Nonthermal superconductivity

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University of Fribourg

Les Diablerets, February 2023

European
Research
Council

FNSNF

Nonthermal superconductivity

in collaboration with:

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Gil Refael (Caltech)
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Yuta Murakami (RIKEN)

Les Diablerets, February 2023

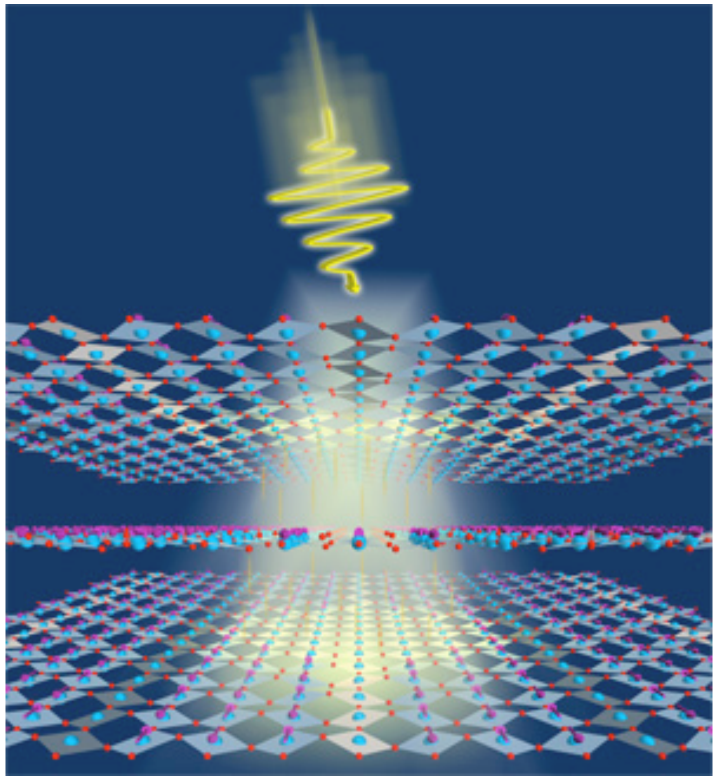
Motivation

“Tuning” of material properties by external driving

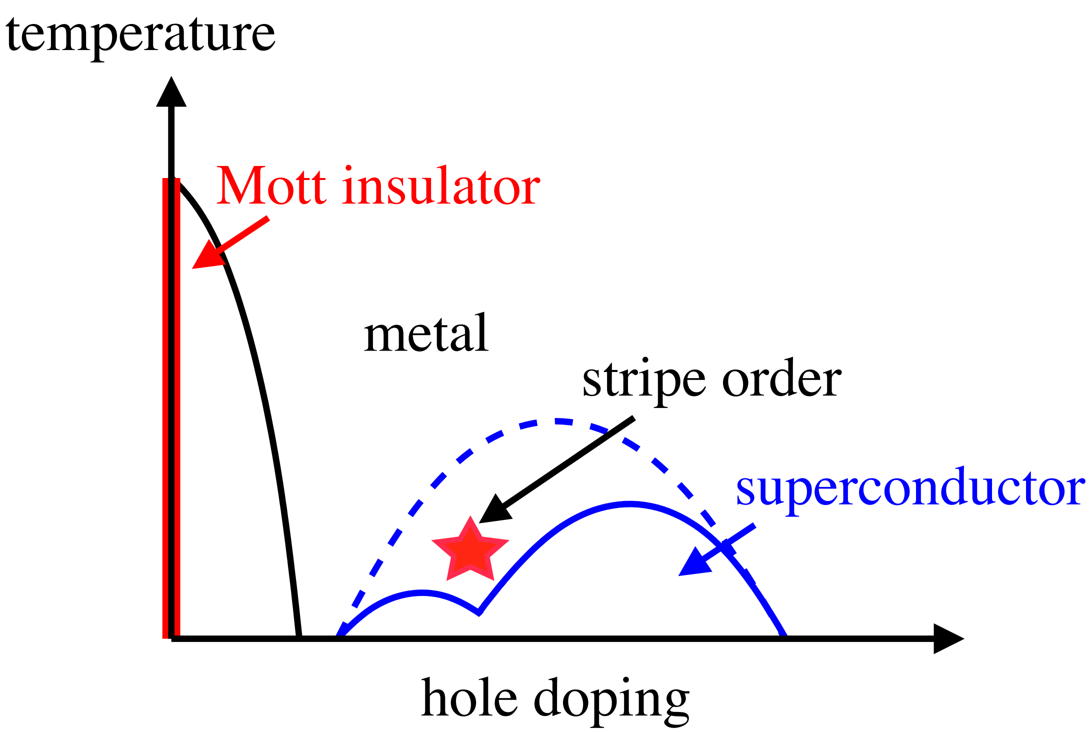
- Enhancement and control of electronic orders

