, N.Tsuji, T. Oka, H.Aoki*

# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Lagrangian density

$$\mathcal{L}[\varphi(x)] = \frac{1}{2}(\partial_\mu \varphi(x))^2 - \frac{1}{2}m_0^2 \varphi(x)^2 - \frac{g_0}{4!} \varphi(x)^4$$

- Spontaneous  $\mathbb{Z}_2$  symmetry breaking for negative (renormalized)  $m^2$
- After Wick rotation, discretization and variable transformation

$$S = \sum_x \left( -2\kappa \sum_\mu \varphi_{x+\hat{\mu}} \varphi_x + \varphi_x^2 + \lambda(\varphi_x^2 - 1)^2 \right)$$

- In the limit  $\lambda \rightarrow \infty$ ,  $\varphi_x = \pm 1$  (Ising model)

# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- **Mean field theory:** mapping to a 0-dimensional effective model

→ replace all interactions by an interaction with a constant **background field  $v$**

- Partition function of the lattice model

$$Z = \int \mathcal{D}[\varphi] \prod_x \exp \left( -\varphi_x^2 - \lambda(\varphi_x^2 - 1)^2 + 2\kappa \sum_{\mu=1}^d \varphi_x \varphi_{x+\hat{\mu}} \right)$$

becomes  $Z_{\text{MF}} = \int_{-\infty}^{\infty} d\varphi \exp \left( -\varphi^2 - \lambda(\varphi^2 - 1)^2 + 2\kappa(2d)v\varphi \right)$

- Self-consistency condition

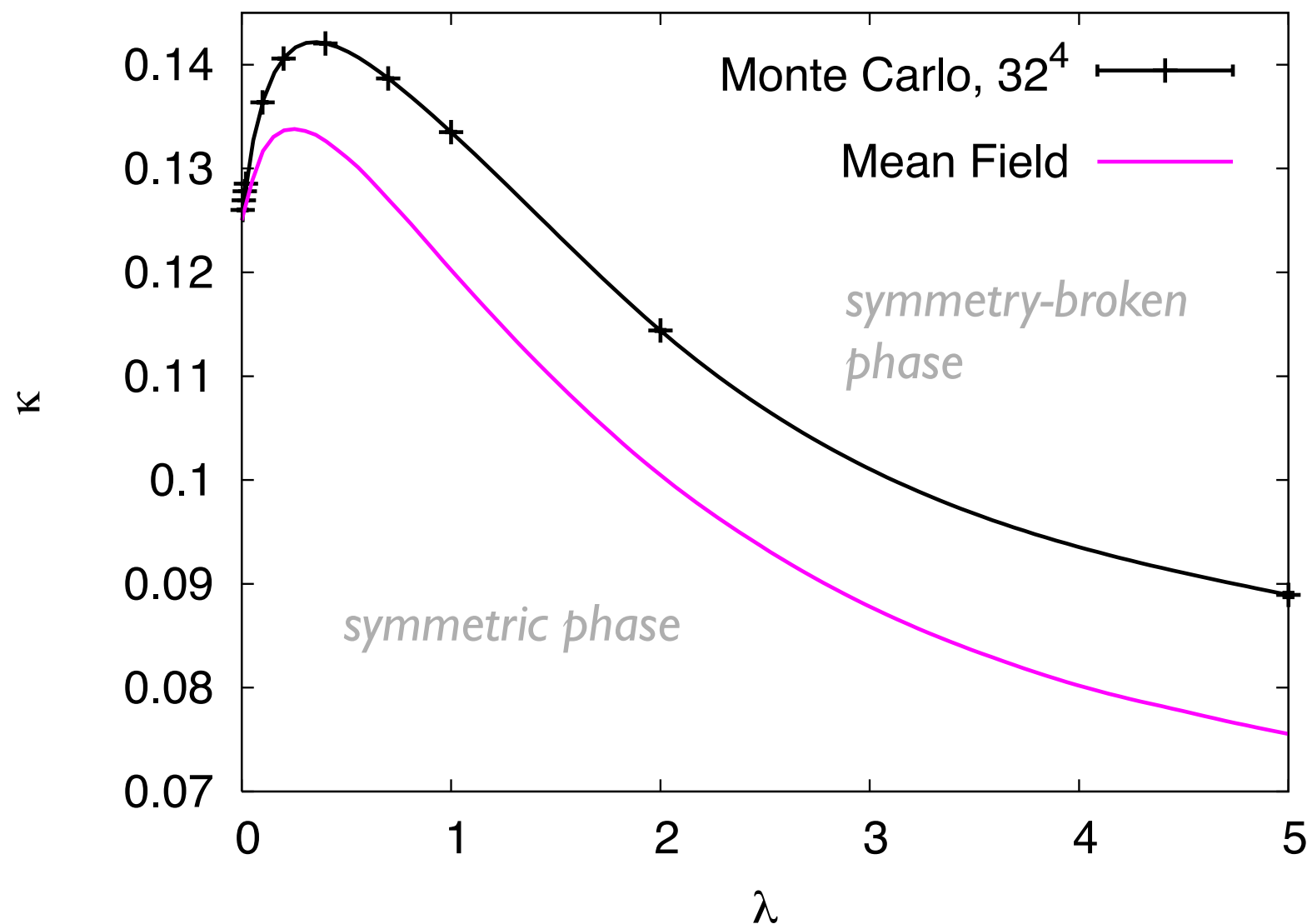
$$v \equiv \langle \varphi \rangle = \frac{1}{Z_{\text{MF}}} \int_{-\infty}^{\infty} \varphi \exp \left( -\varphi^2 - \lambda(\varphi^2 - 1)^2 + 2\kappa(2d)v\varphi \right)$$

# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Mean field theory:** Phase diagram ( $d=3+1$ )



# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- **Dynamical mean field theory:** mapping to a  $(0+1)$ -dimensional effective model

→ explicitly treat fluctuations in one dimension, freeze fluctuations in the  $(d-1)$  other dimensions

- Dynamical dimension:  $t$  (with conjugate momentum  $\omega$ )

Frozen dimensions:  $x_1, \dots, x_{d-1}$  (conjugate momenta  $k_1, \dots, k_{d-1}$ )

*This convention allows to study finite-temperature behavior by varying the extent of the dynamical dimension*

- Breaks Lorentz invariance, but let's try it anyhow ...

# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- **Dynamical mean field theory:** mapping to a (0+1)-dimensional effective model

→ explicitly treat fluctuations in one dimension, freeze fluctuations in the (d-1) other dimensions

- Schematically:

$$Z = \int \mathcal{D}[\varphi] \exp \left( 2\kappa \sum_x \sum_{\mu} \varphi_x \varphi_{x+\hat{\mu}} - \sum_x V(\varphi_x) \right)$$

$$Z_{\text{DMFT}} = \int \mathcal{D}[\varphi] \exp \left( - \sum_{t,t'} K^{-1}(t-t') \varphi_t \varphi_{t'} - \sum_t V(\varphi_t) + h \sum_t \varphi_t \right)$$

*non-zero in the  
symmetry-broken  
phase*



*effect of the frozen dimensions on the local dynamics*

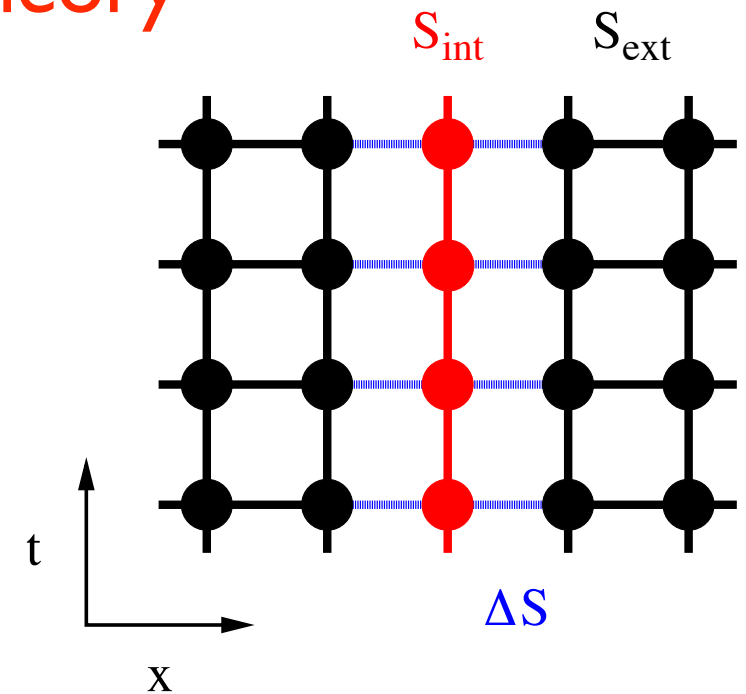
# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Cavity construction:** separate action into *internal*  $x = (\vec{0}, t)$  and *external*  $x \neq (\vec{0}, t)$  degrees of freedom

$$S = S_{\text{int}} + \Delta S + S_{\text{ext}}$$



$$S_{\text{int}} = \sum_t \left[ -2\kappa \varphi_{\text{int},t+1} \varphi_{\text{int},t} + \varphi_{\text{int},t}^2 + \lambda(\varphi_{\text{int},t}^2 - 1)^2 \right]$$

$$\Delta S = -2\kappa \sum_t \sum_{\langle \text{int}, \text{ext} \rangle} \varphi_{\text{int},t} \varphi_{\text{ext},t}$$

$$S_{\text{ext}} = \sum_{x \neq (\vec{0}, t)} \left[ -2\kappa \sum_{\nu} \varphi_{x+\hat{\nu}} \varphi_x + \varphi_x^2 + \lambda(\varphi_x^2 - 1)^2 \right]$$

- Expand  $\exp(-\Delta S)$  and integrate out the external degrees of freedom

# DMFT for quantum field theories

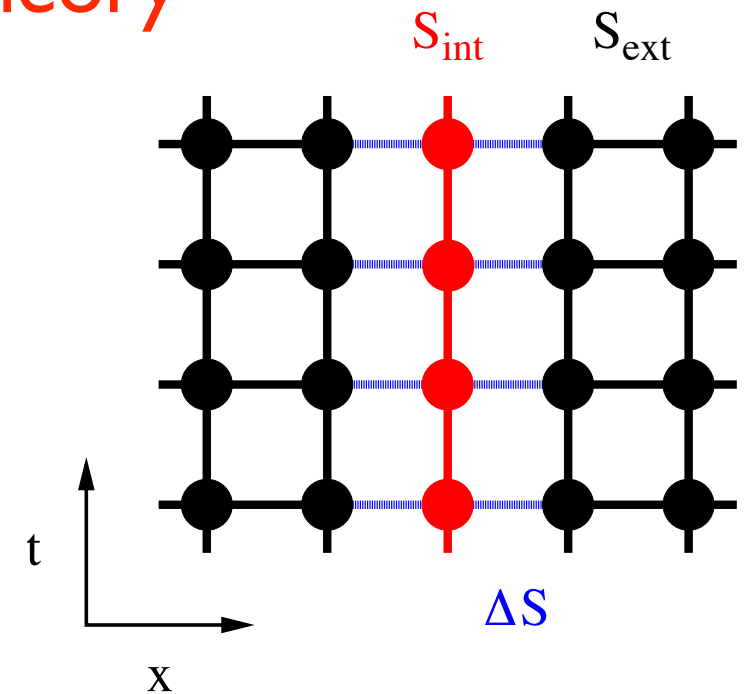
- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Cavity construction:** to allow for symmetry breaking, we write

$$\varphi_{\text{ext},t} = \phi_{\text{ext}} + \delta\varphi_{\text{ext},t}, \quad \langle \varphi_{\text{ext}} \rangle = \phi_{\text{ext}}$$

$$\varphi_{\text{int},t} = \phi_{\text{int}} + \delta\varphi_{\text{int},t}, \quad \langle \varphi_{\text{int}} \rangle = \phi_{\text{int}}$$



$$\Delta S = -\kappa \sum_t \left( 2(d-1)\phi_{\text{ext}}^\dagger \delta\varphi_{\text{int},t} + \sum_{\langle \text{int}, \text{ext} \rangle} \delta\varphi_{\text{int},t}^\dagger \delta\varphi_{\text{ext},t} \right) + f(\varphi_{\text{ext}})$$

$$\equiv \underbrace{S_1}_{\substack{\uparrow \\ \text{can be included in } S_{\text{int}}}} + \sum_t \underbrace{\delta S}_{\substack{\uparrow \\ \text{can be included in } S_{\text{ext}}}} + f(\varphi_{\text{ext}})$$

- Expand  $\exp(-\delta S)$

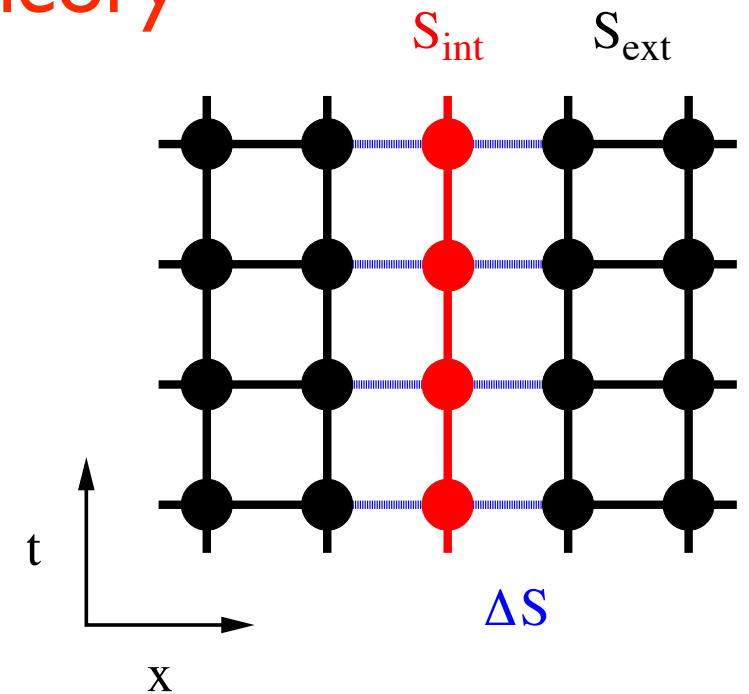
# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Cavity construction:** Terms up to second order yield

$$Z = Z_{\text{ext}} \int \mathcal{D}\varphi_{\text{int}} \exp(-S_{\text{int}} - S_1) \times \left( 1 - \sum_t \langle \delta S(t) \rangle_{\text{ext}} + \frac{1}{2} \sum_{t,t'} \langle \delta S(t) \delta S(t') \rangle_{\text{ext}} + \dots \right)$$



- First order term is zero because proportional to  $\langle \delta \varphi_{\text{ext}} \rangle_{\text{ext}} = 0$

- Second order term is non-zero:

**“hybridization function”**



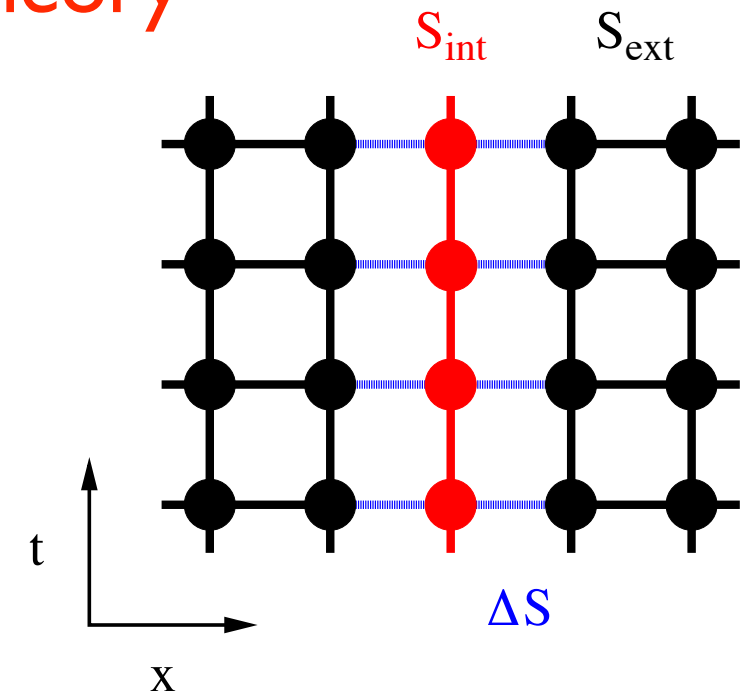
$$\langle \delta S(t) \delta S(t') \rangle_{\text{ext}} \equiv \delta \varphi_{\text{int},t}^\dagger \Delta(t - t') \delta \varphi_{\text{int},t'}$$

# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Cavity construction:** After re-exponentiation and switching back from  $\delta\varphi$  to  $\varphi$  we find the effective single-site action



$$S_{\text{imp}} = \sum_{t,t'} \varphi_t K_{\text{imp},c}^{-1}(t-t') \varphi_{t'} + \lambda \sum_t (\varphi_t^2 - 1)^2 - h \sum_t \varphi_t$$

$$\tilde{K}_{\text{imp},c}^{-1}(\omega) = 1 - 2\kappa \cos(\omega) - \tilde{\Delta}(\omega) \quad \text{Fourier transform of nn interaction in time}$$

$$h = 2\phi_{\text{ext}}(2\kappa(d-1) - \tilde{\Delta}(0)) \quad \text{because action written in terms of phi}$$

- We call it “impurity action” (condensed-matter convention)

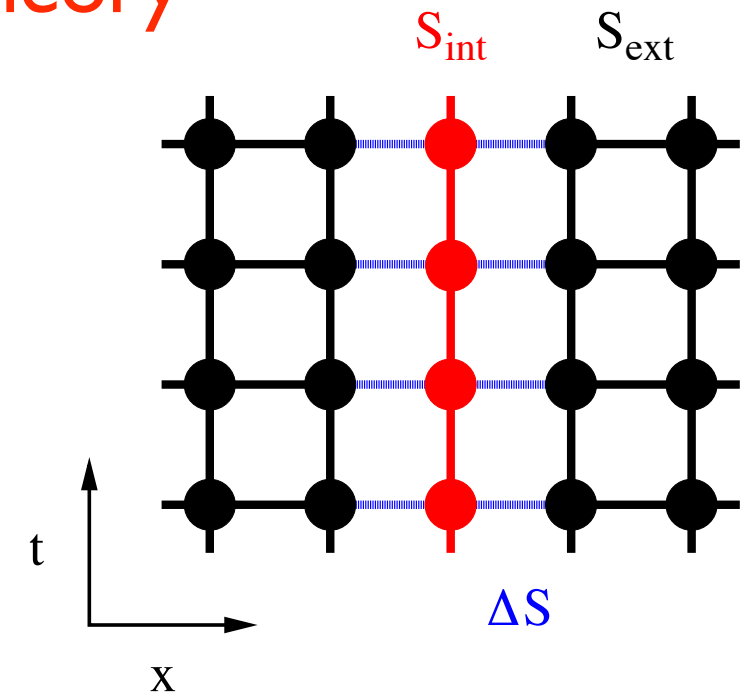
# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Dynamical mean field equations:**

Hybridization function  $\Delta$  and  $\phi_{\text{ext}}$  are fixed by self-consistency conditions



$$S_{\text{imp}} = \sum_{t,t'} \varphi_t K_{\text{imp},c}^{-1}(t-t') \varphi_{t'} + \lambda \sum_t (\varphi_t^2 - 1)^2 - h \sum_t \varphi_t$$

$$\tilde{K}_{\text{imp},c}^{-1}(\omega) = 1 - 2\kappa \cos(\omega) - \tilde{\Delta}(\omega)$$

$$h = 2\phi_{\text{ext}}(2\kappa(d-1) - \tilde{\Delta}(0))$$

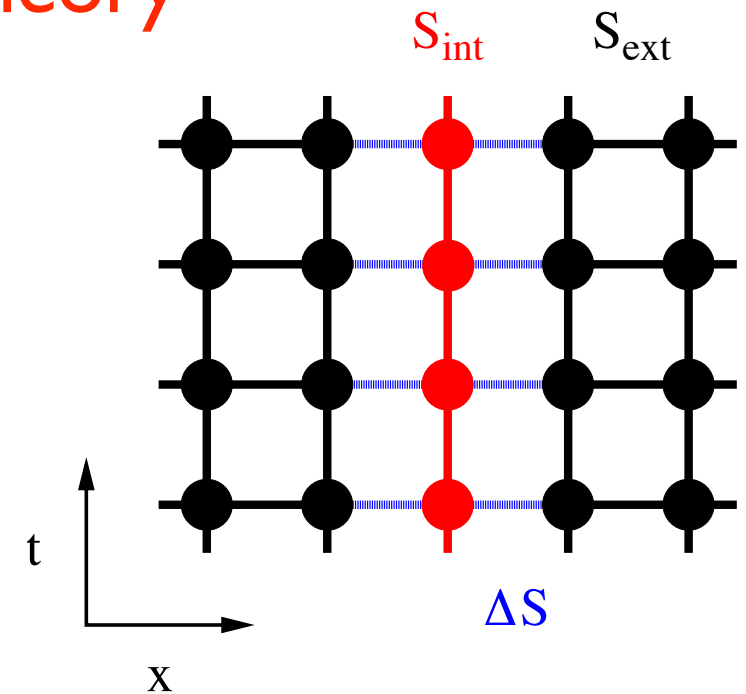
# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Dynamical mean field equations:**

Hybridization function  $\Delta$  and  $\phi_{\text{ext}}$  are fixed by self-consistency conditions



- Local lattice Green's function

$$\tilde{G}_{\text{loc}}(\omega) = \sum_k \frac{1}{\tilde{G}_0^{-1}(k, \omega) + \tilde{\Sigma}(k, \omega)}$$

*DMFT approximation: identify lattice and impurity self-energy*

$$\tilde{G}_0^{-1}(k, \omega) = 1 - 2\kappa \sum_{i=1}^d \cos(k_i)$$

*GF of the d-dimensional free theory*

- Impurity Green's function

$$\tilde{G}_{\text{imp}}(\omega) = \frac{1}{\tilde{K}_{\text{imp},c}^{-1}(\omega) + \tilde{\Sigma}_{\text{imp}}(\omega)} = \frac{1}{1 - 2\kappa \cos(\omega) - \tilde{\Delta}(\omega) + \tilde{\Sigma}_{\text{imp}}(\omega)}$$

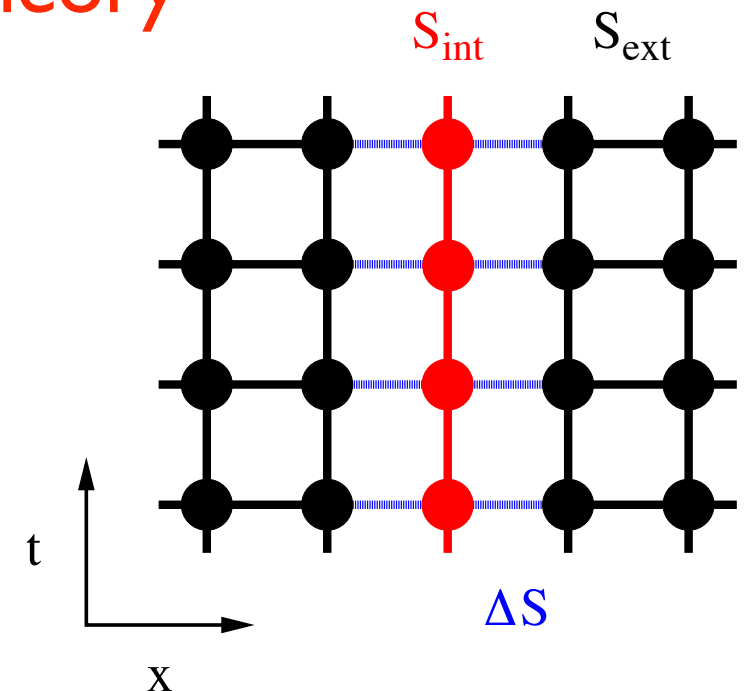
# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Dynamical mean field equations:**