  e. g. *light-induced high-temperature superconductivity (?)*

  cuprates: Fausti et al., Science (2011), Kaiser et al., PRB (2014)



phonons excited by THz pulse



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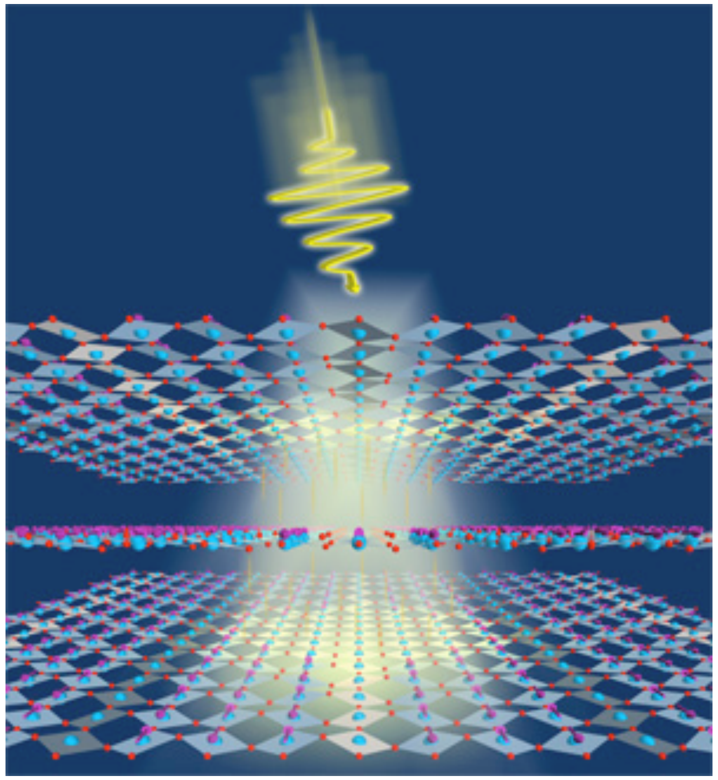

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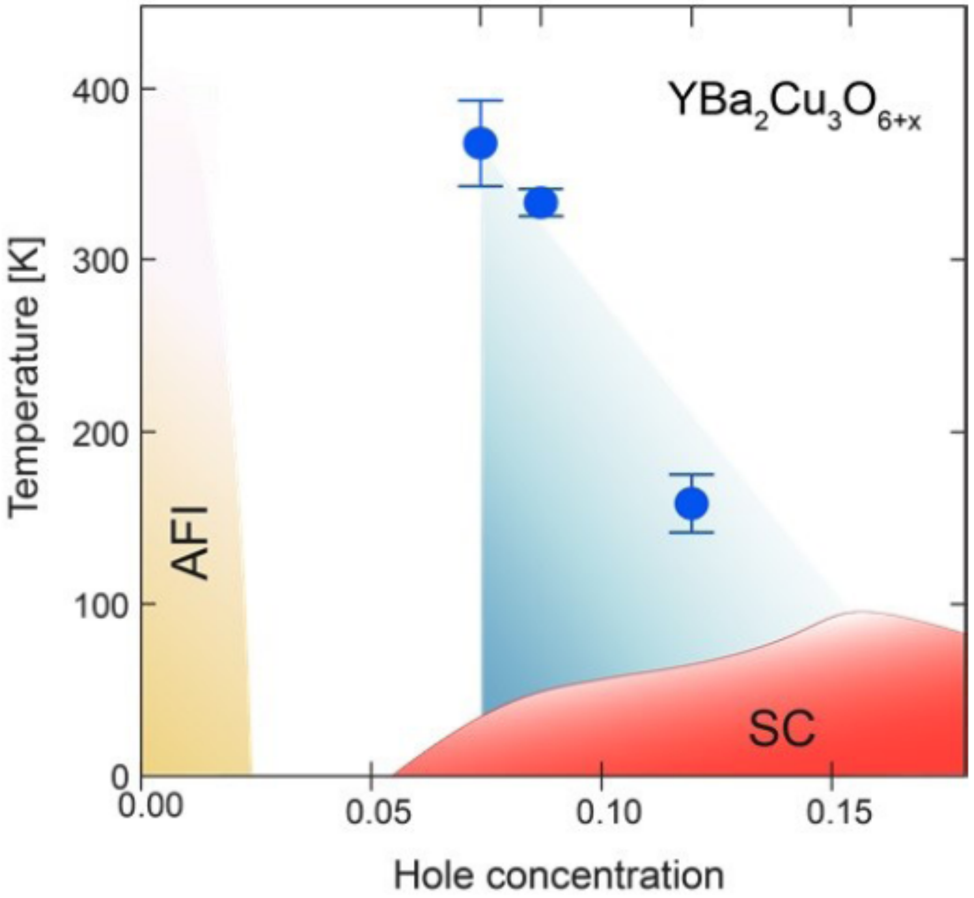


Motivation

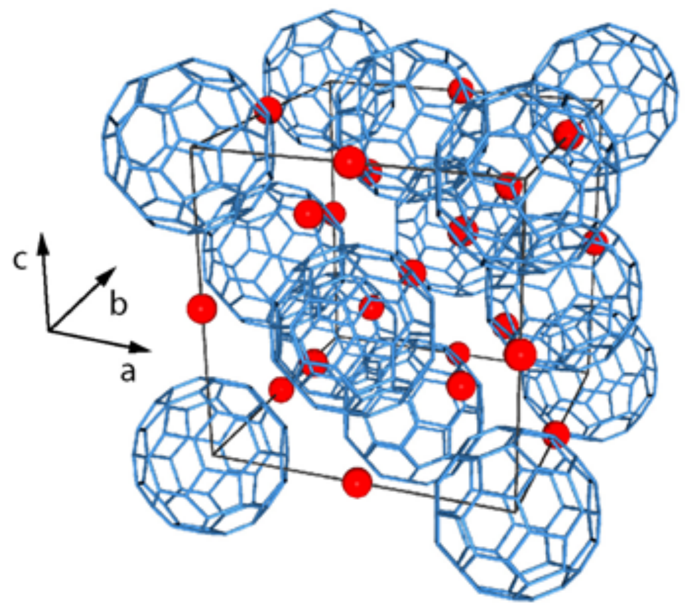
“Tuning” of material properties by external driving

- Enhancement and control of electronic orders

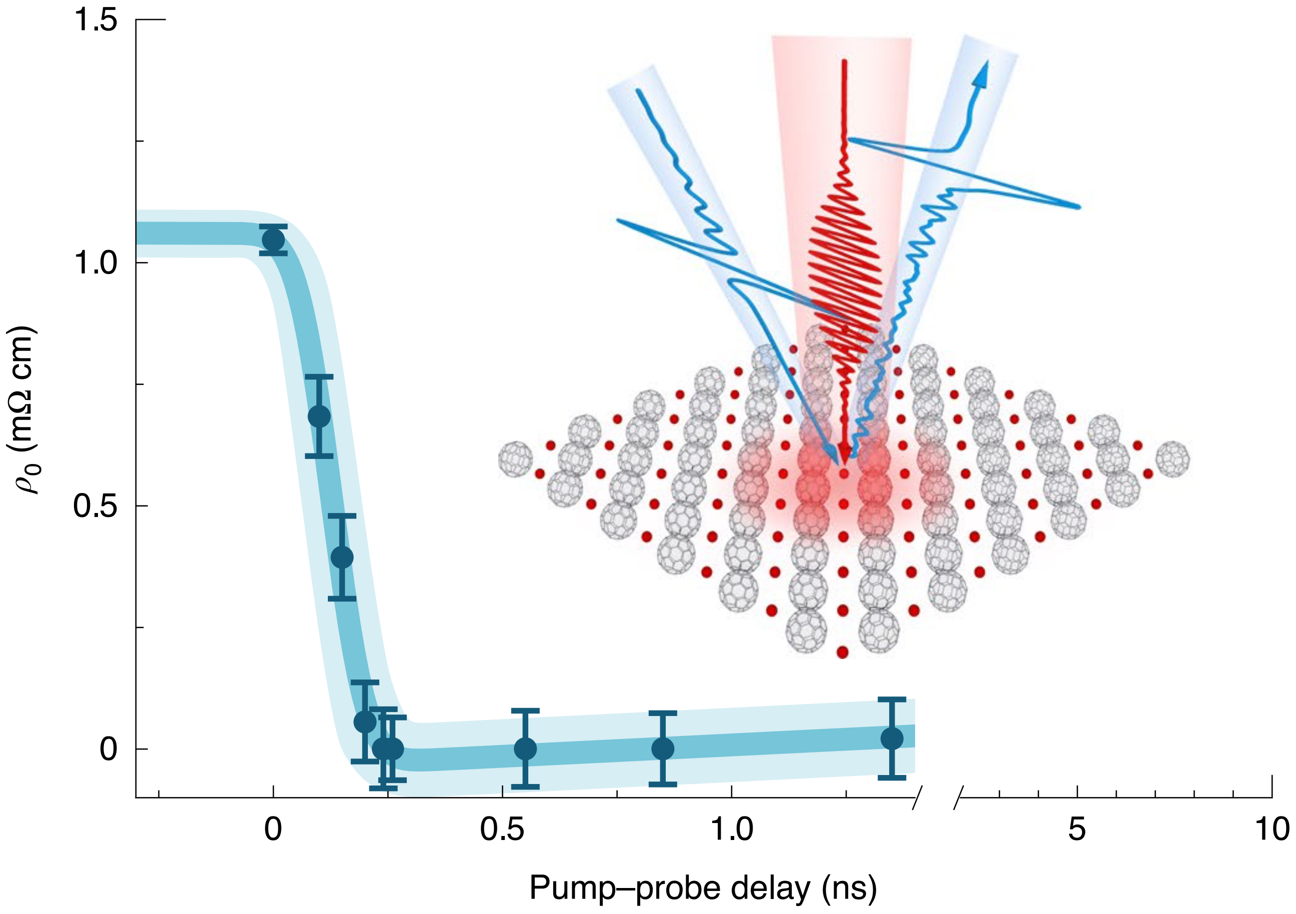
  e. g. *light-induced high-temperature superconductivity (?)*