Hybridization function  $\Delta$  and  $\phi_{\text{ext}}$  are fixed by self-consistency conditions



- Local lattice Green's function

$$\tilde{G}_{\text{loc}}(\omega) = \sum \frac{1}{\tilde{G}_{\text{imp}}^{-1}(\omega) + \tilde{\Delta}(\omega) - 2\kappa \sum_{i=1}^{d-1} \cos k_i}$$

- Self-consistency equations:

$$\begin{aligned} \tilde{G}_{\text{imp}}(\omega) &= \tilde{G}_{\text{loc}}(\omega) \\ \langle \varphi \rangle_{S_{\text{imp}}} &= \phi_{\text{ext}} \end{aligned}$$

*substitution yields an implicit equation for the hybridization function*

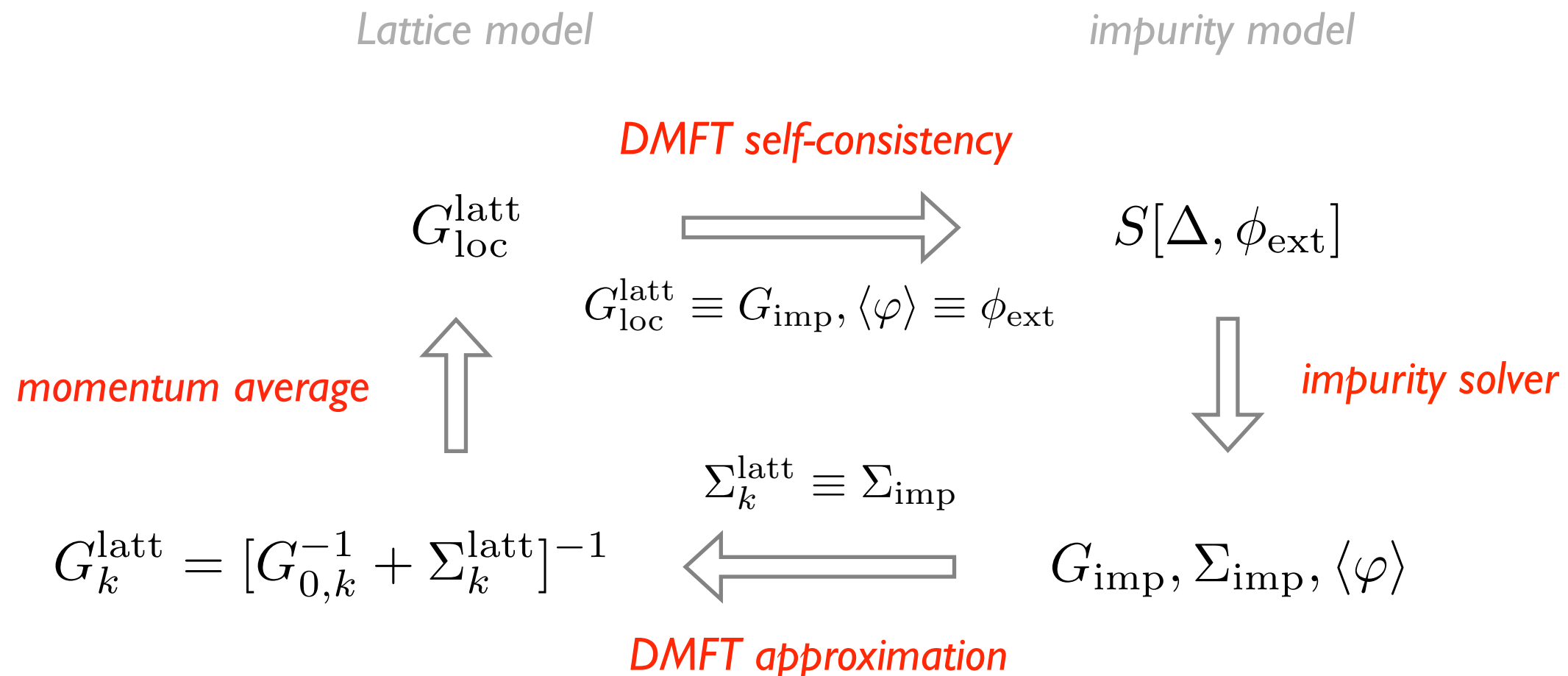
# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Dynamical mean field equations:**

Hybridization function  $\Delta$  and  $\phi_{\text{ext}}$   
are fixed by self-consistency conditions

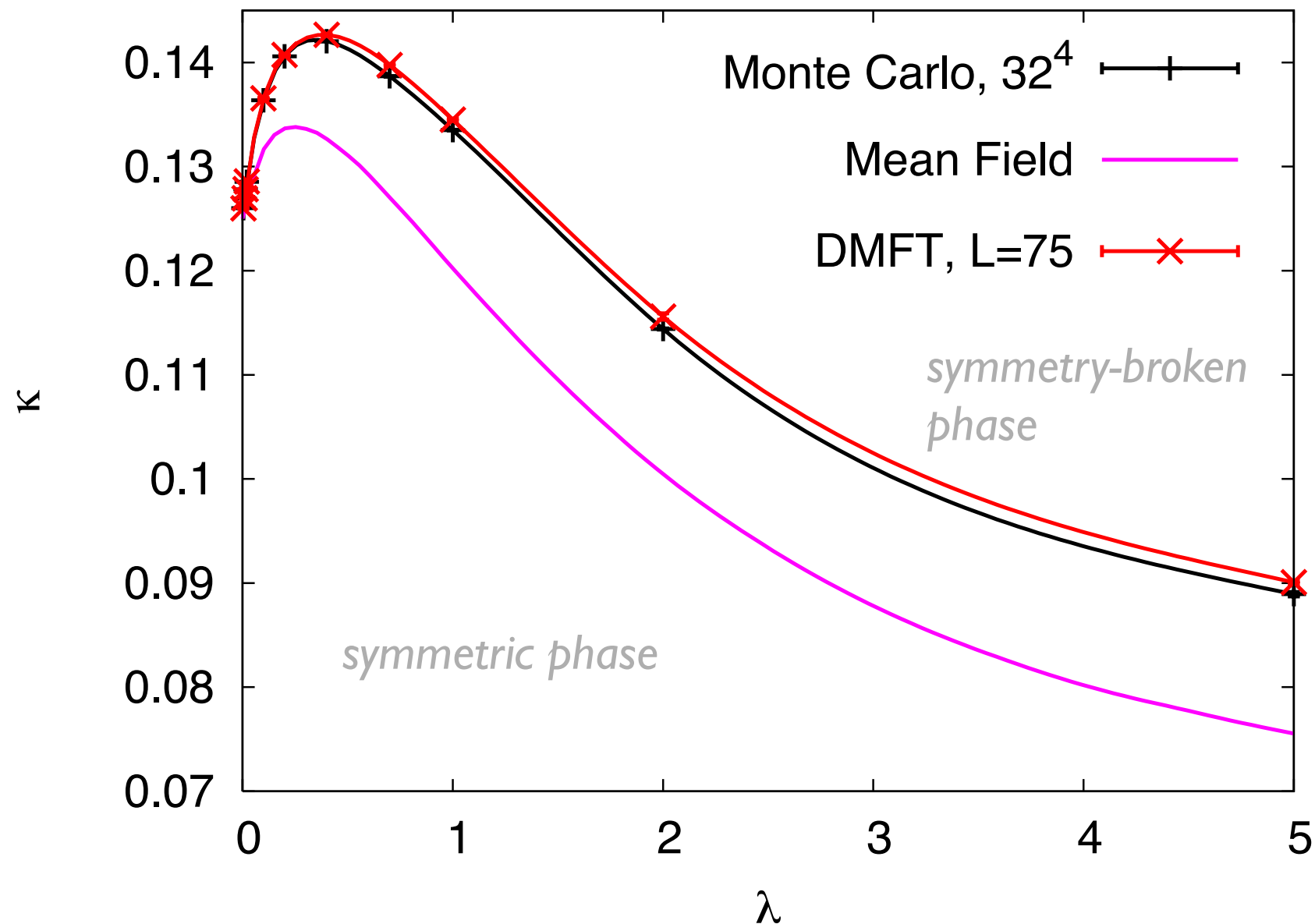


# DMFT for quantum field theories

- Simple example: **real, scalar  $\varphi^4$  quantum field theory**

*Akerlund, de Forcrand, Georges & Werner (2013)*

- Dynamical mean field phase diagram ( $d=3+1$ ):**

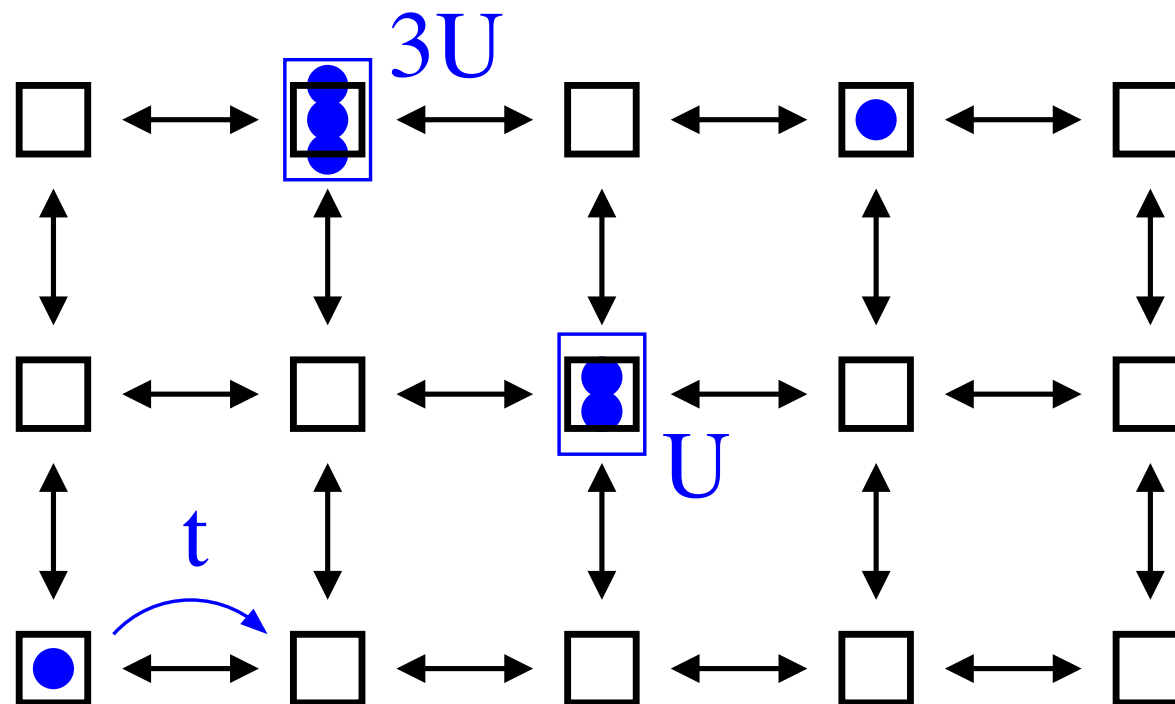


# DMFT for Bosons

- Simple example: **Bose-Hubbard model**

*Fisher, Grinstein, Weichmann & Fisher (1989)*

$$H = -t \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i$$



- Mott-Insulator to superfluid transition at low temperature

# DMFT for Bosons

- Simple example: **Bose-Hubbard model**
- Derivation of DMFT formalism analogous to the  $\varphi^4$  case

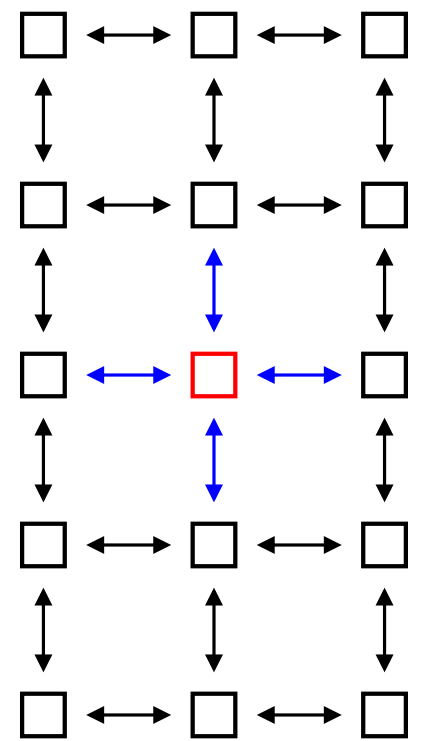
*Anders, Pollet, Gull, Troyer & Werner (2011)*

- Split action of the lattice model into  $S = S_{\text{int}} + \Delta S + S_{\text{ext}}$

$$S_{\text{int}} = \int_0^\beta d\tau \left[ -\mu b_{\text{int}}^\dagger b_{\text{int}} + \frac{U}{2} n_{\text{int}} (n_{\text{int}} - 1) \right]$$

$$\Delta S = -t \int_0^\beta \sum_{\langle \text{int}, \text{ext} \rangle} (b_{\text{int}}^\dagger b_{\text{ext}} + b_{\text{ext}}^\dagger b_{\text{int}})$$

$$S_{\text{ext}} = \int_0^\beta d\tau \left[ -\mu b_{\text{ext}}^\dagger b_{\text{ext}} + \frac{U}{2} n_{\text{ext}} (n_{\text{ext}} - 1) \right]$$

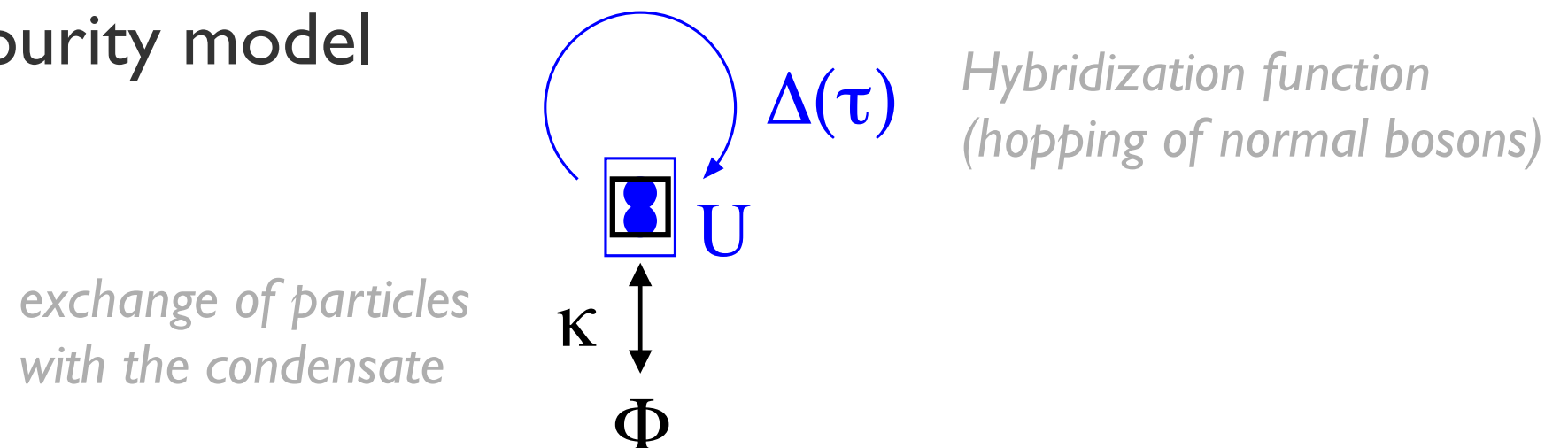


- To allow for symmetry breaking (condensation), write

$$b_{\text{ext}} = \phi_{\text{ext}} + \delta b_{\text{ext}}, \quad b_{\text{int}} = \phi_{\text{int}} + \delta b_{\text{int}}$$

# DMFT for Bosons

- Simple example: **Bose-Hubbard model**
- Derivation of DMFT formalism analogous to the  $\varphi^4$  case  
*Anders, Pollet, Gull, Troyer & Werner (2011)*
- Expand  $\exp(-\Delta S)$ , integrate out external degrees of freedom
- End up with an impurity model



$$S_{\text{imp}} = -\frac{1}{2} \int_0^\beta \mathbf{b}^\dagger(\tau) \mathbf{\Delta}(\tau - \tau') \mathbf{b}(\tau') + \int_0^\beta d\tau \left[ -\mu n(\tau) + \frac{U}{2} n(\tau) [n(\tau) - 1] \right] - \kappa \Phi^\dagger \int_0^\beta d\tau \mathbf{b}(\tau)$$

# DMFT for Bosons

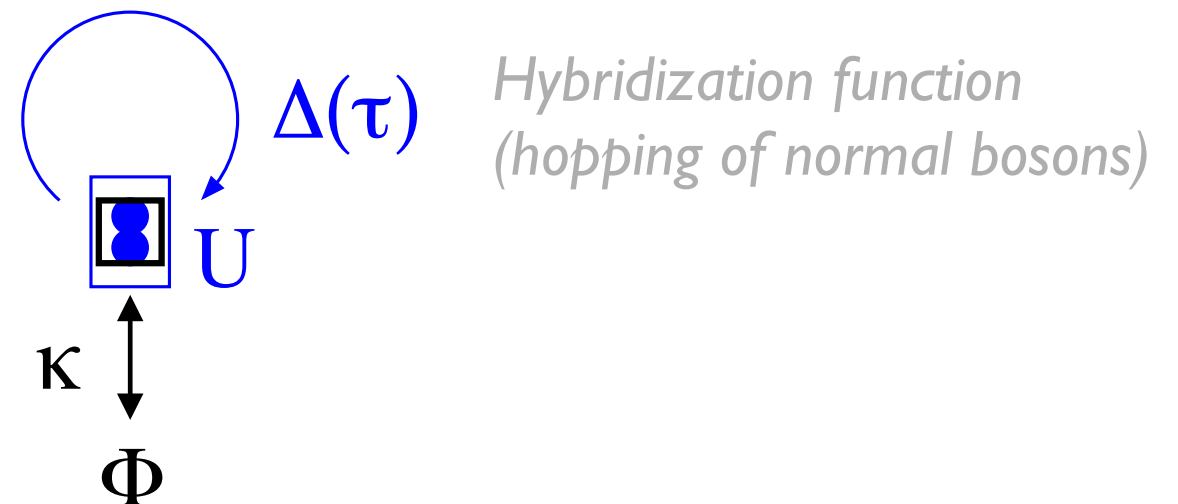
- Simple example: **Bose-Hubbard model**
- Derivation of DMFT formalism analogous to the  $\varphi^4$  case  
*Anders, Pollet, Gull, Troyer & Werner (2011)*
- Expand  $\exp(-\Delta S)$ , integrate out external degrees of freedom

- End up with an impurity model

*Nambu notation*



*exchange of particles  
with the condensate*



- $\Delta$  and  $\Phi$  fixed by the DMFT self-consistency condition  
*approximation: identification of lattice and impurity self-energy*

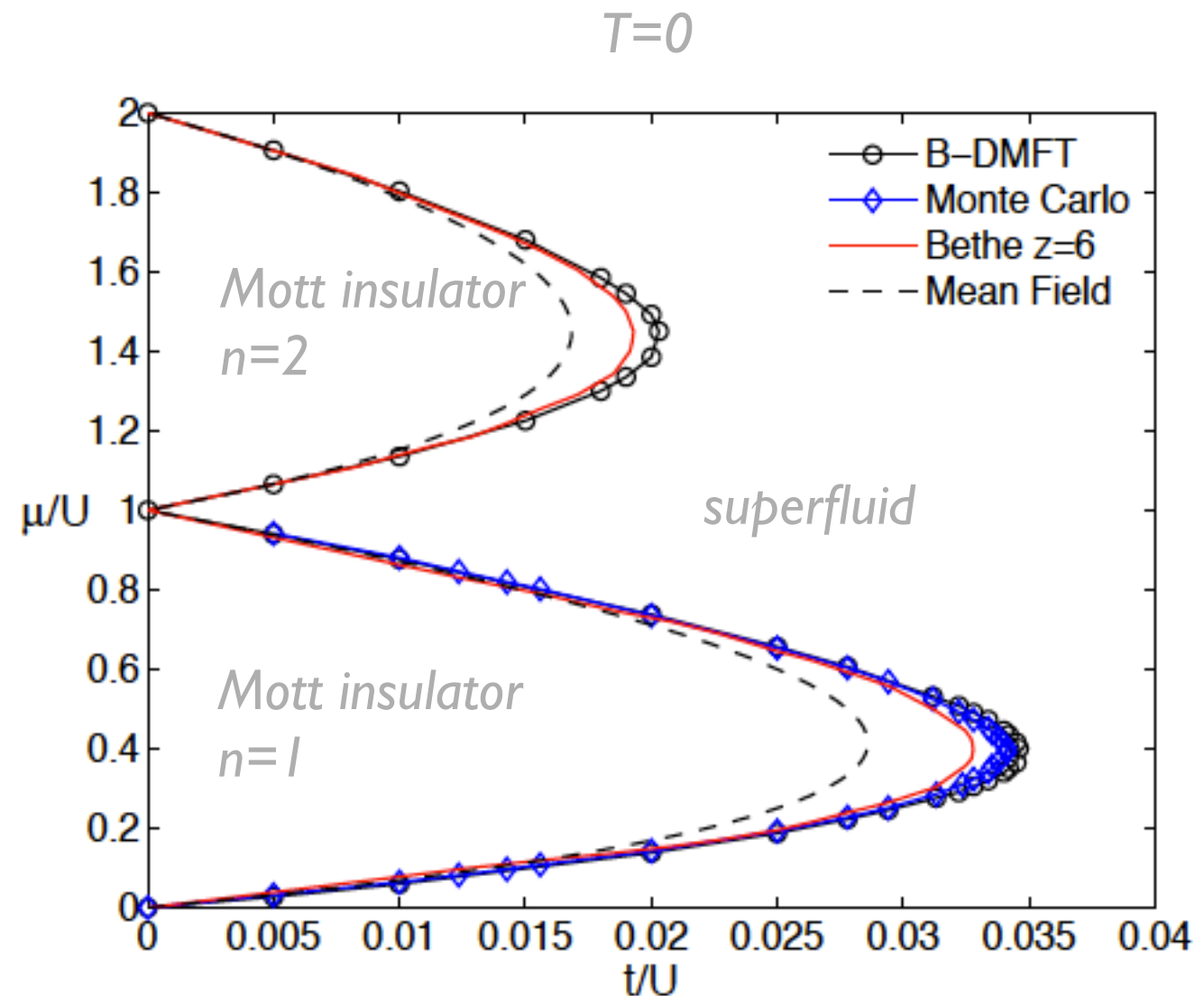
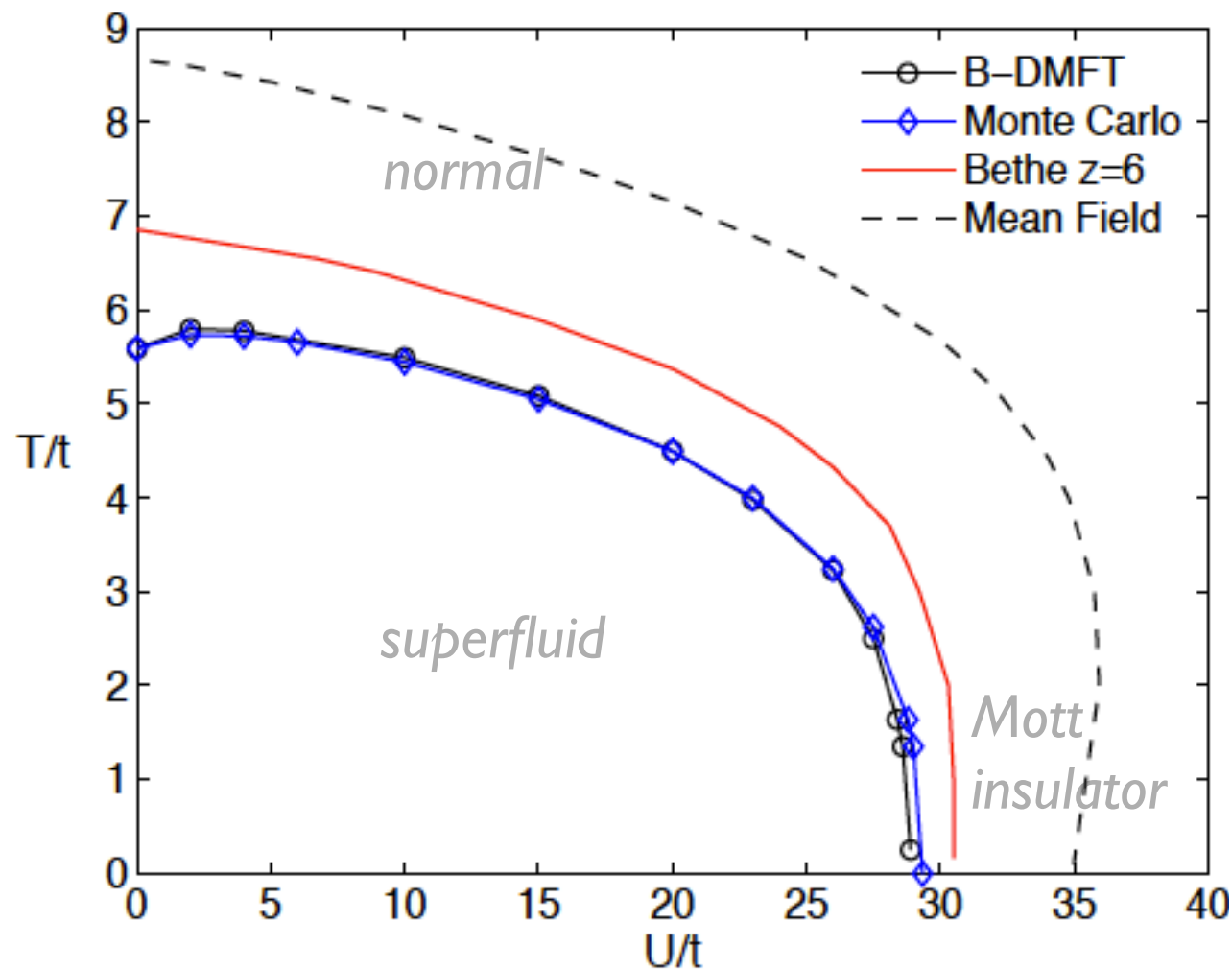
$$\Phi = \langle \mathbf{b}(\tau) \rangle_{S_{\text{imp}}}, \quad \mathbf{G}_{\text{loc}}^{\text{latt}} = \mathbf{G}_{\text{imp},c} \quad [= -\langle T \mathbf{b}(\tau) \mathbf{b}^\dagger(0) \rangle_{S_{\text{imp}}} + \Phi \Phi^\dagger]$$