fullerides: Budden et al., Nature Phys. (2021)

stronger pump pulse (300fs - 300 ps)



K_3C_{60}



Goal

- Explore nonthermal superconductivity in Hubbard models

1) Entropy cooling mechanism for producing "cold" photo-doped states

2) eta-pairing in photo-doped Mott insulators on bipartite lattices

3) Chiral superconductivity in photo-doped Mott insulators on frustrated lattices

5) Effective equilibrium approach for photo-doped Mott systems

6) Spin, charge and eta-spin separation in photo-doped 1D systems

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numerical results based on dynamical mean field theory (DMFT)

5) Effective equilibrium approach for photo-doped Mott systems

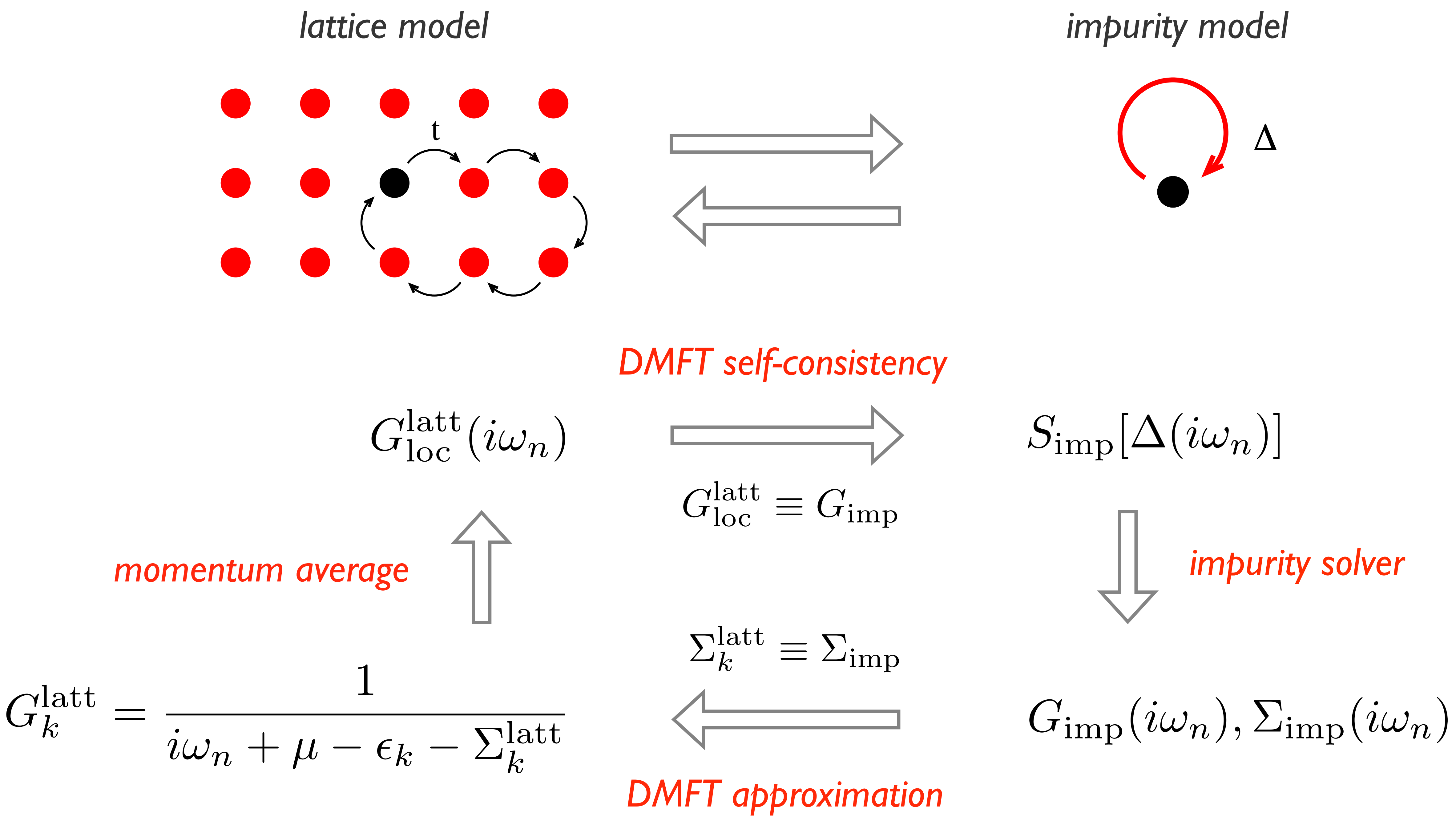
6) Spin, charge and eta-spin separation in photo-doped 1D systems

numerical results based on iterated time-evolving block decimation (iTEBD)

Method

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

  Georges & Kotliar, PRB (1992)



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

DMFT self-consistency

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

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

impurity solver

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

$$\Sigma^{\text{latt}}_k \equiv \Sigma_{\text{imp}}$$

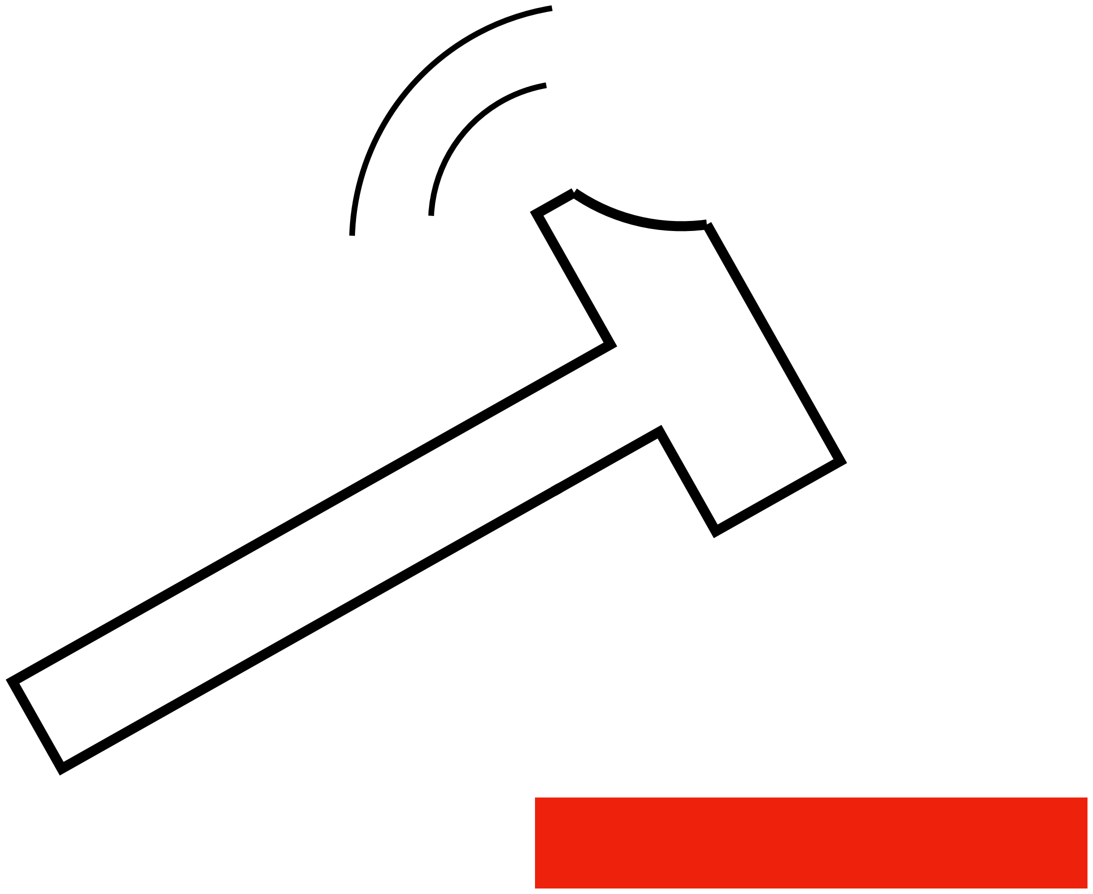
DMFT approximation

$$G^{\text{latt}}_k = \frac{1}{i\omega_n + \mu - \epsilon_k - \Sigma^{\text{latt}}_k}$$