# DMFT for Bosons

- Simple example: **Bose-Hubbard model**
- Derivation of DMFT formalism analogous to the  $\varphi^4$  case

*Anders, Pollet, Gull, Troyer & Werner (2011)*

- Results: Phase diagram ( $d=3+1$ )



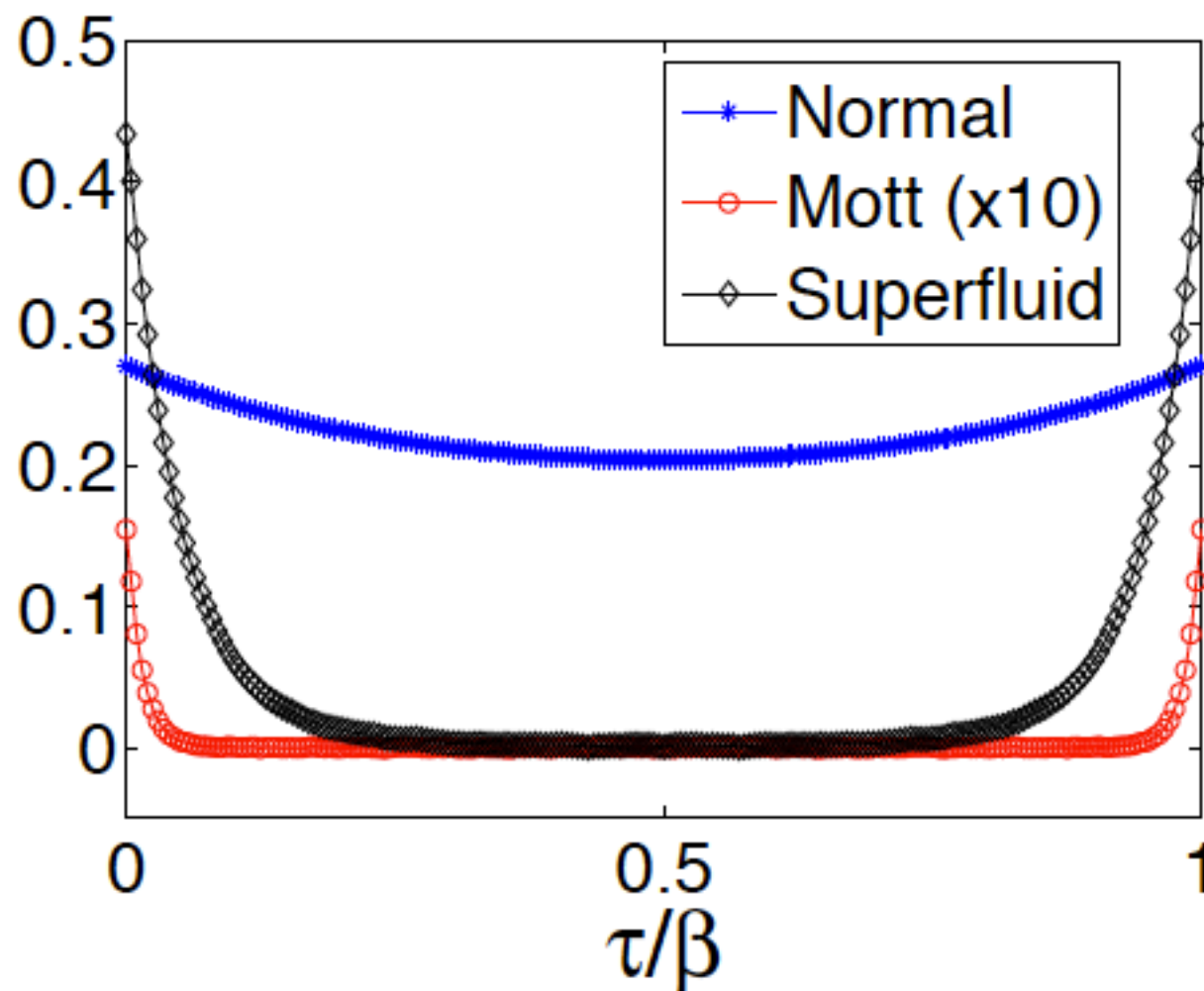
# DMFT for Bosons

- Simple example: **Bose-Hubbard model**
- Derivation of DMFT formalism analogous to the  $\varphi^4$  case

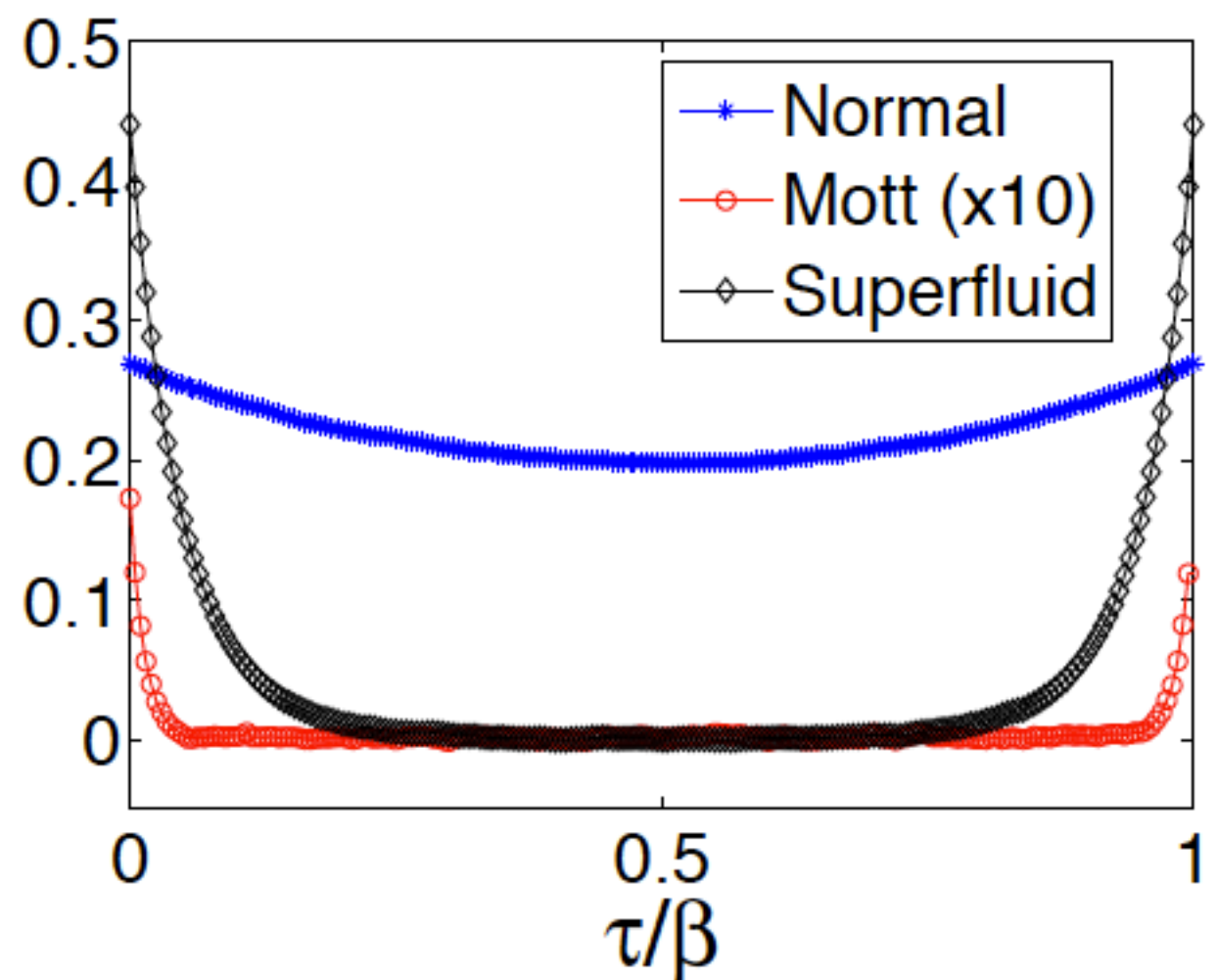
*Anders, Pollet, Gull, Troyer & Werner (2011)*

- Results: Connected density-density correlation functions ( $d=3+1$ )

DMFT



lattice QMC

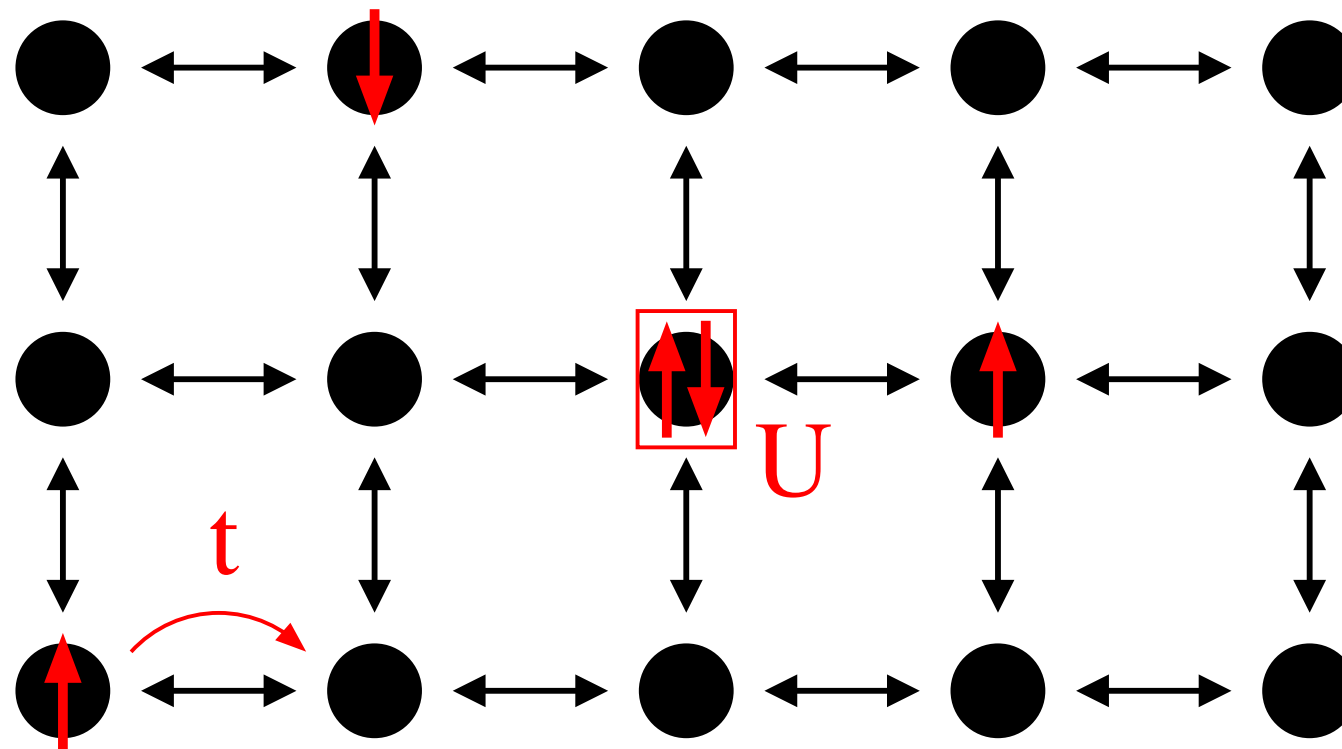


# DMFT for Fermions

- Simple example: **single-band Hubbard model**

*Gutzwiller, Kanamori, Hubbard (1963)*

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu \sum_{i,\sigma} n_{i,\sigma}$$



- Describes Mott transition, magnetic and superconducting transitions

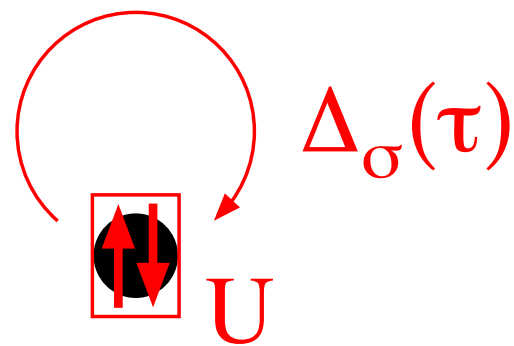
# DMFT for Fermions

- Simple example: **single-band Hubbard model**

*Gutzwiller, Kanamori, Hubbard (1963)*

- **Dynamical mean field theory:** Mapping to a quantum impurity model

*Georges & Kotliar (1992)*



*Hybridization function  
(describes hopping of electrons  
into the lattice and back)*

- Hybridization functions  $\Delta_\sigma$  fixed by DMFT self-consistency condition

*approximation: identification of lattice and impurity self-energy*

$$G_{\text{loc},\sigma}^{\text{latt}} = G_{\text{imp},\sigma}$$

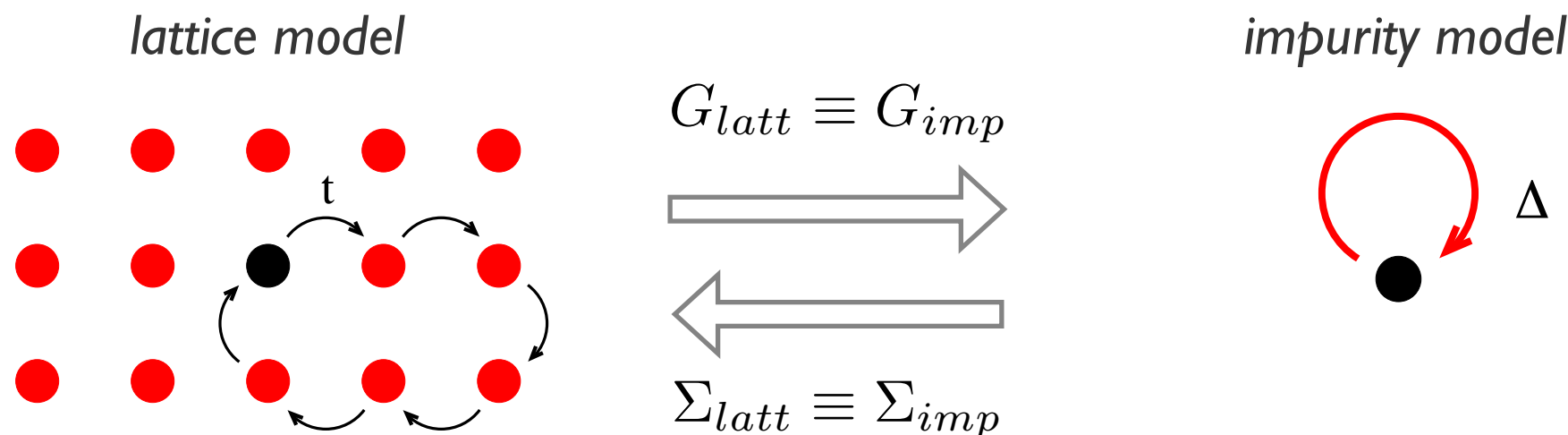
# DMFT for Fermions

- Simple example: **single-band Hubbard model**

*Gutzwiller, Kanamori, Hubbard (1963)*

- **Dynamical mean field theory:** Mapping to a quantum impurity model

*Georges & Kotliar (1992)*



- Various numerical approaches to solve the impurity problem:  
*weak-coupling perturbation theory, strong-coupling perturbation theory, exact diagonalization, NRG, QMC, ...*

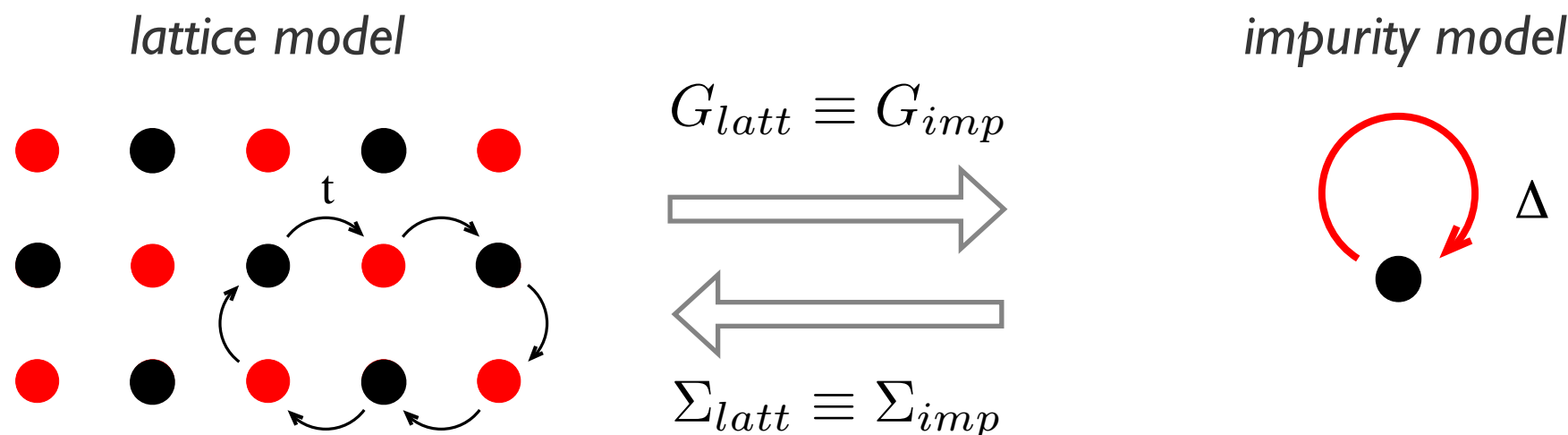
# DMFT for Fermions

- Simple example: **single-band Hubbard model**

*Gutzwiller, Kanamori, Hubbard (1963)*

- Dynamical mean field theory:** Mapping to a quantum impurity model

*Georges & Kotliar (1992)*



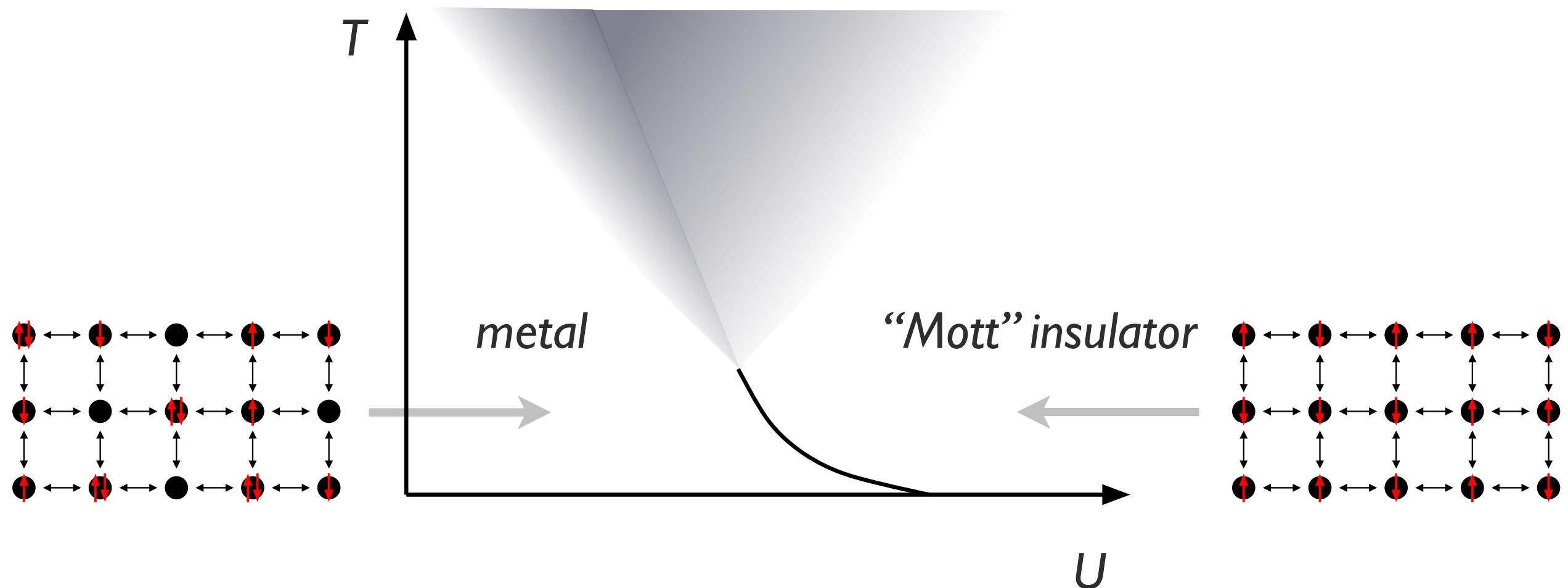
- Single-site DMFT can treat two-sublattice order (e. g. AFM)

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

- Pure Neel order:  $\text{Bath}_{B,\sigma} = \text{Bath}_{A,\bar{\sigma}}$

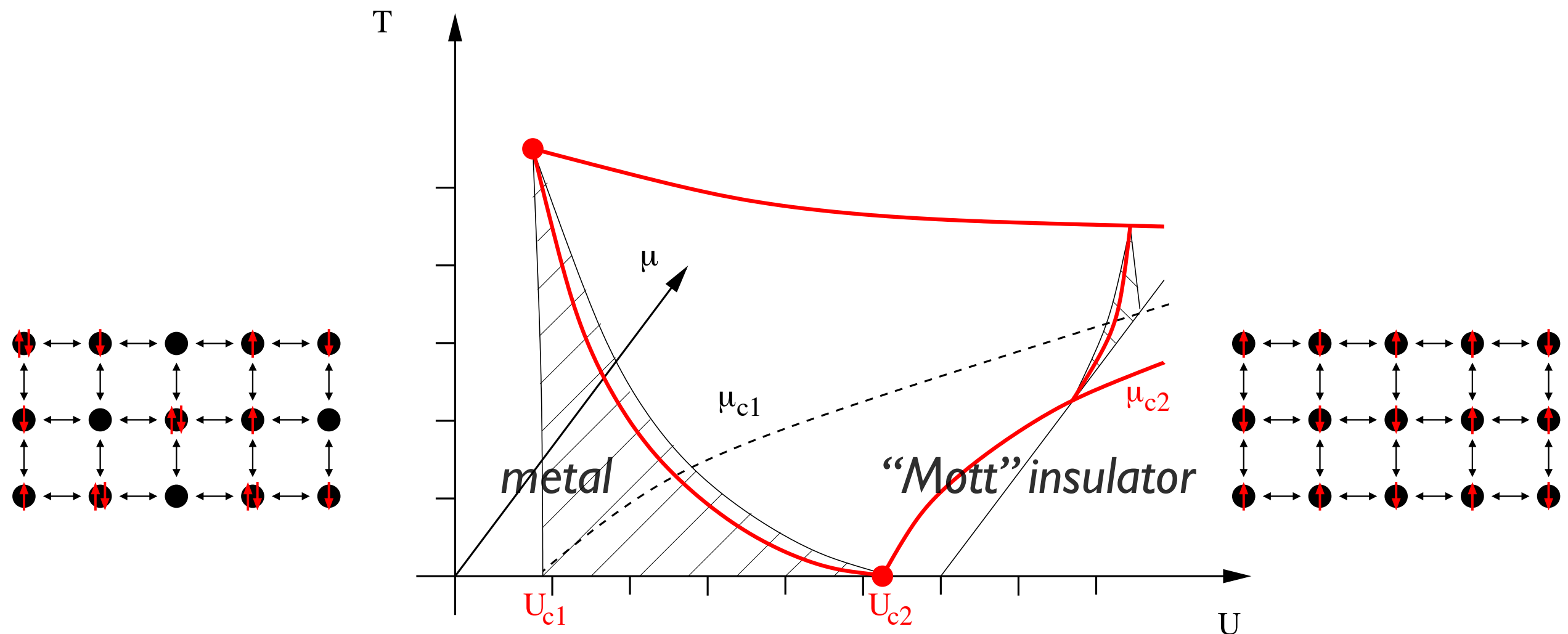
# DMFT for Fermions

- Equilibrium DMFT phase diagram (half-filling)
- Paramagnetic calculation: Metal - Mott insulator transition at low  $T$
- Smooth crossover at high  $T$



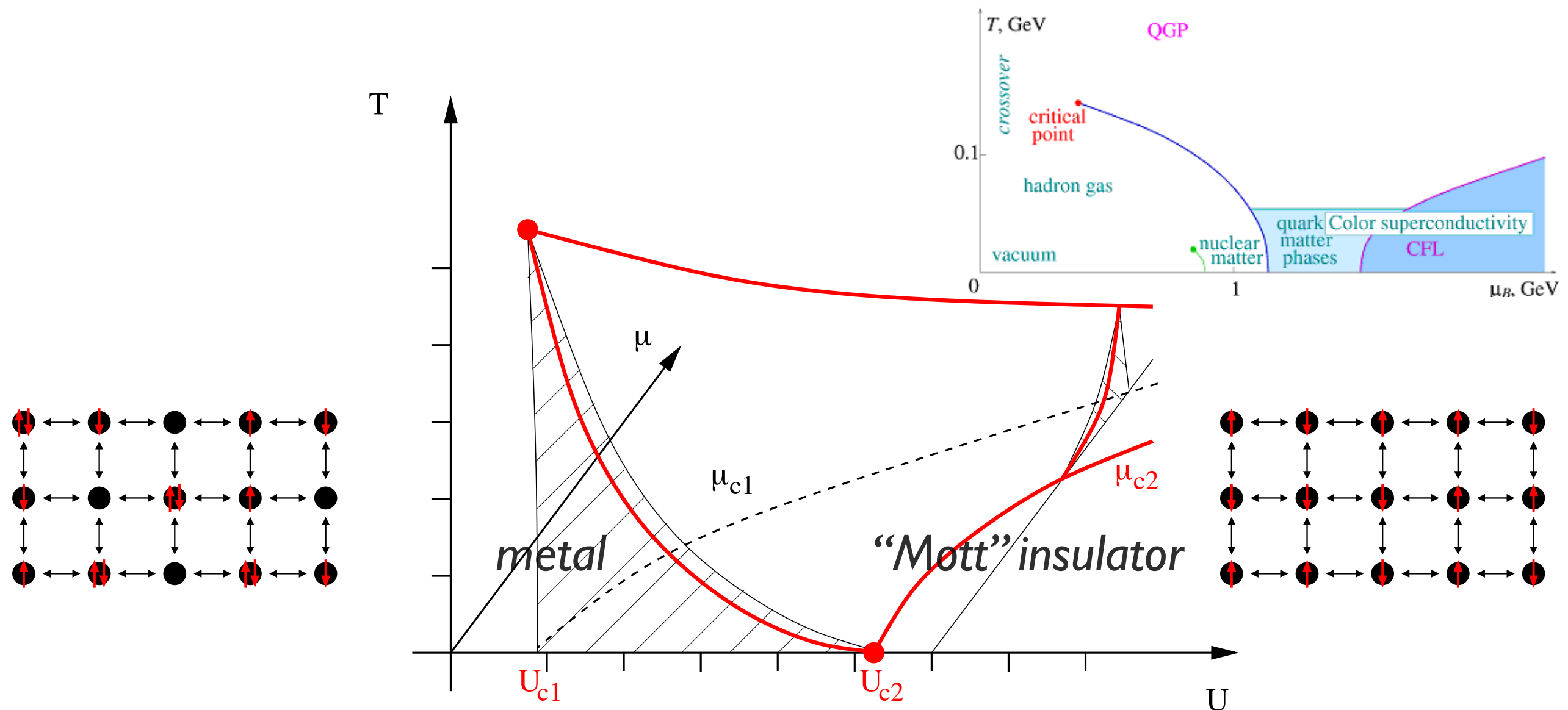
# DMFT for Fermions

- Equilibrium DMFT phase diagram
- Paramagnetic calculation: Metal - Mott insulator transition at low  $T$
- Doping-driven metallization upon increasing  $\mu$



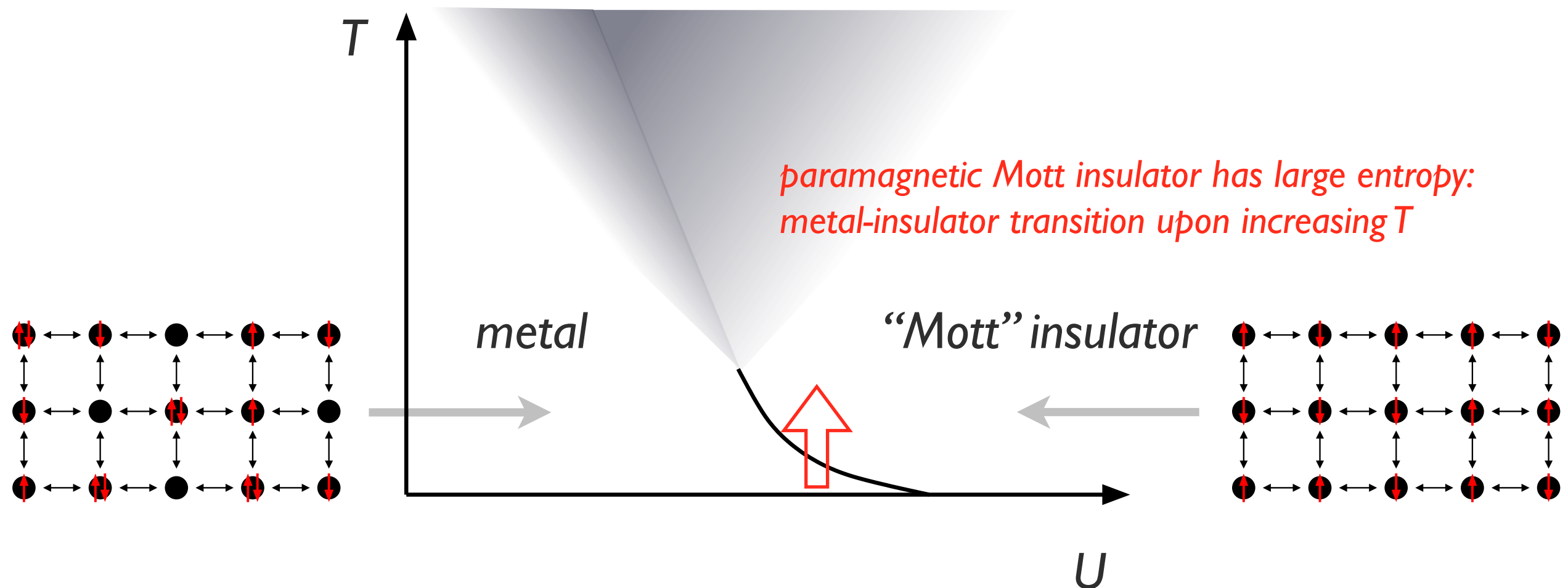
# DMFT for Fermions

- Equilibrium DMFT phase diagram
- Paramagnetic calculation: Metal - Mott insulator transition at low  $T$
- Doping-driven metallization upon increasing  $\mu$



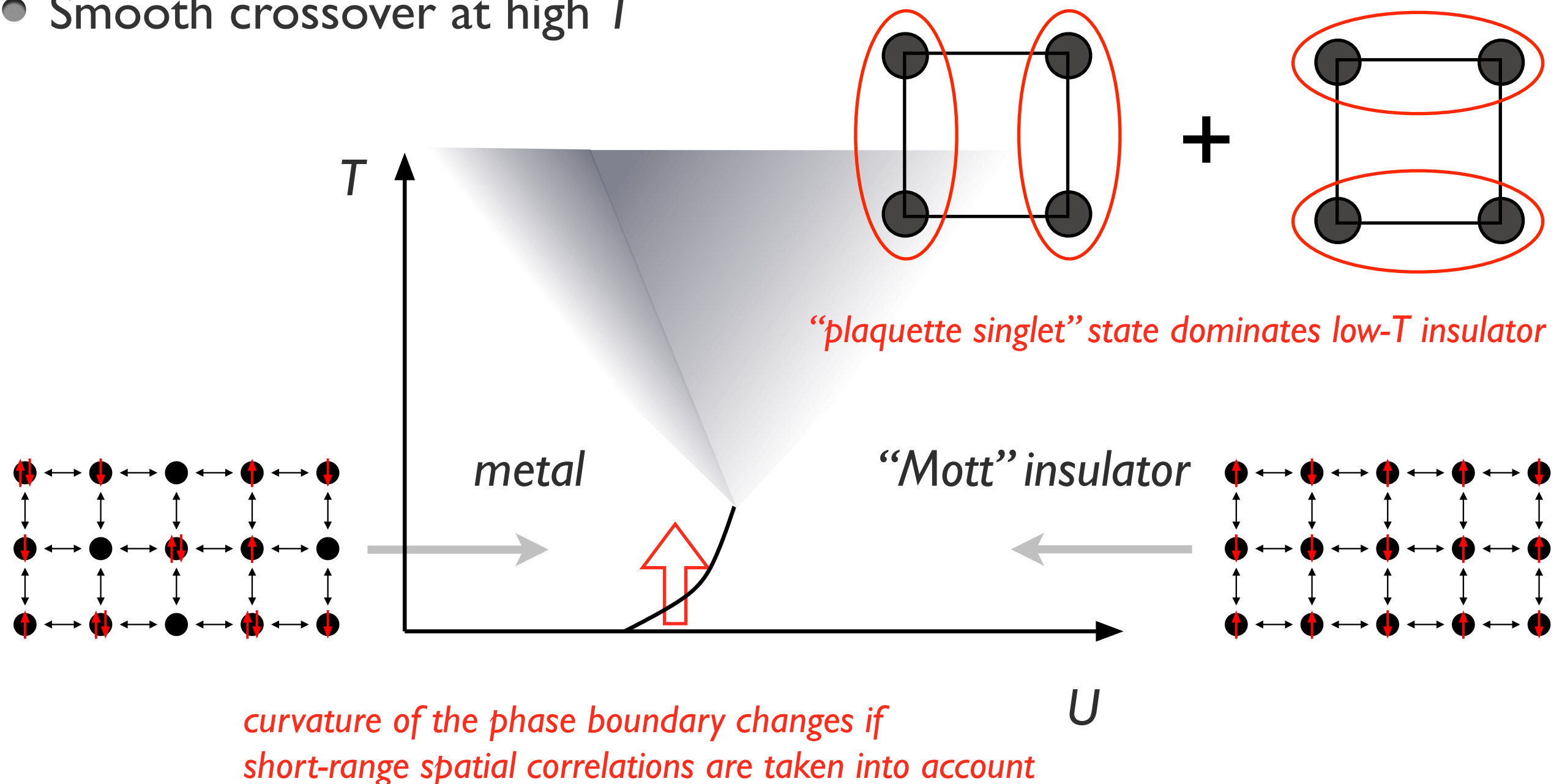
# DMFT for Fermions

- Equilibrium DMFT phase diagram (half-filling)
- Paramagnetic calculation: Metal - Mott insulator transition at low  $T$
- Smooth crossover at high  $T$



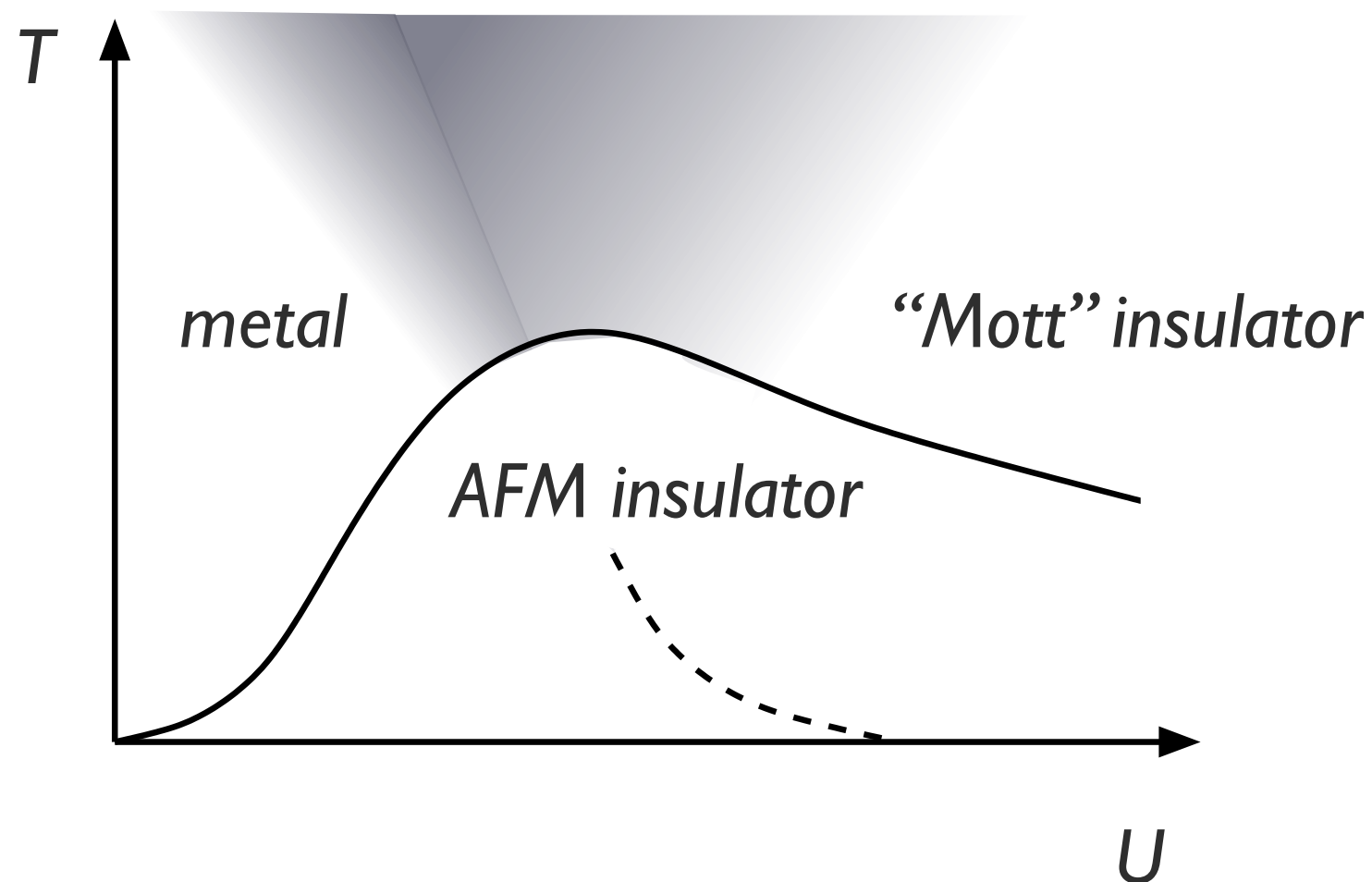
# DMFT for Fermions

- Equilibrium DMFT phase diagram (half-filling)
- Paramagnetic calculation: Metal - Mott insulator transition at low  $T$
- Smooth crossover at high  $T$



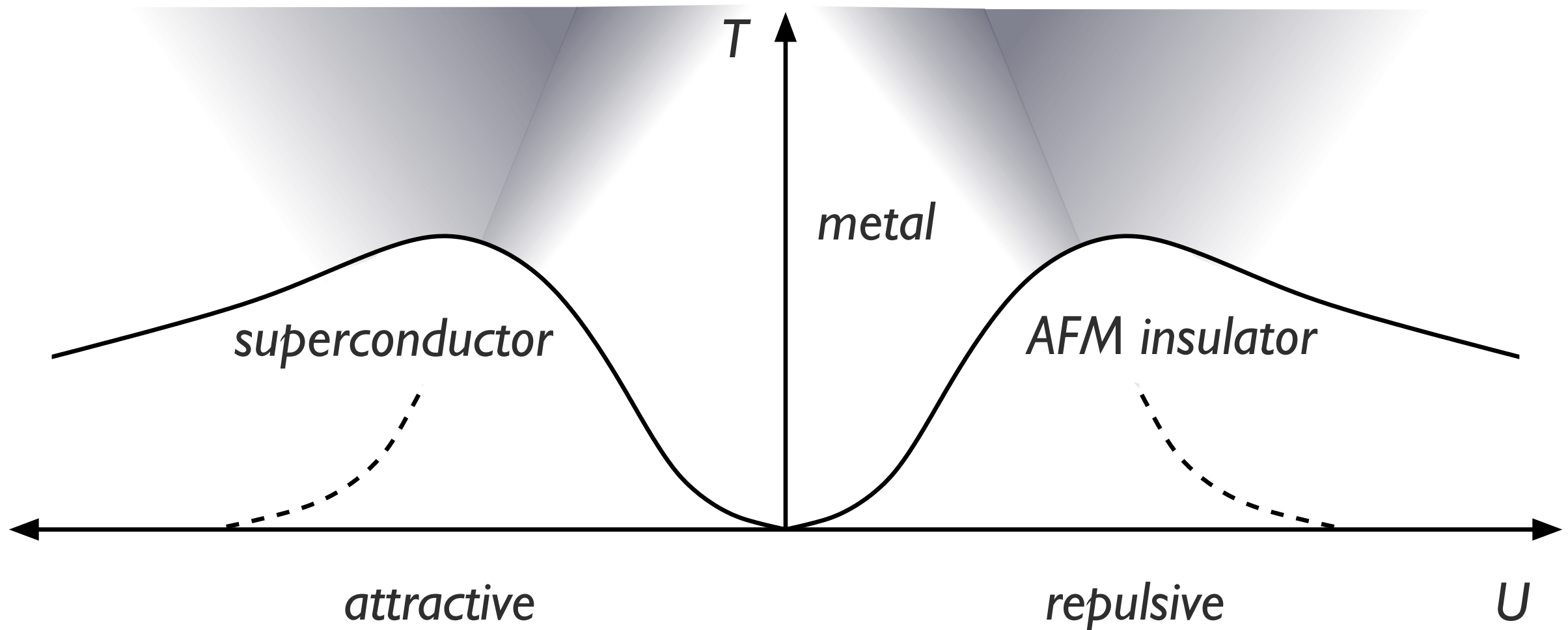
# DMFT for Fermions

- Equilibrium DMFT phase diagram (half-filling)
- With 2-sublattice order: Antiferromagnetic insulator at low  $T$
- Smooth crossover at high  $T$