momentum average

Conceptual question

Appearance of “fragile” electronic orders in highly nonequilibrium states



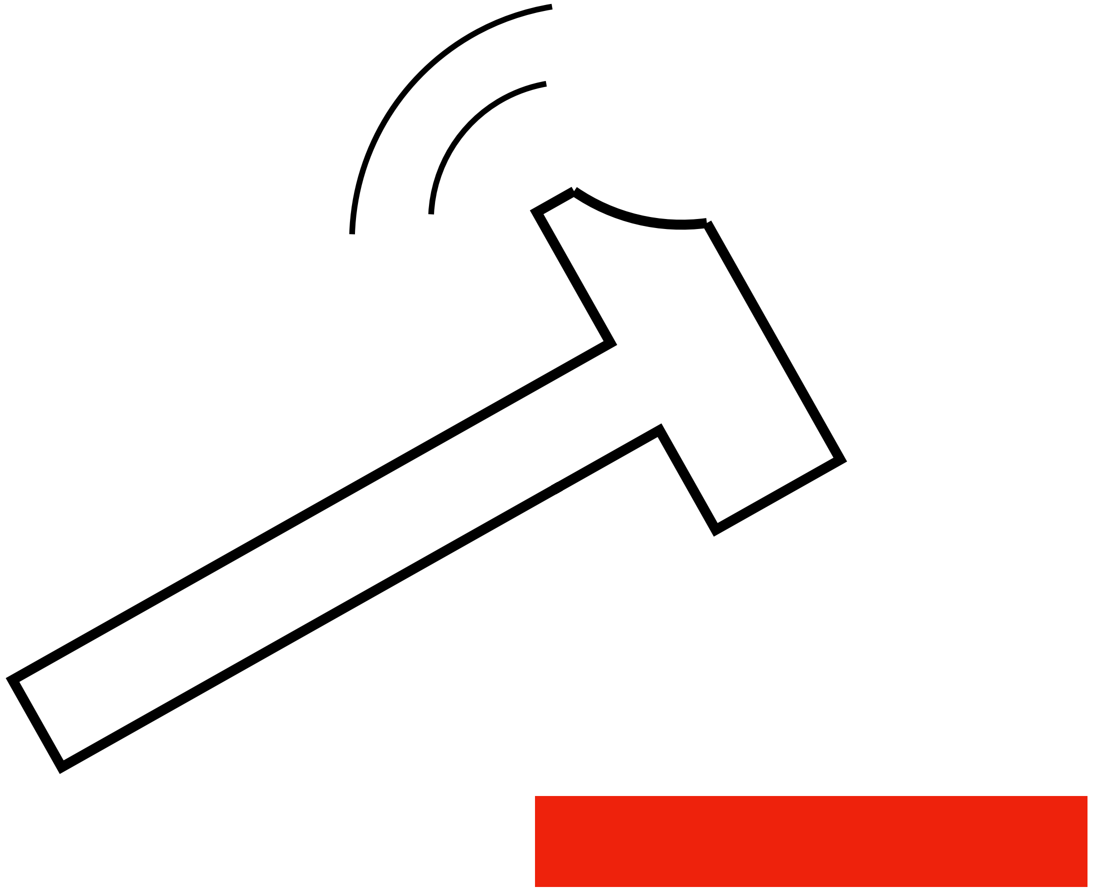
correlated electron system

Conceptual question

Appearance of "fragile" electronic orders in highly nonequilibrium states

- Need to find ways to avoid heating