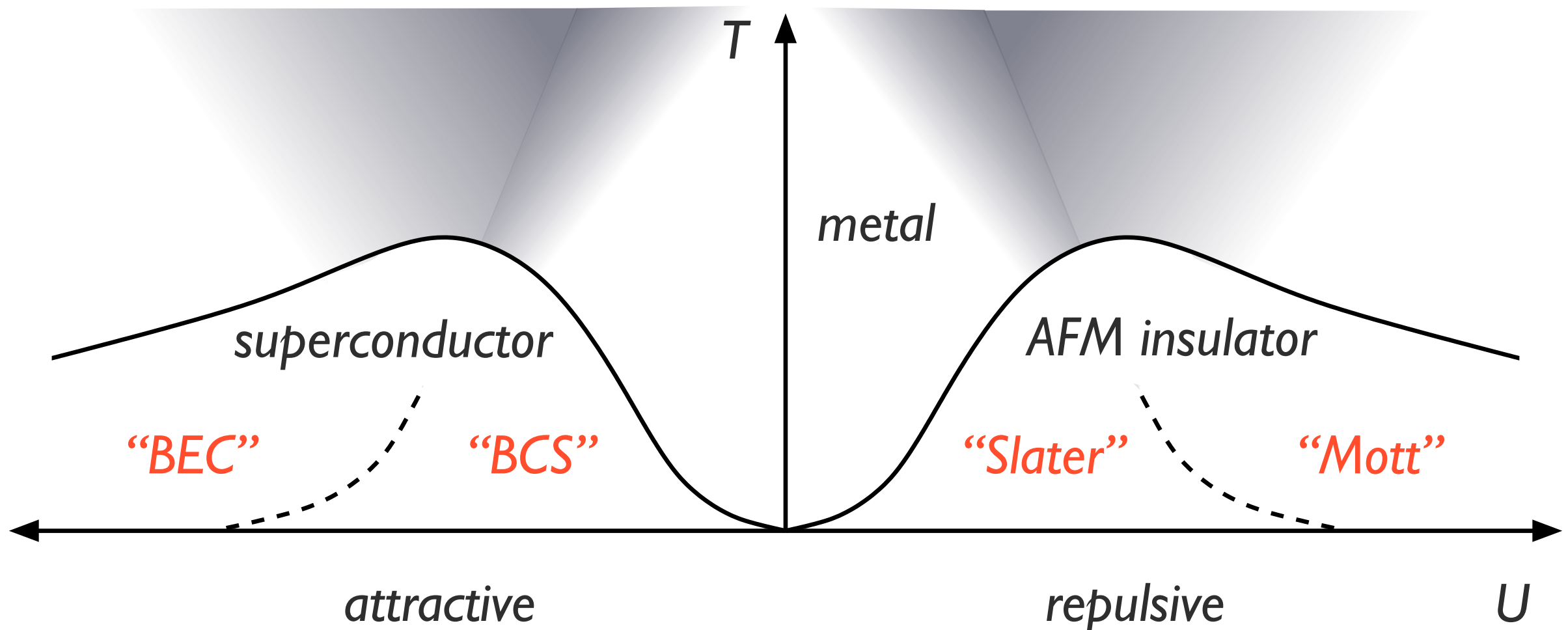
# DMFT for Fermions

- Equilibrium DMFT phase diagram (half-filling)
- Transformation  $c_{i\uparrow} \rightarrow c_{i\uparrow}^\dagger$  ( $i \in A$ ),  $c_{i\uparrow} \rightarrow -c_{i\uparrow}^\dagger$  ( $i \in B$ )  
maps repulsive model onto attractive model



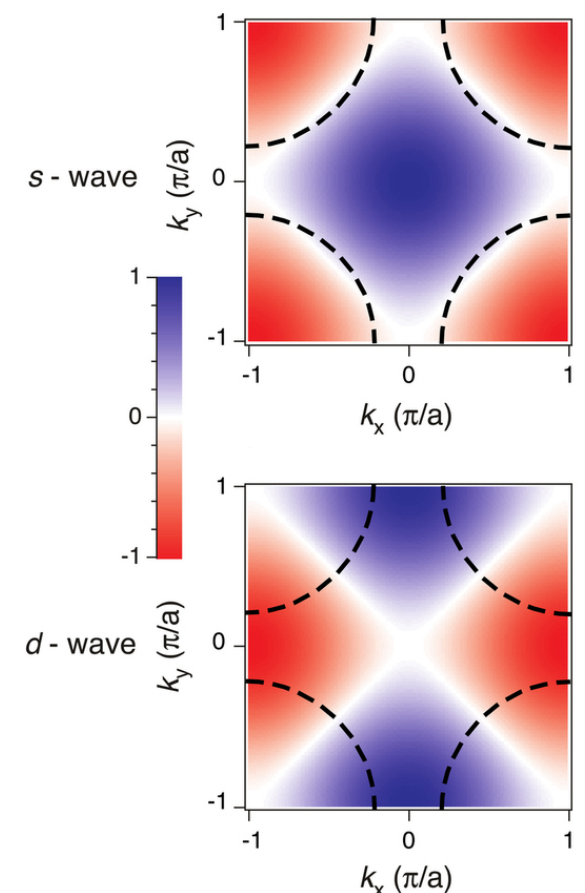
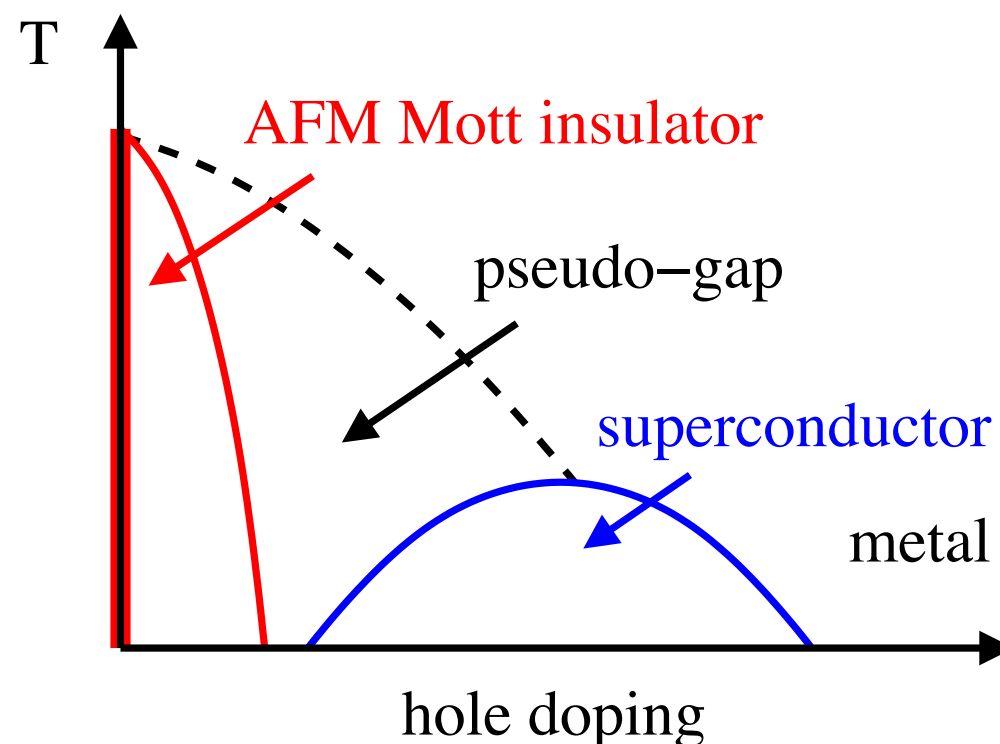
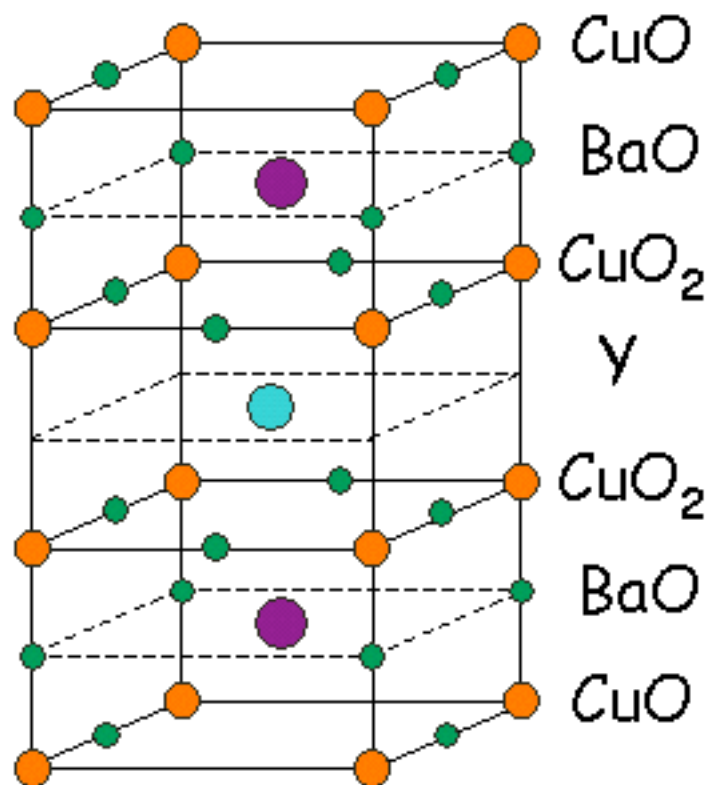
# DMFT for Fermions

- Equilibrium DMFT phase diagram (half-filling)
- Half-filling: transformation  $c_{i\uparrow} \rightarrow c_{i\uparrow}^\dagger$  ( $i \in A$ ),  $c_{i\uparrow} \rightarrow -c_{i\uparrow}^\dagger$  ( $i \in B$ )  
maps repulsive model onto attractive model



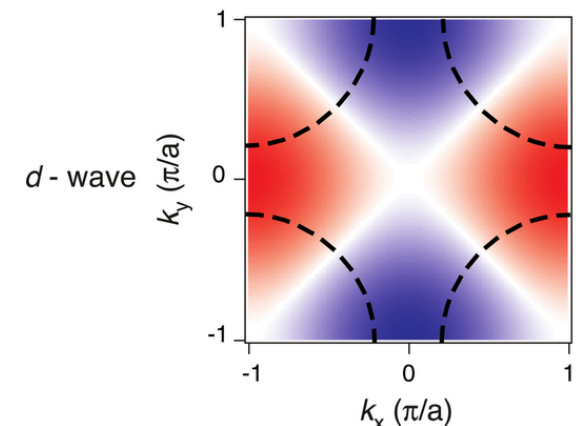
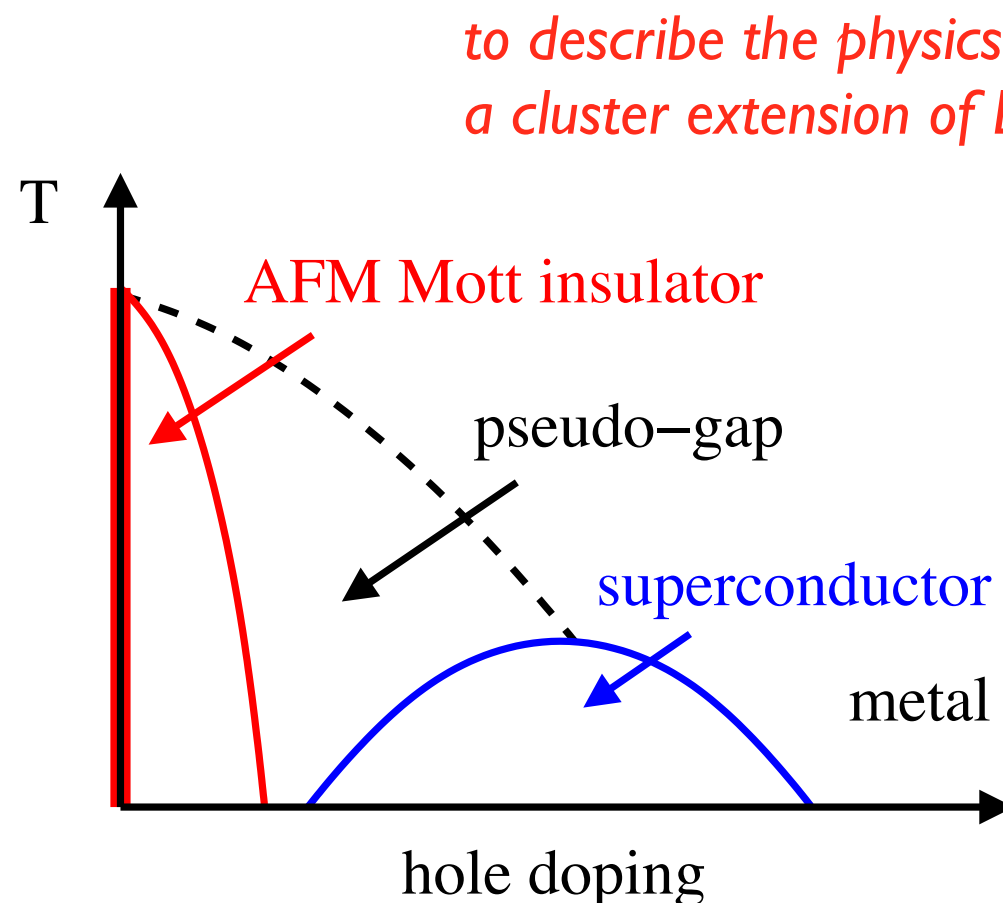
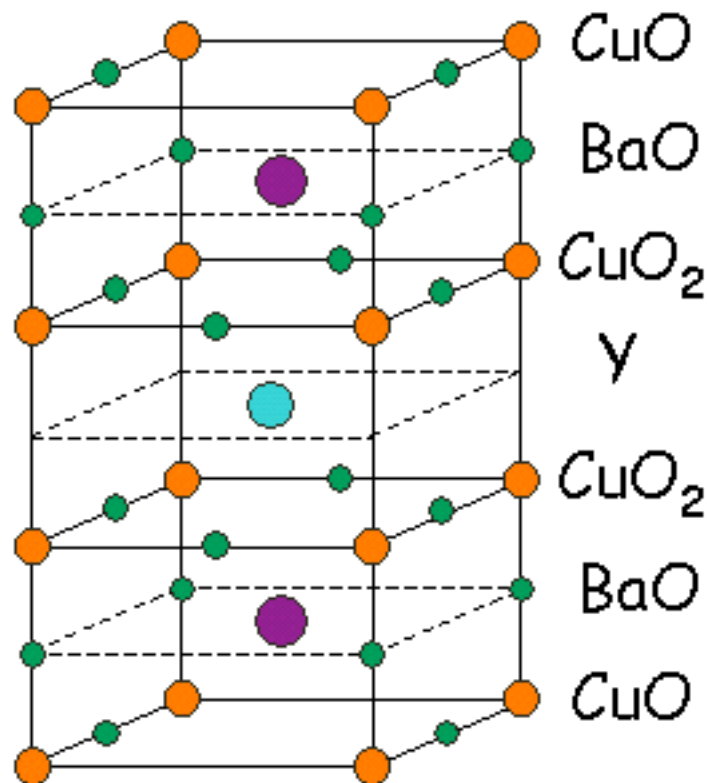
# DMFT for Fermions

- 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- $T_c$  (cuprate) superconductors



# DMFT for Fermions

- 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- $T_c$  (cuprate) superconductors

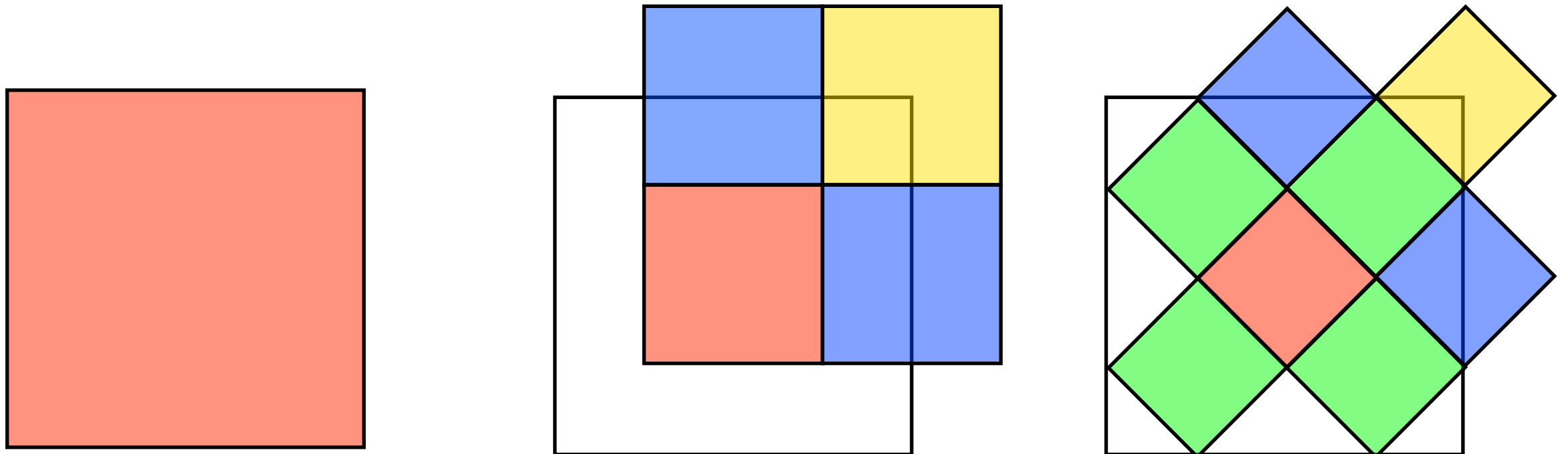


# DMFT for Fermions

- 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

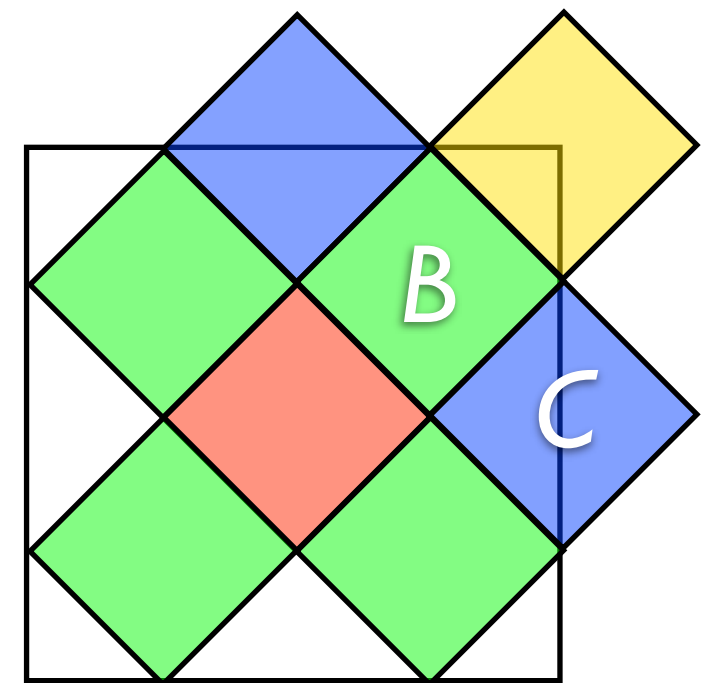
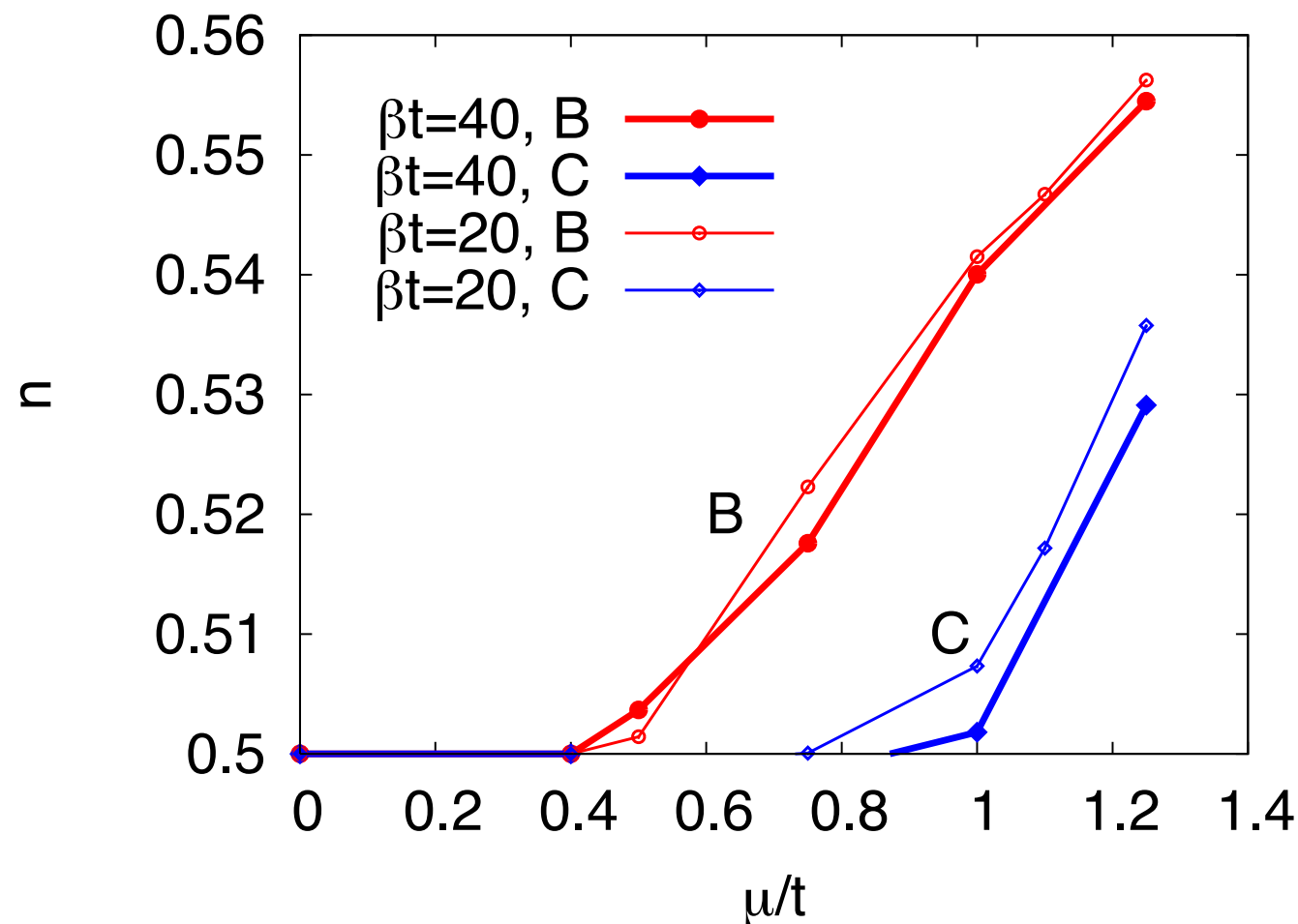
$$\Sigma(p, \omega) = \sum_a \phi_a(p) \Sigma_a(\omega)$$

- “Tiling” of the Brillouin zone



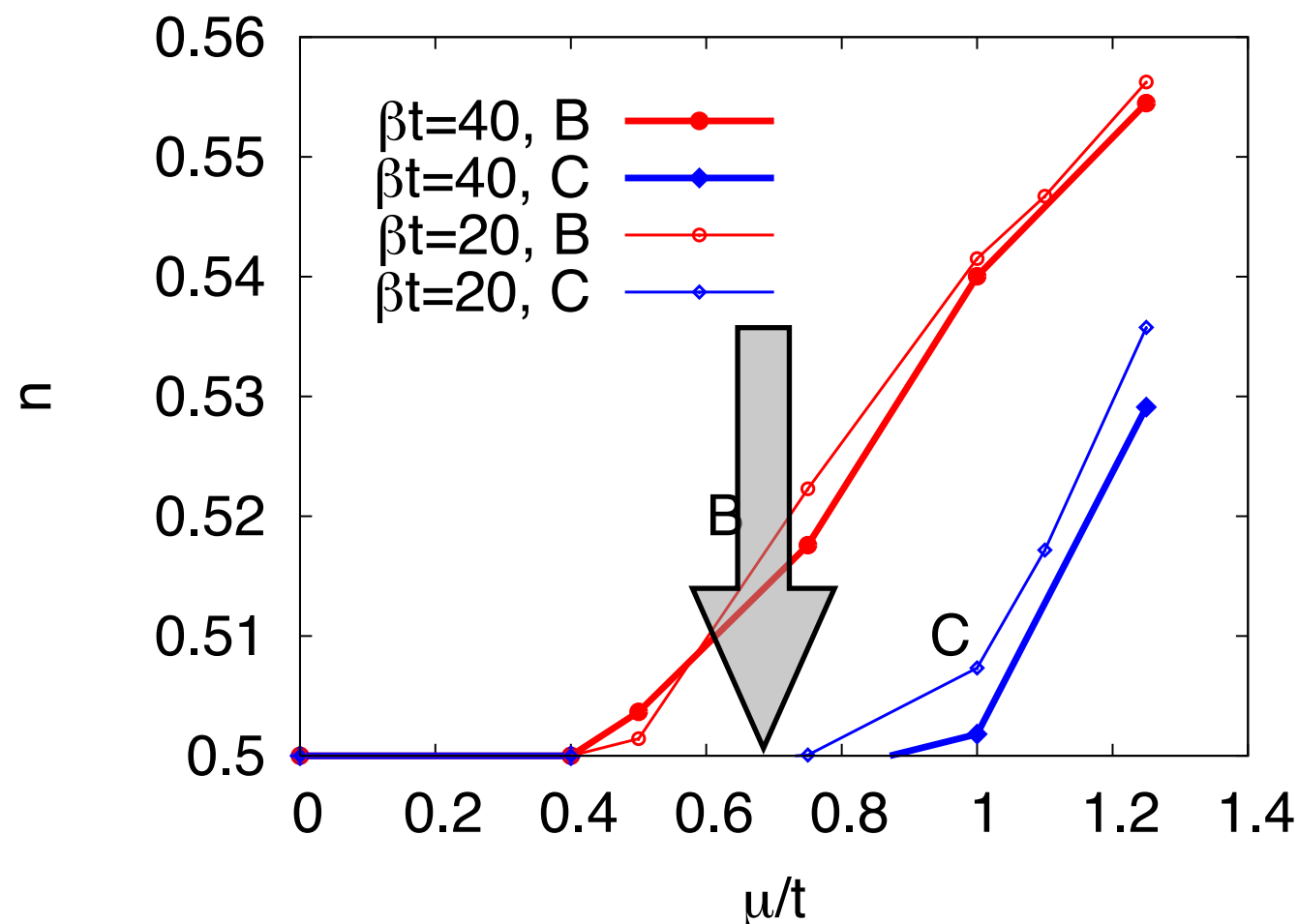
# DMFT for Fermions

- Low-dimensional systems
- Cluster DMFT self-consistently embeds a cluster of  $N_c$  sites into a fermionic bath *Hettler, Prushke, Krishnamurthy & Jarrell (1998)*
- Doping driven insulator-metal transition in the 8-site cluster DMFT
  - first 8% of dopants go into the *B* sector *Werner, Gull, Parcollet & Millis (2010)*

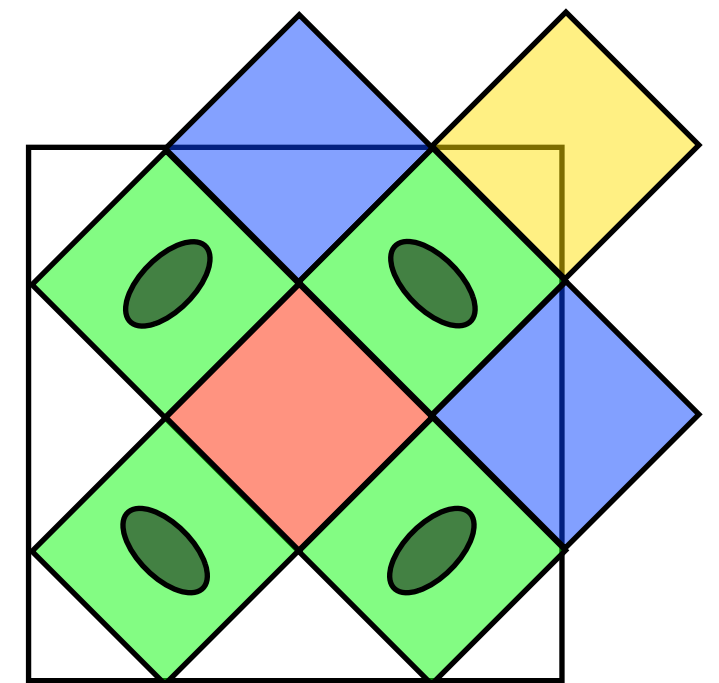


# DMFT for Fermions

- Low-dimensional systems
- Cluster DMFT self-consistently embeds a cluster of  $N_c$  sites into a fermionic bath *Hettler, Prushke, Krishnamurthy & Jarrell (1998)*
- Doping driven insulator-metal transition in the 8-site cluster DMFT
  - first 8% of dopants go into the *B* sector *Werner, Gull, Parcollet & Millis (2010)*

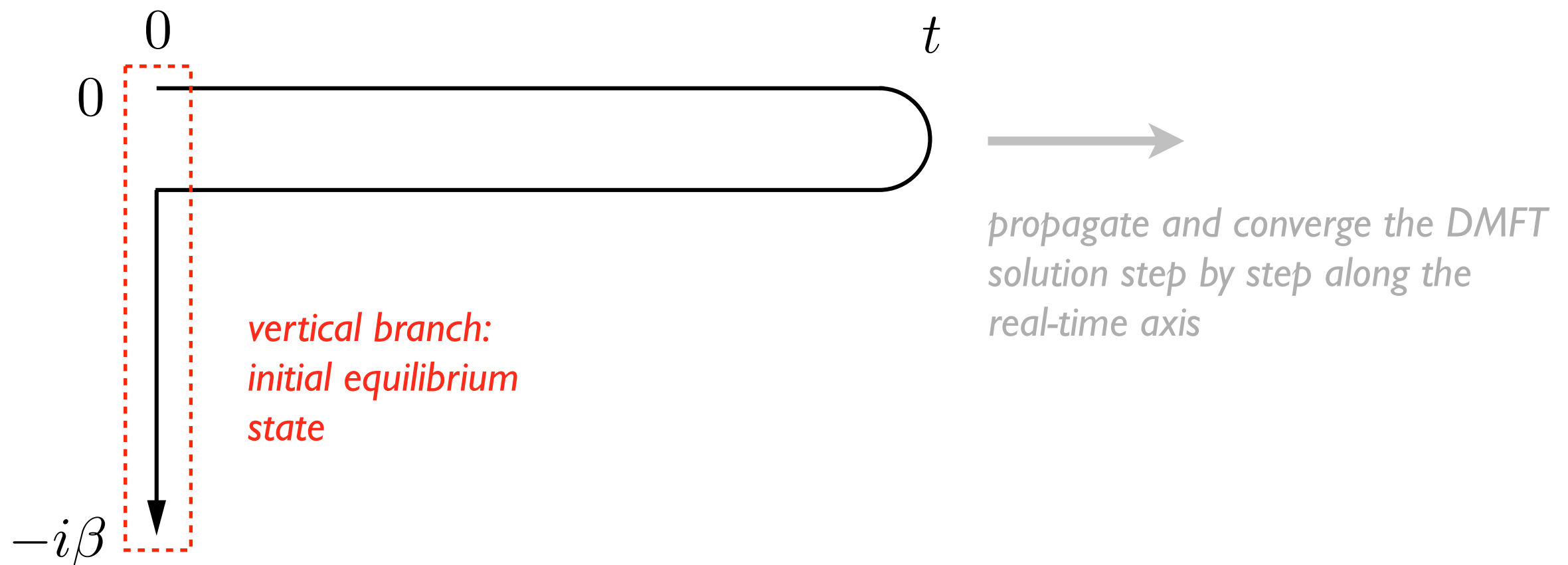


*Pseudogap phase as a momentum-selective Mott state*



# Nonequilibrium DMFT

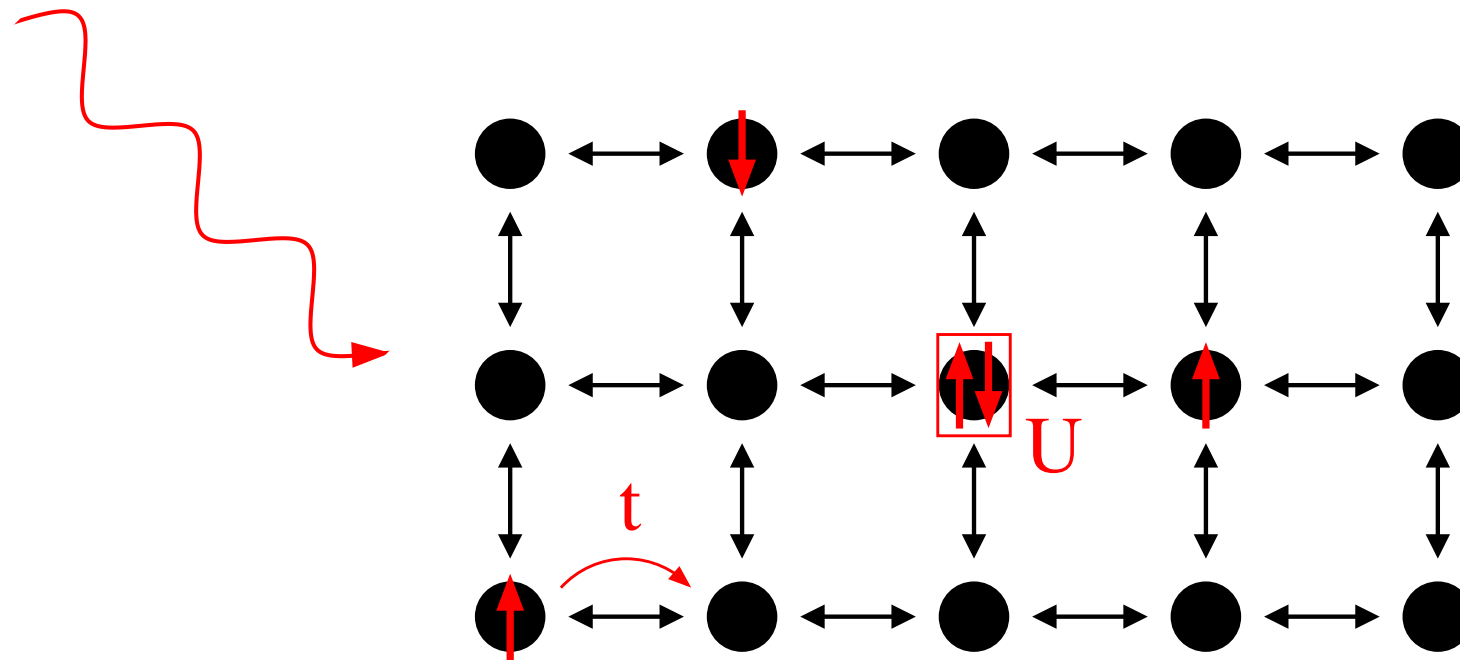
- **DMFT accurately treats time-dependent fluctuations**  
→ can be directly applied to nonequilibrium systems *Freericks et al. (2006)*
- **Equilibrium:** solve DMFT equations on the imaginary-time interval  
*Time-translation invariance: can use Fourier transformation*
- **Nonequilibrium:** solve DMFT equations on the **Kadanoff-Baym contour** *Integral-differential equations of Volterra type*



# Nonequilibrium DMFT

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

*Freericks et al. (2006)*



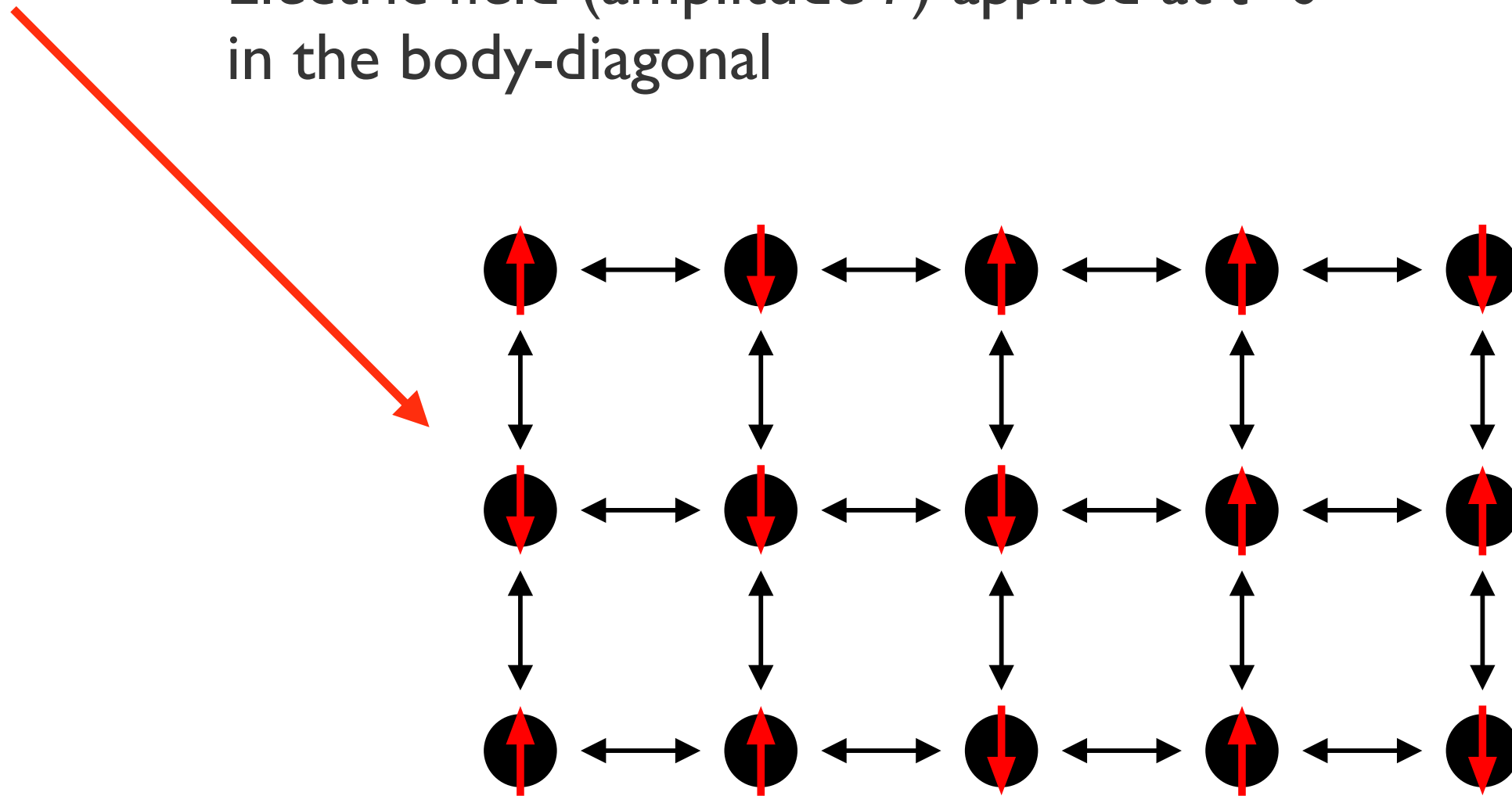
- Peierls substitution:  $\varepsilon(k) \rightarrow \varepsilon(k - eA(t))$
- Lattice: hypercubic, infinite-d limit  $\rho(\varepsilon) = \frac{1}{\sqrt{\pi}W} \exp(-\varepsilon^2/W^2)$

# DC electric fields

- Dielectric breakdown of the Mott insulator

*Eckstein, Oka, & Werner (2011); Eckstein & Werner (2013)*

Electric field (amplitude  $F$ ) applied at  $t=0$   
in the body-diagonal

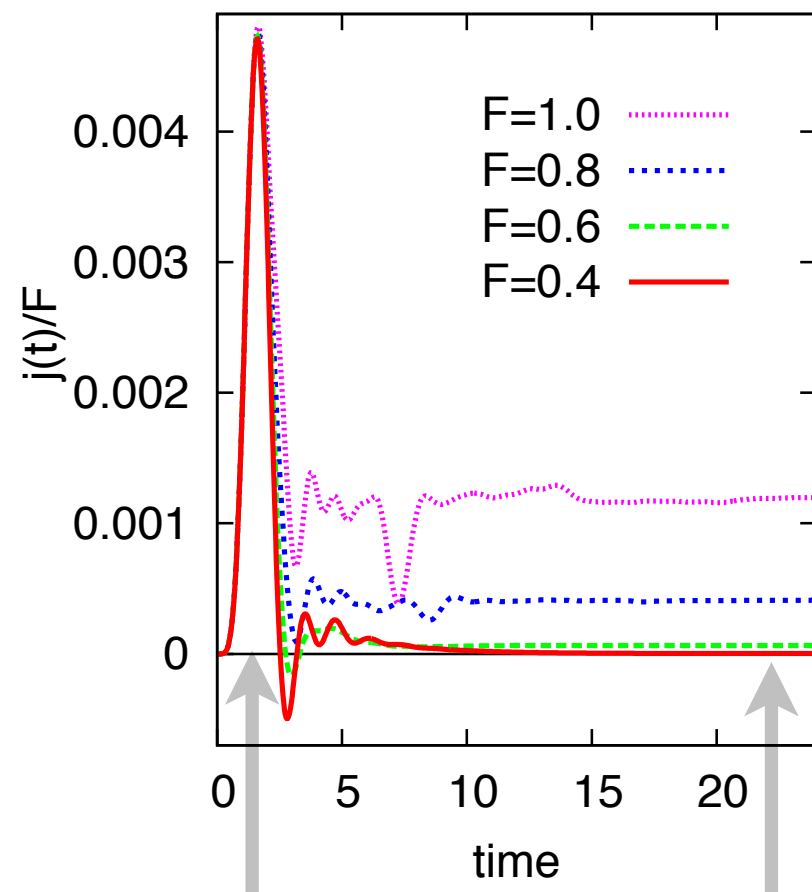


# DC electric fields

- Dielectric breakdown of the Mott insulator

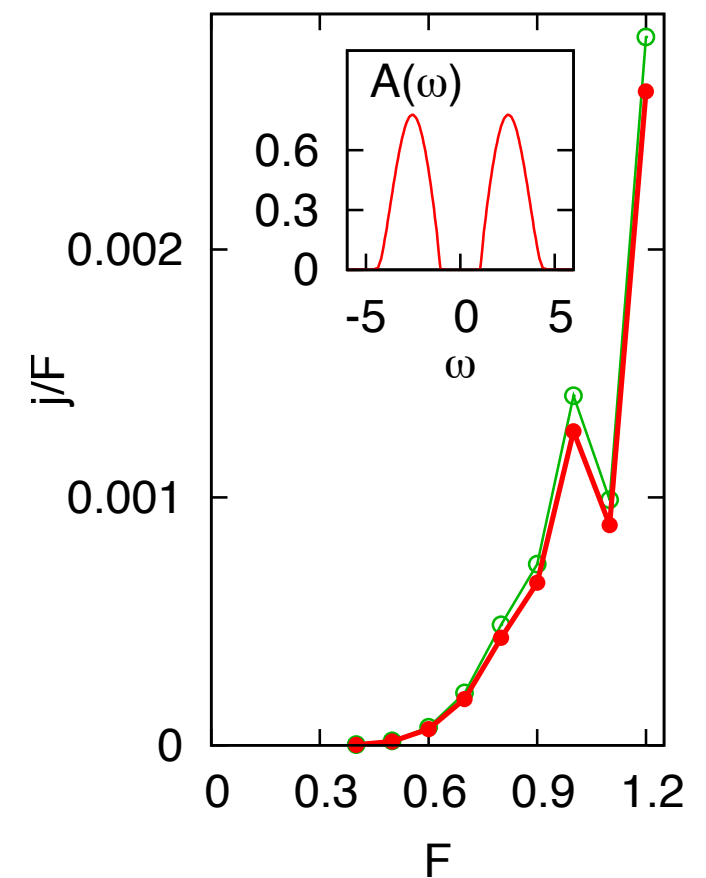
*Eckstein, Oka, & Werner (2011); Eckstein & Werner (2013)*

- Time evolution of the current and double occupancy



*build-up of a polarization*

*quasi-steady state*



*quasi-steady current follows a threshold-law:*

$$j/F \propto \exp(-F_{\text{th}}/F)$$

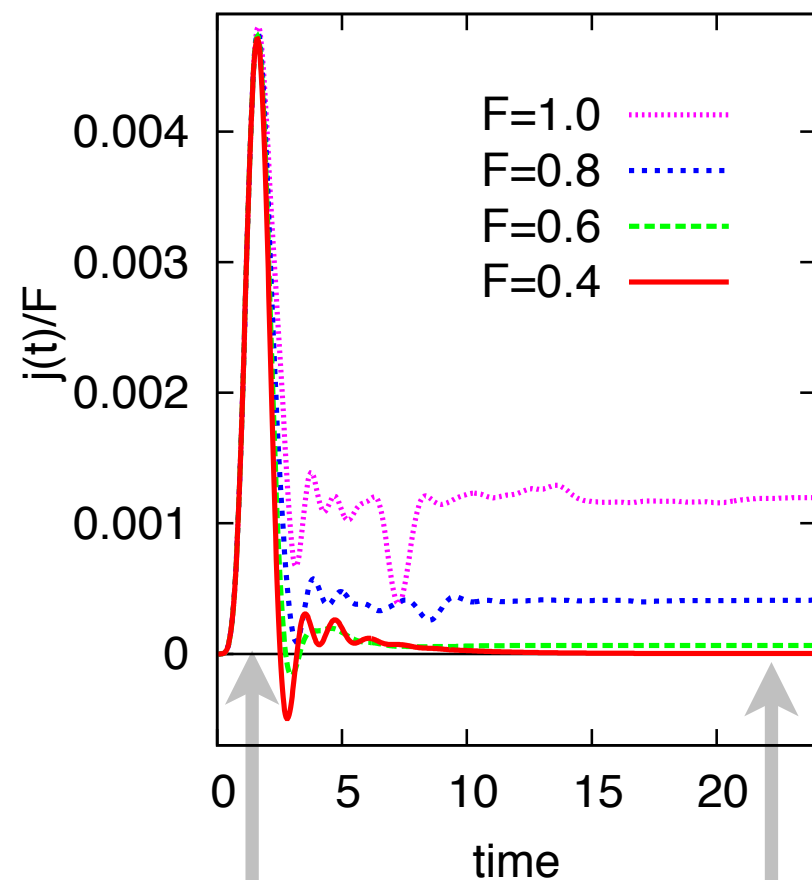
# DC electric fields

- **Dielectric breakdown of the Mott insulator**

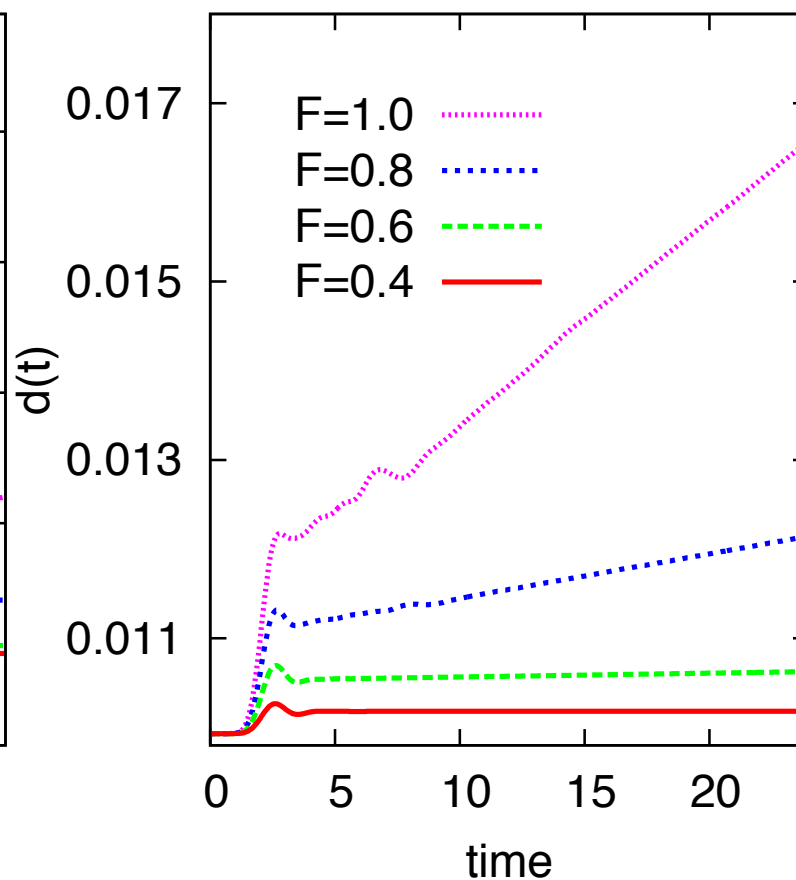
*Eckstein, Oka, & Werner (2011); Eckstein & Werner (2013)*