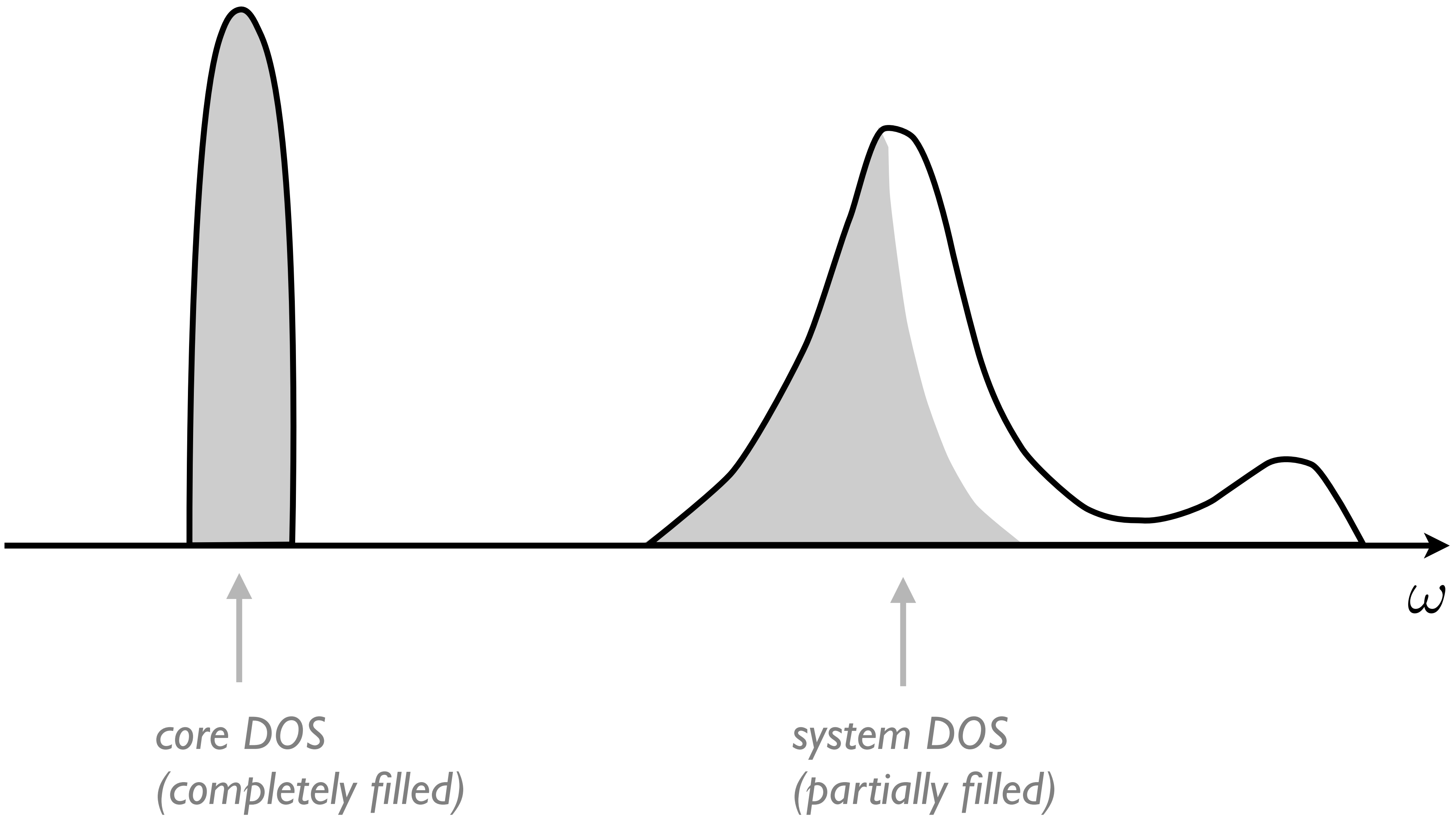
→ entropy cooling



correlated electron system

Entropy cooling ("evaporative cooling")

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



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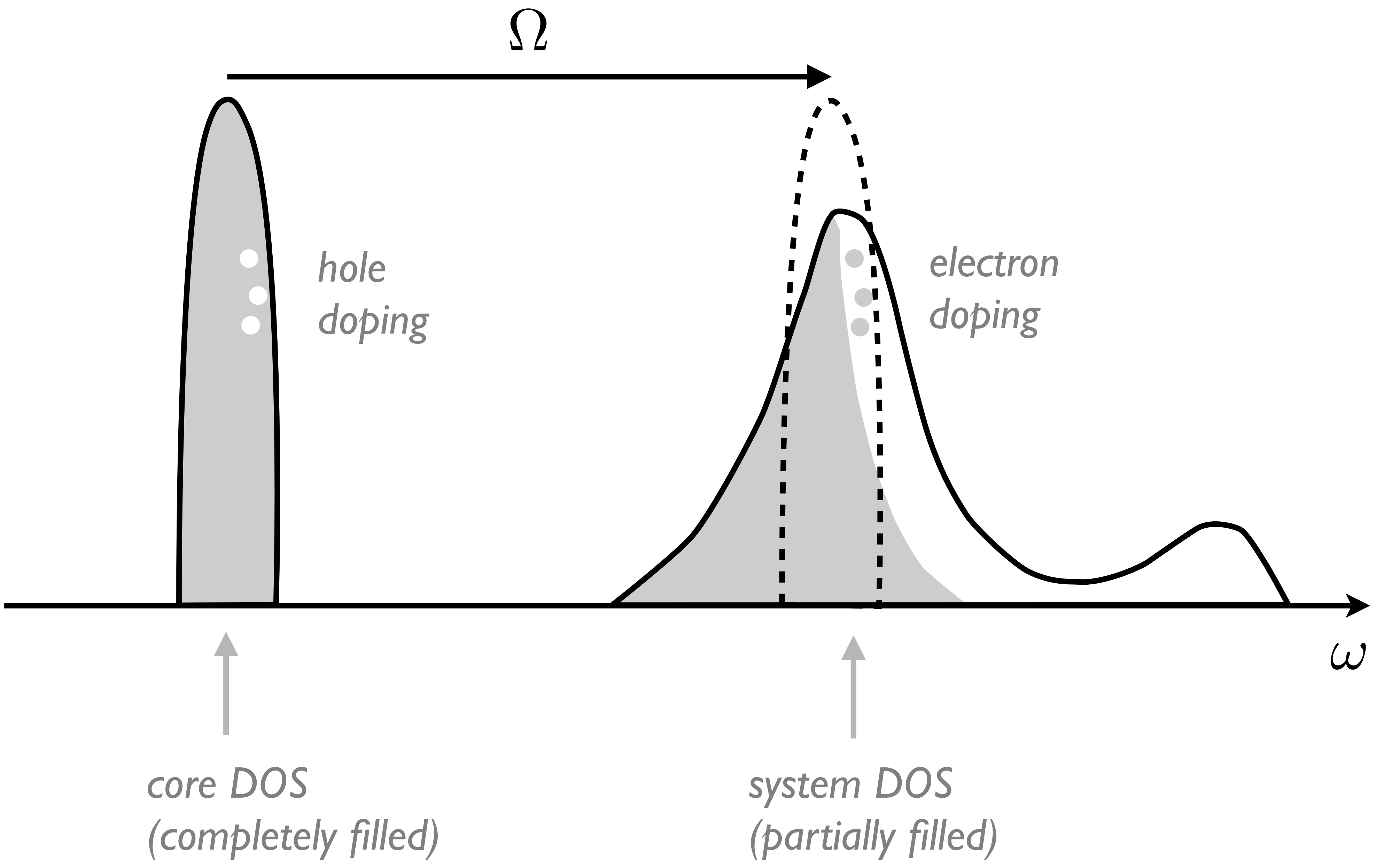