- Time evolution of the current and double occupancy

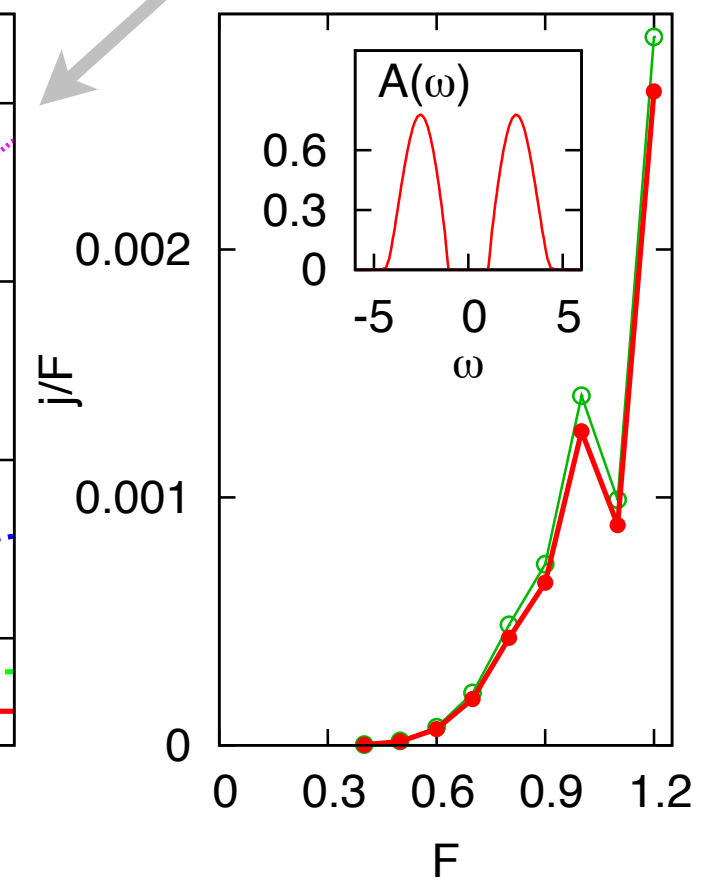
*constant production of  
doublon-hole pairs*



*build-up of a polarization*



*quasi-steady state*



*quasi-steady current follows a threshold-law:*

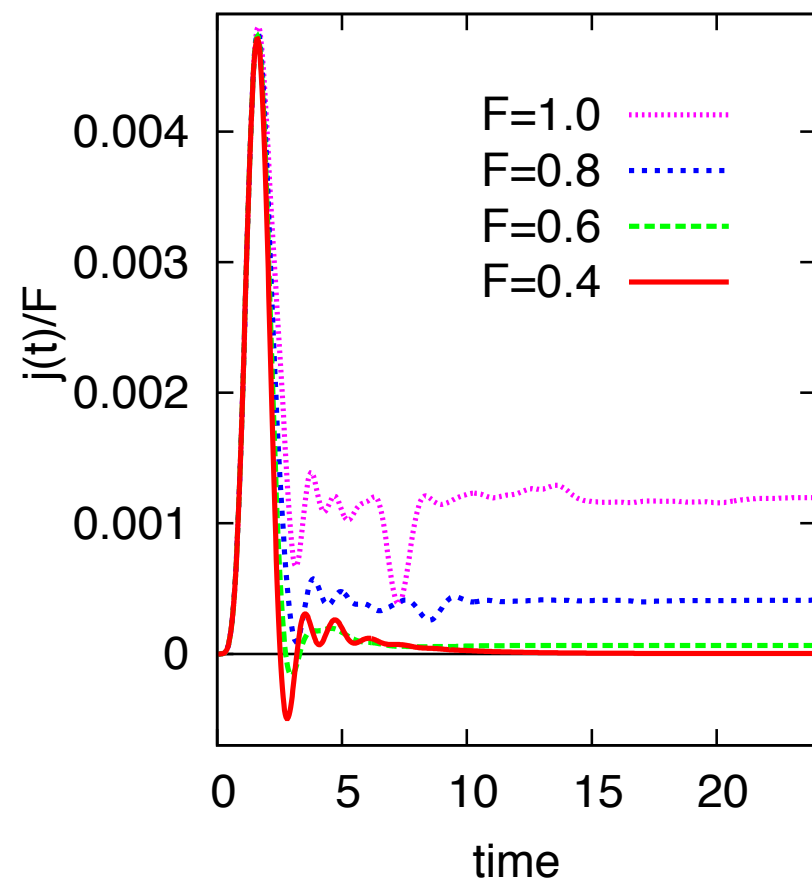
$$j/F \propto \exp(-F_{th}/F)$$

# DC electric fields

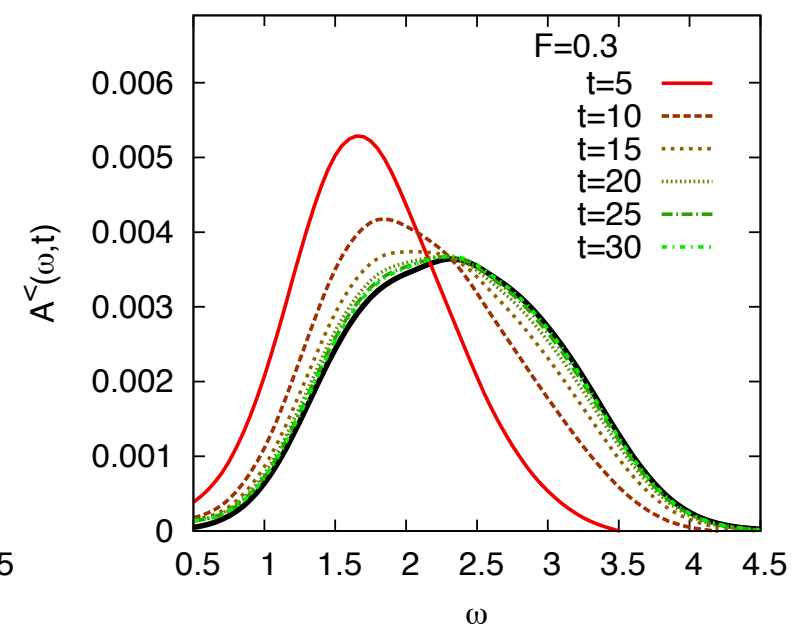
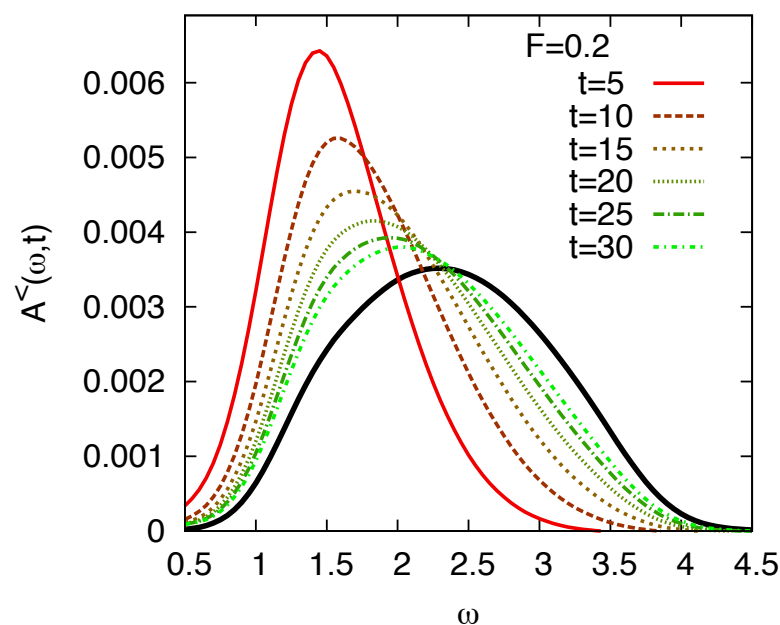
- **Dielectric breakdown of the Mott insulator**

*Eckstein, Oka, & Werner (2011); Eckstein & Werner (2013)*

- Why is there a steady-state current if number of carriers increases?



*time-dependent occupation function compared to a rescaled spectral function (black)*

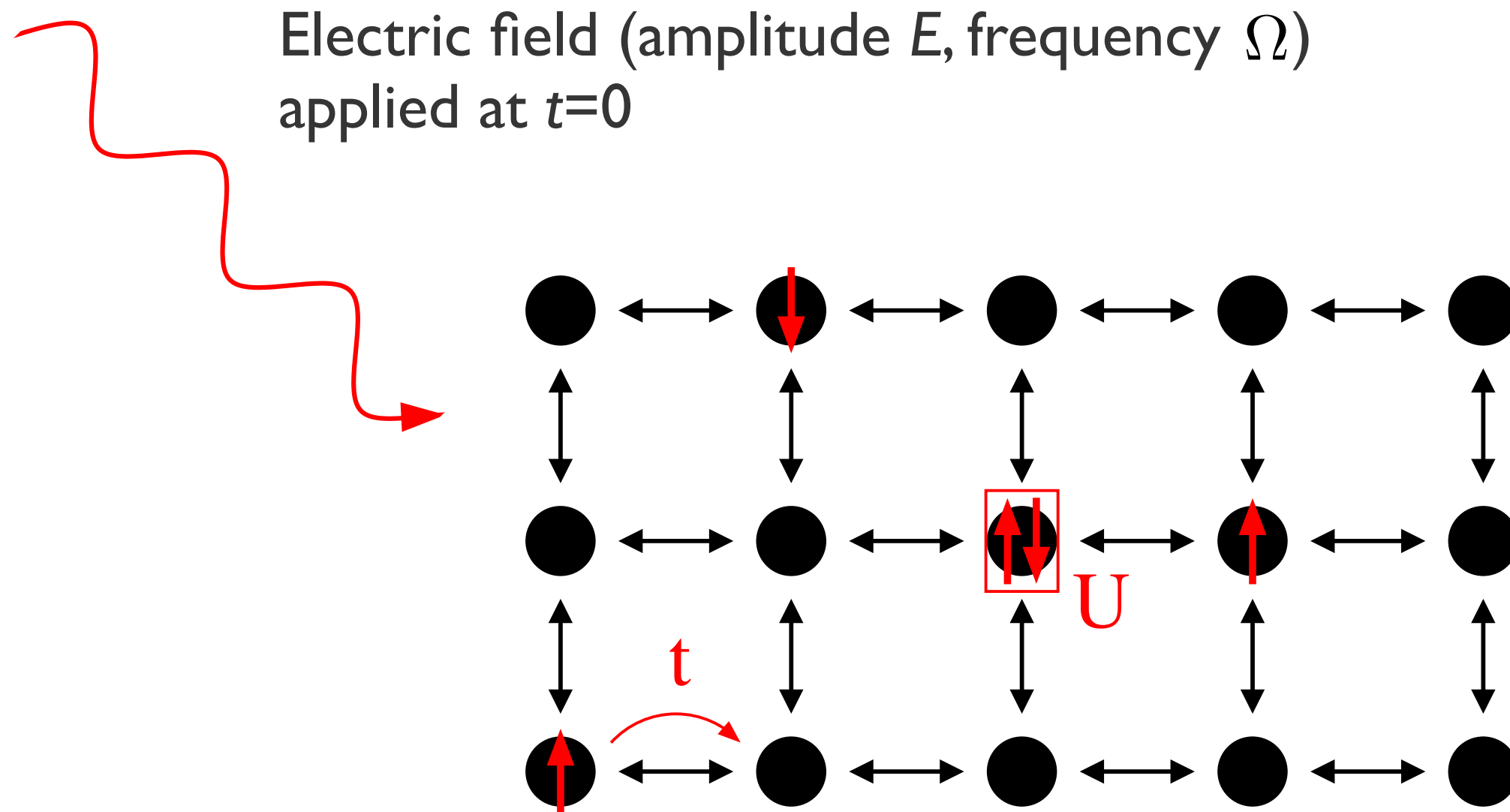


- Doublons (and holes) quickly heat up to infinite temperature!  
→ no contribution to the current

# DC electric fields

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

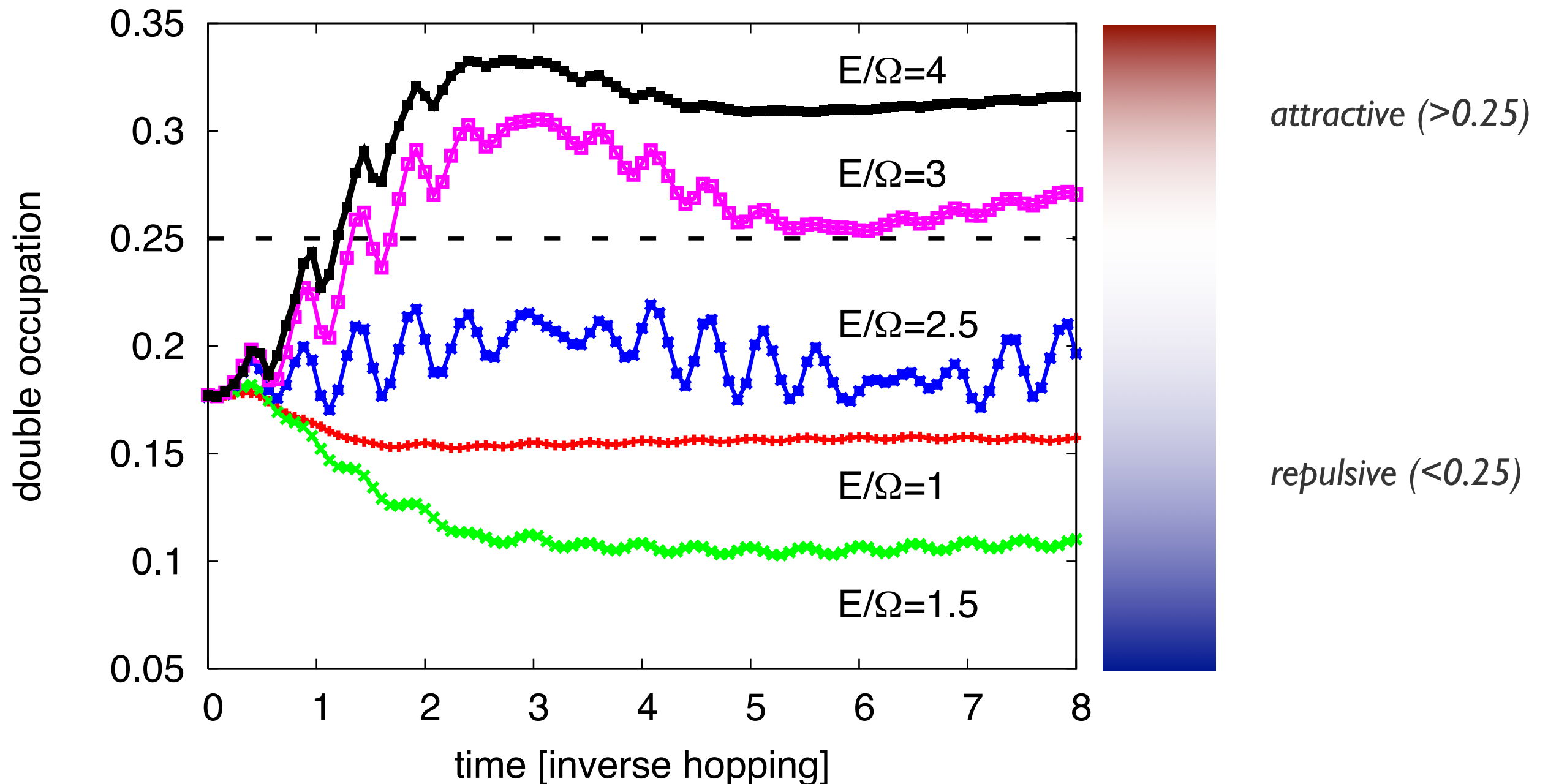
*Tsuji, Oka, Werner and Aoki (2011)*



# Periodic electric fields

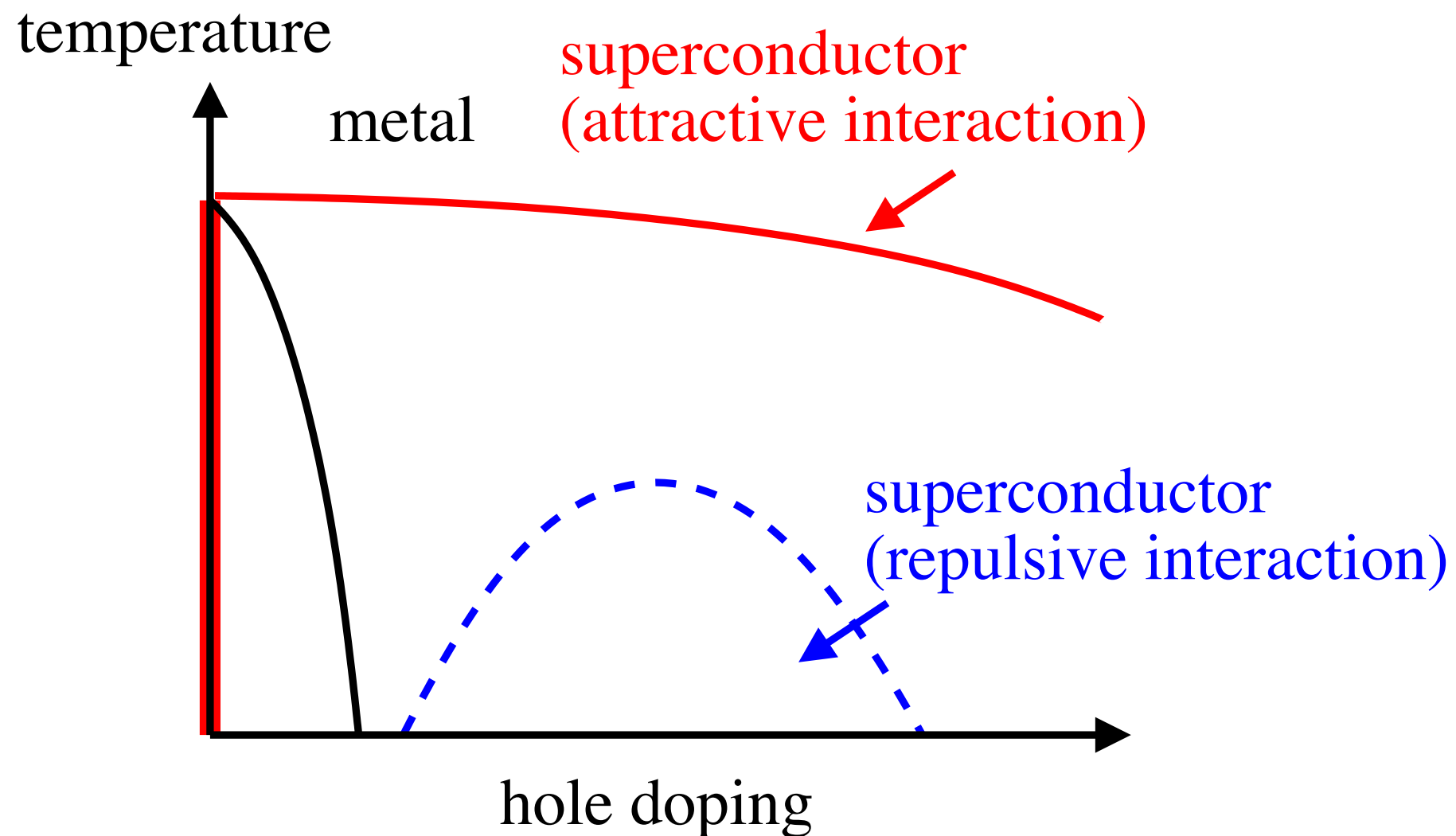
- AC-field quench in the Hubbard model (metal phase)

*Tsuji, Oka, Werner and Aoki (2011)*



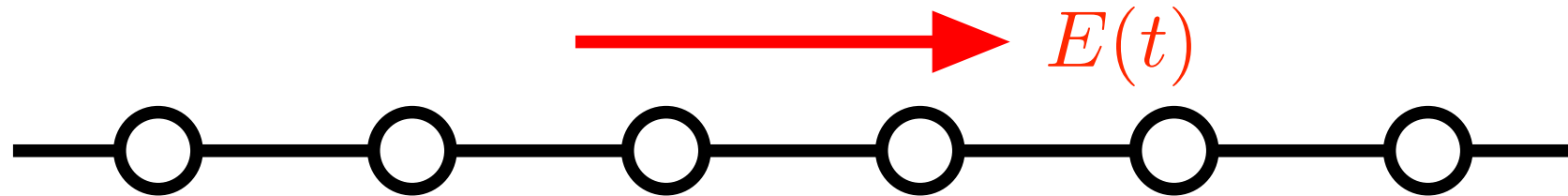
# Periodic electric fields

- AC-field quench in the Hubbard model (metal phase)
  - Sign inversion of the interaction: repulsive  $\leftrightarrow$  attractive
  - *Dynamically generated* high- $T_c$  superconductivity?



# Origin of the attractive interaction

- Periodic E-field leads to a population inversion



- Gauge with pure vector potential

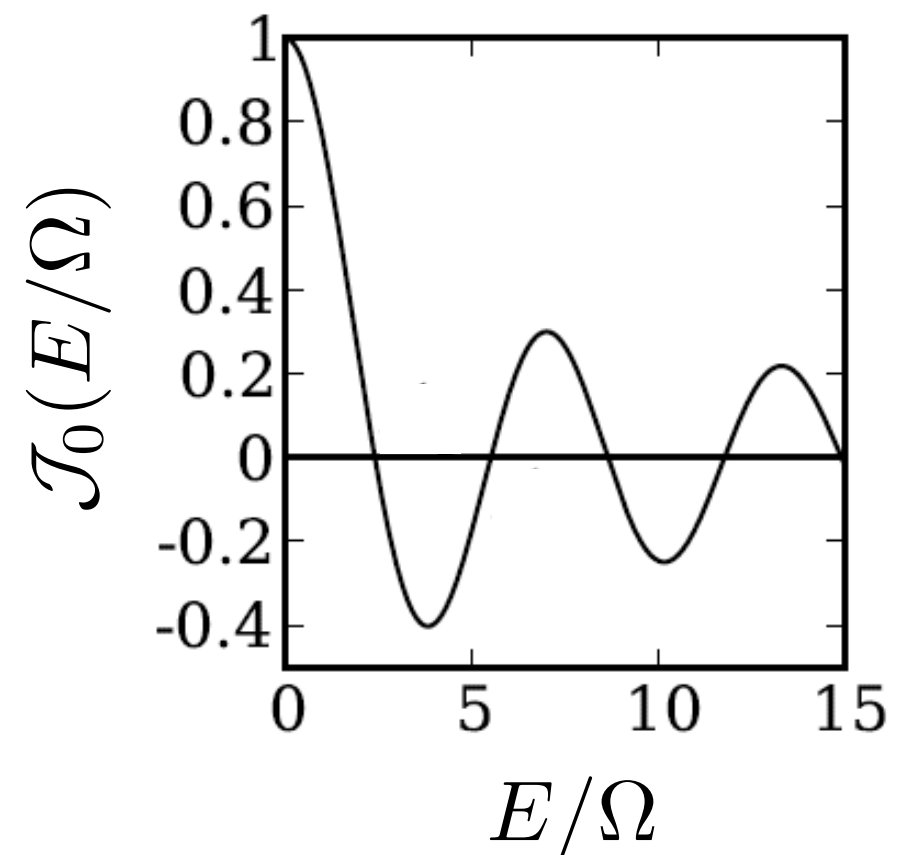
$$E(t) = E \cos(\Omega t) = -\partial_t A(t)$$

$$\Rightarrow A(t) = -\left(E/\Omega\right) \sin(\Omega t)$$

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

- Renormalized dispersion

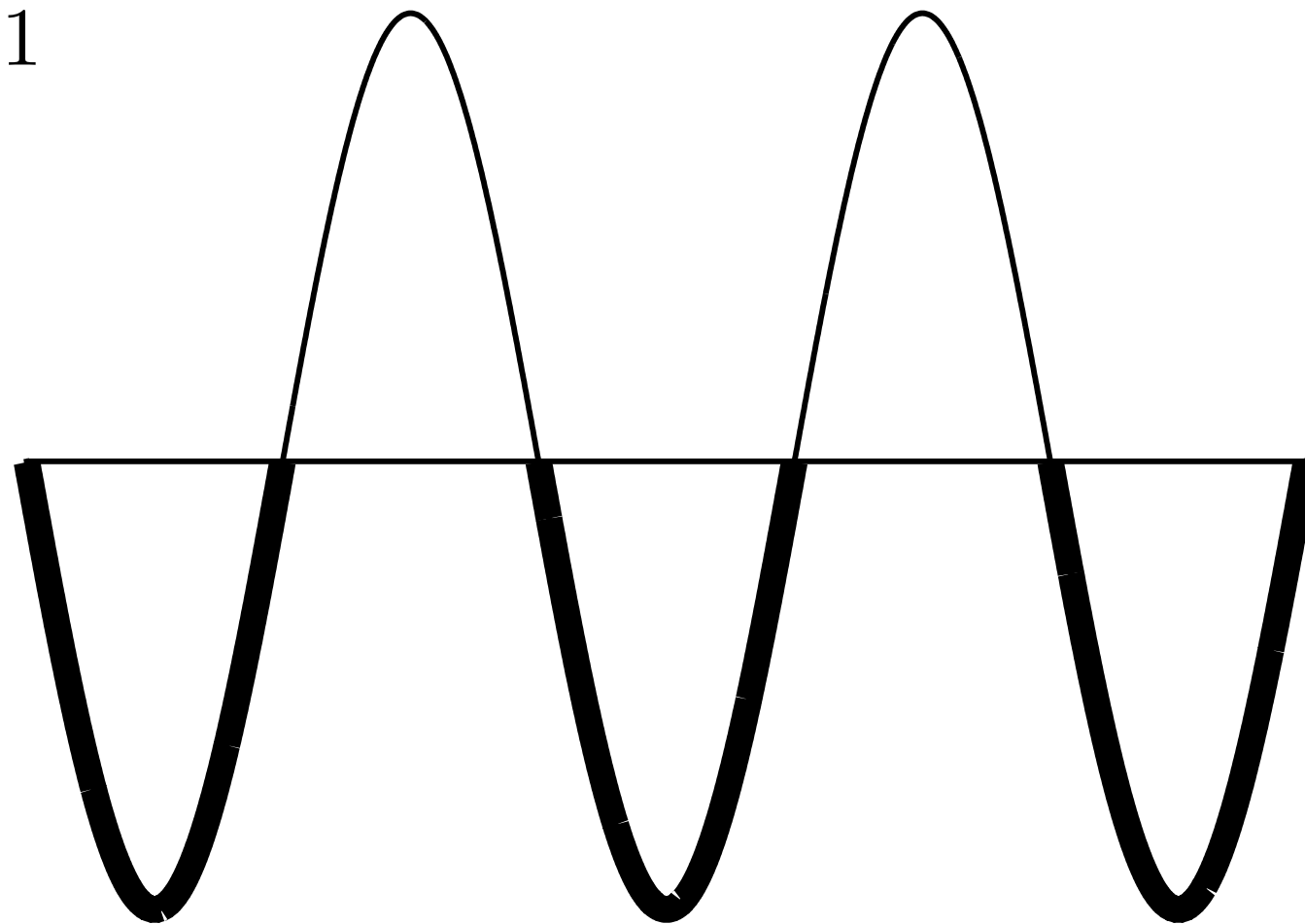
$$\overline{\epsilon}_k = \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} dt \epsilon_{k-A(t)} = \mathcal{J}_0(E/\Omega) \epsilon_k$$



# Origin of the attractive interaction

- Periodic E-field leads to a population inversion

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



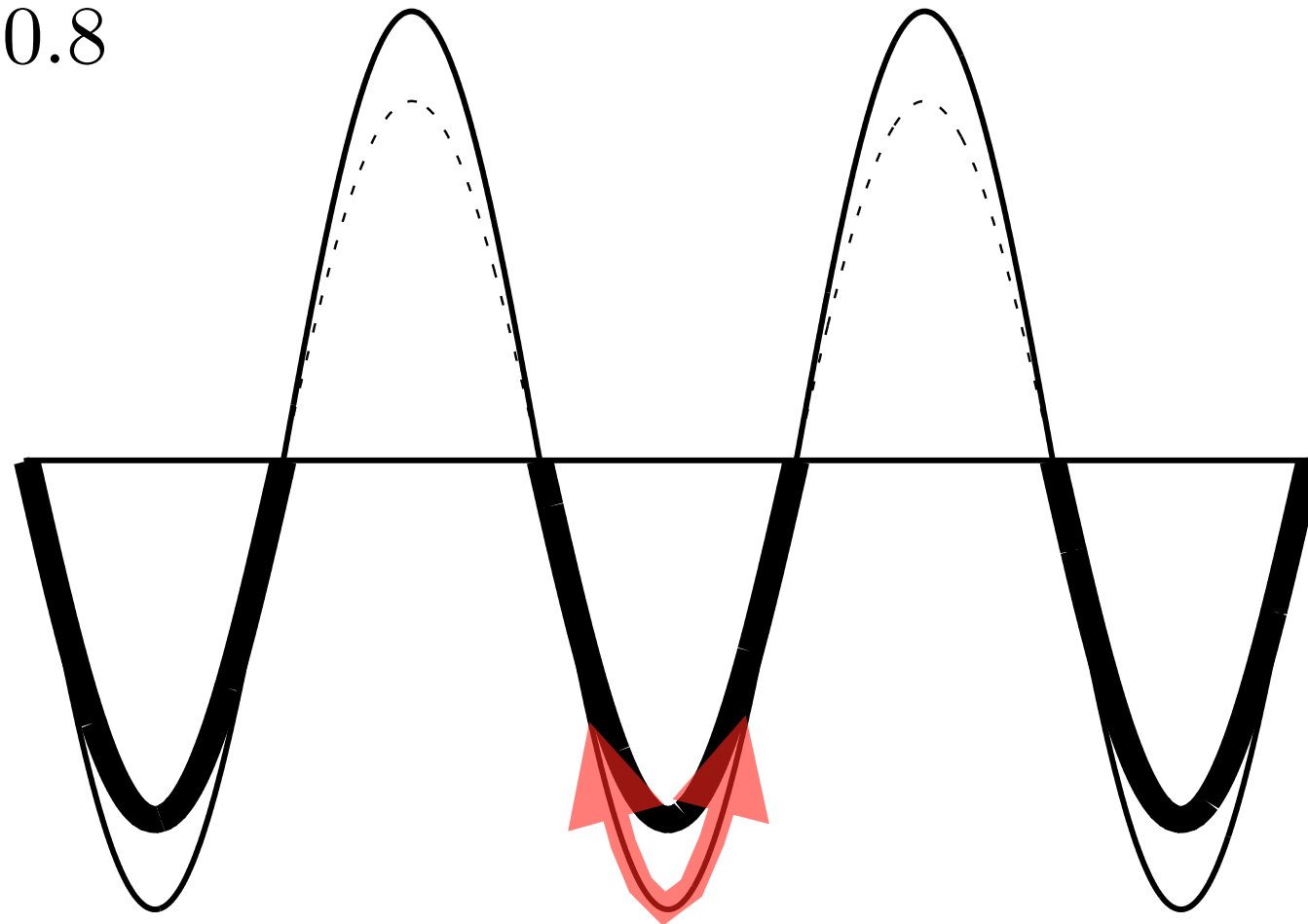
- Renormalized dispersion

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

# Origin of the attractive interaction

- Periodic E-field leads to a population inversion

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



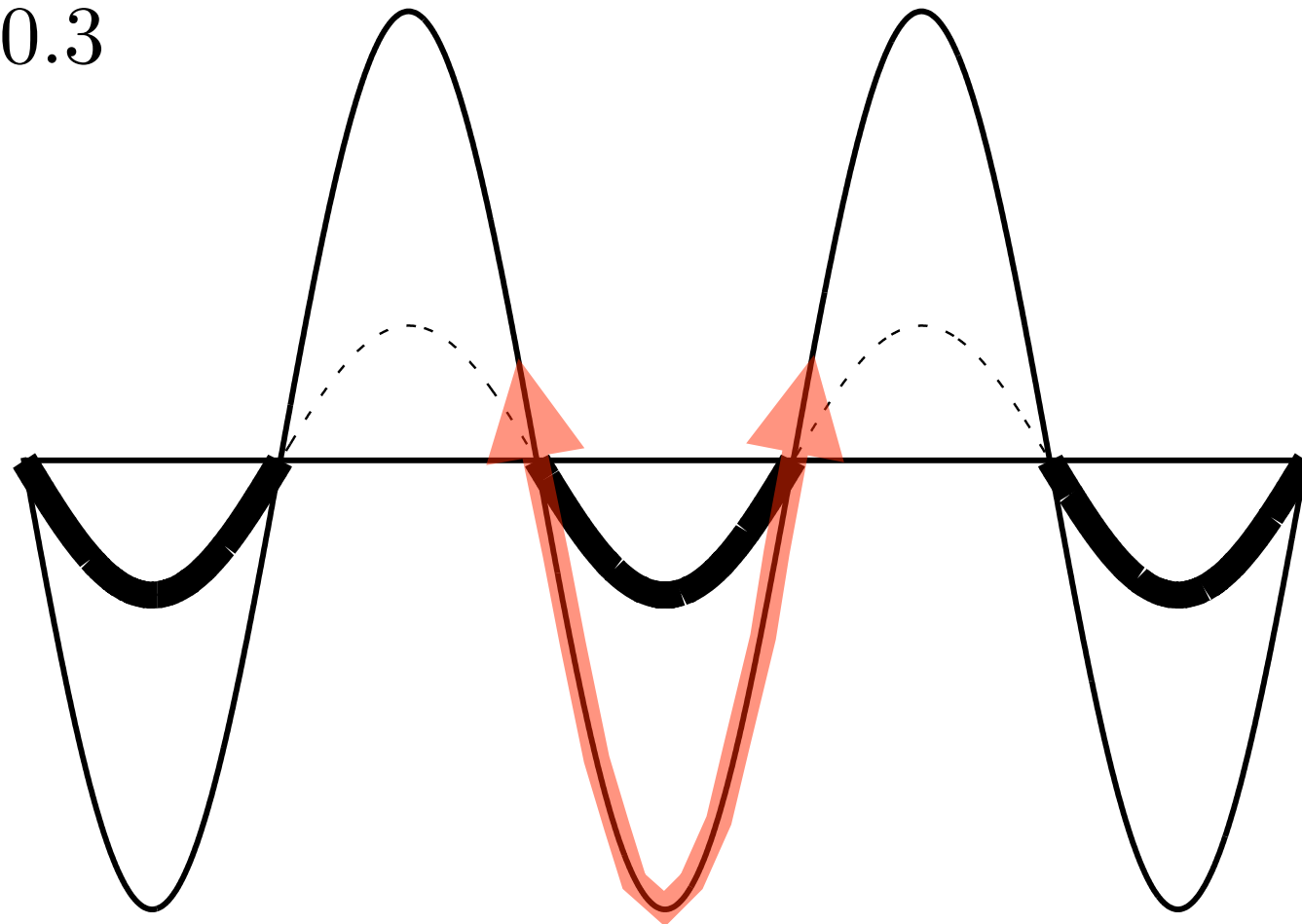
- Renormalized dispersion

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

# Origin of the attractive interaction

- Periodic E-field leads to a population inversion

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



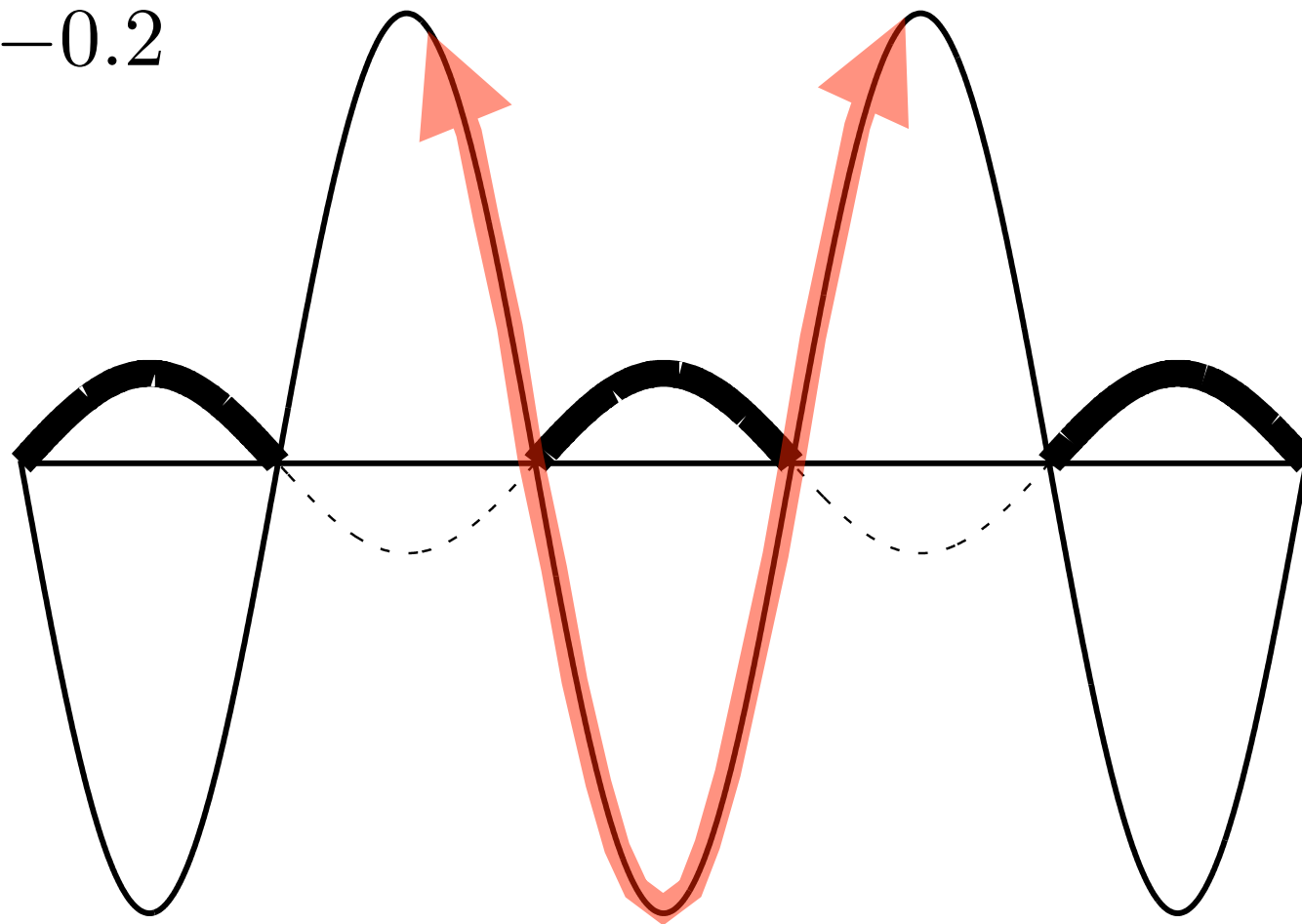
- Renormalized dispersion

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

# 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  $U < 0, T > 0$

$$\begin{aligned} \tilde{T} < 0, \mathcal{J}_0 < 0 \quad \rho &\propto \exp \left( -\frac{1}{\tilde{T}} \left[ \sum_{k\sigma} \mathcal{J}_0 \epsilon_k n_{k\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \right] \right) \\ T_{\text{eff}} = \frac{\tilde{T}}{\mathcal{J}_0} > 0 \quad &= \exp \left( -\frac{1}{T_{\text{eff}}} \left[ \sum_{k\sigma} \epsilon_k n_{k\sigma} + \frac{U}{\mathcal{J}_0} \sum_i n_{i\uparrow} n_{i\downarrow} \right] \right) \end{aligned}$$

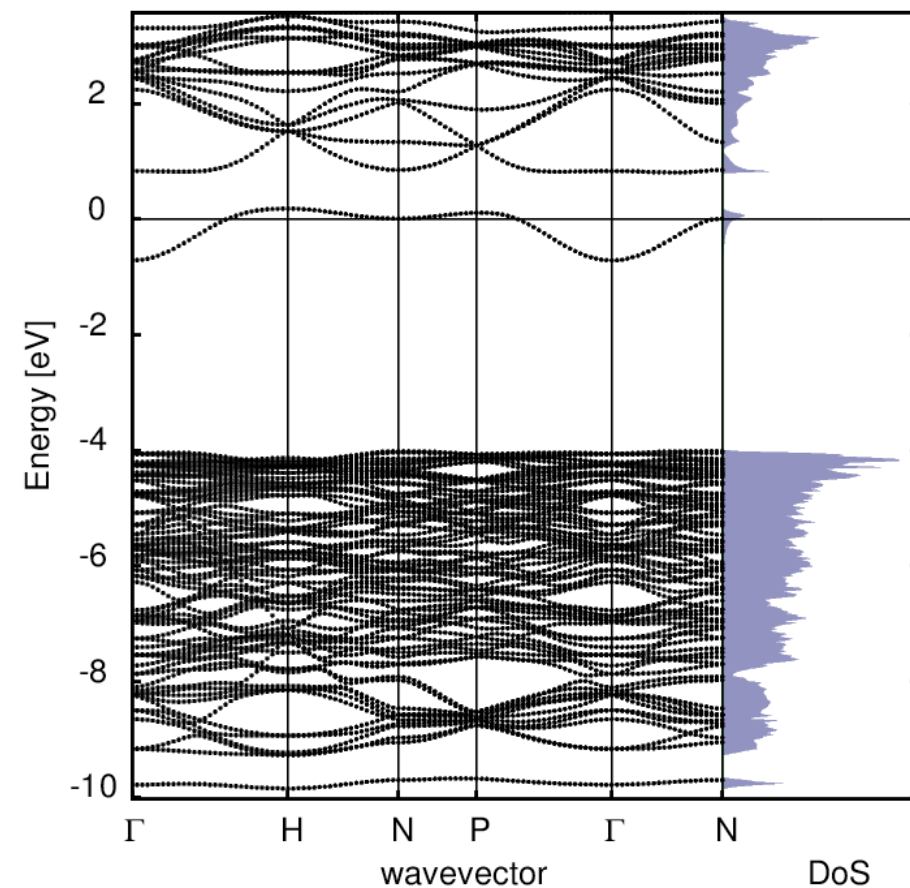
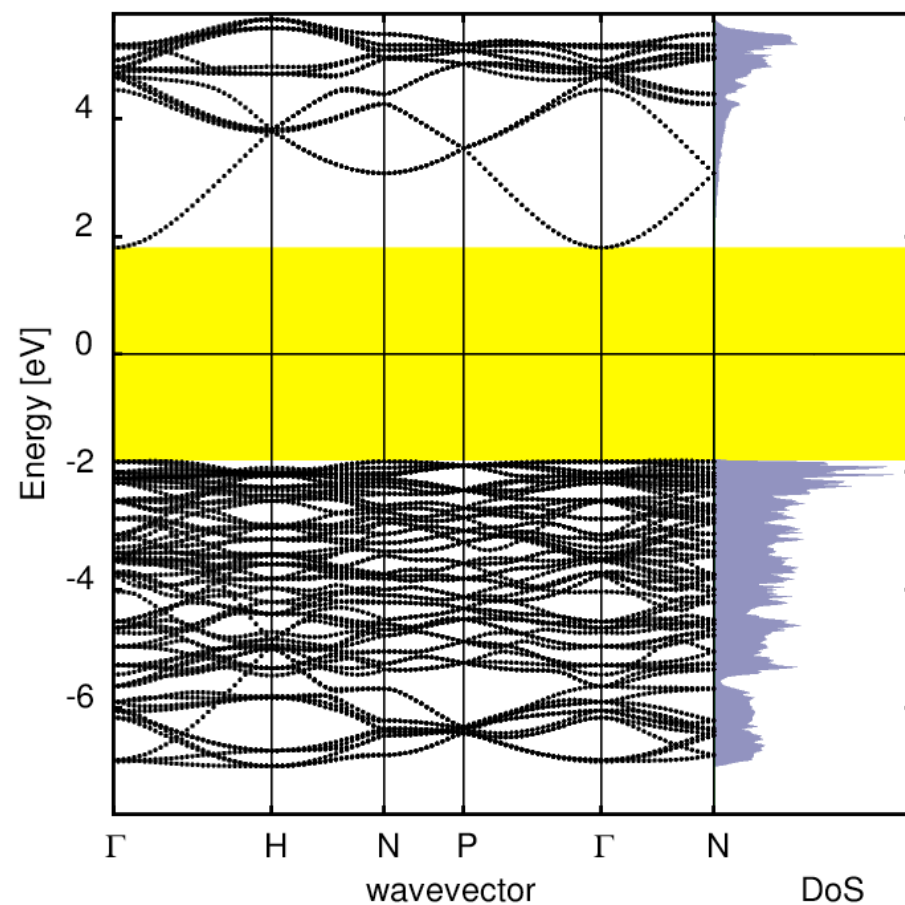
- Effective interaction of the  $T_{\text{eff}} > 0$  state

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

# Experimental realization?

- Potentially interesting material: Sn doped  $\text{In}_2\text{O}_3$ 
  - Transparent conductor
  - Single s-band crossing the Fermi level

*band structure by Bernard Delley (PSI)*



# Summary

- *Overview of DMFT.*
  - *Basic idea: neglect spatial fluctuations, keep dynamical fluctuations*
  - *Map  $(d+1)$  dimensional lattice to a  $(0+1)$  dimensional impurity model*
- *Phasediagram of the Hubbard model.*
  - *Importance of short-range spatial correlations in  $d=2$*
  - *Relationship to cuprate physics*
- *Extension to nonequilibrium problems.*
  - *Dielectric breakdown of a Mott insulator in strong DC fields*
  - *Dynamical band-flipping and interaction conversion by AC fields*