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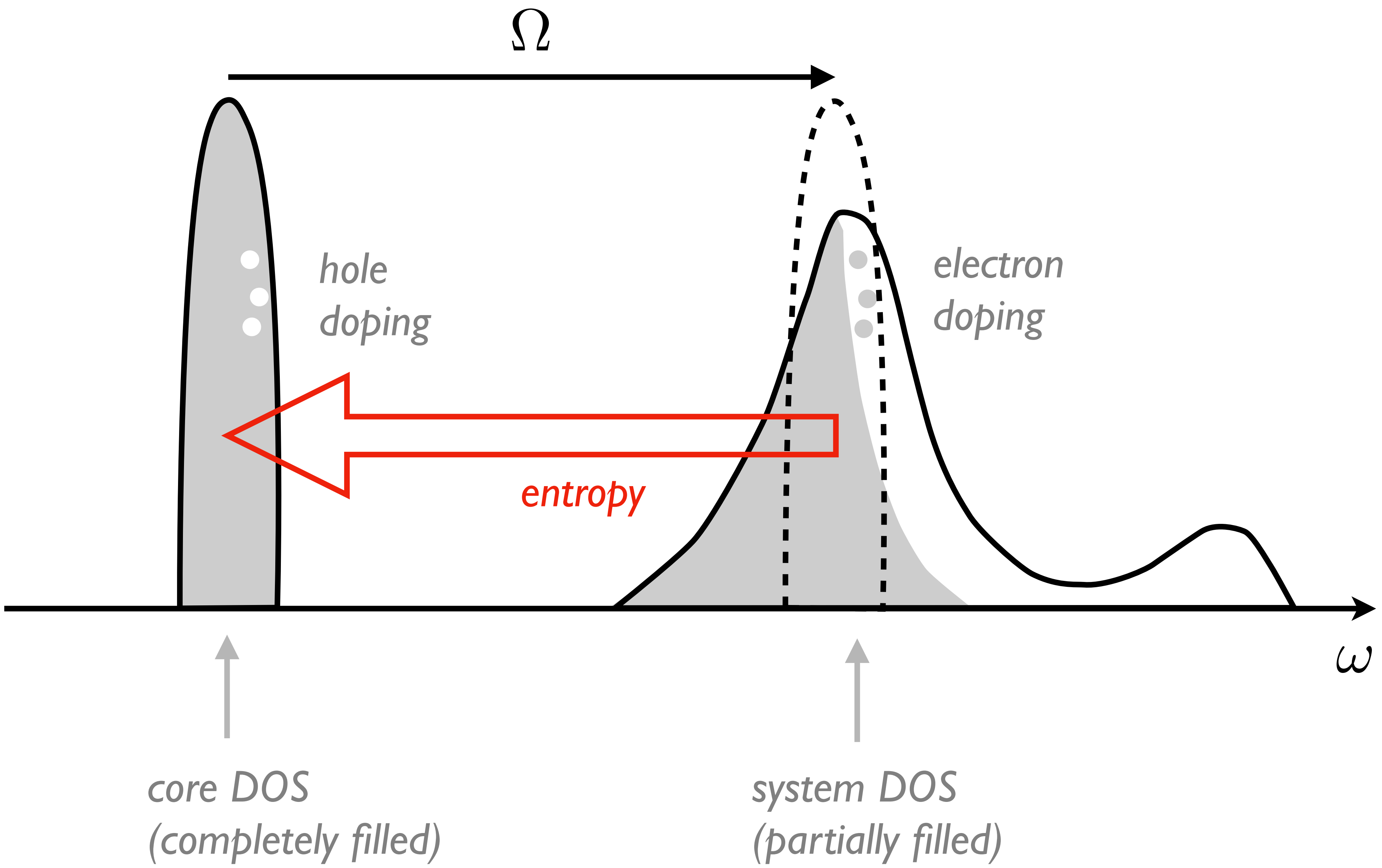
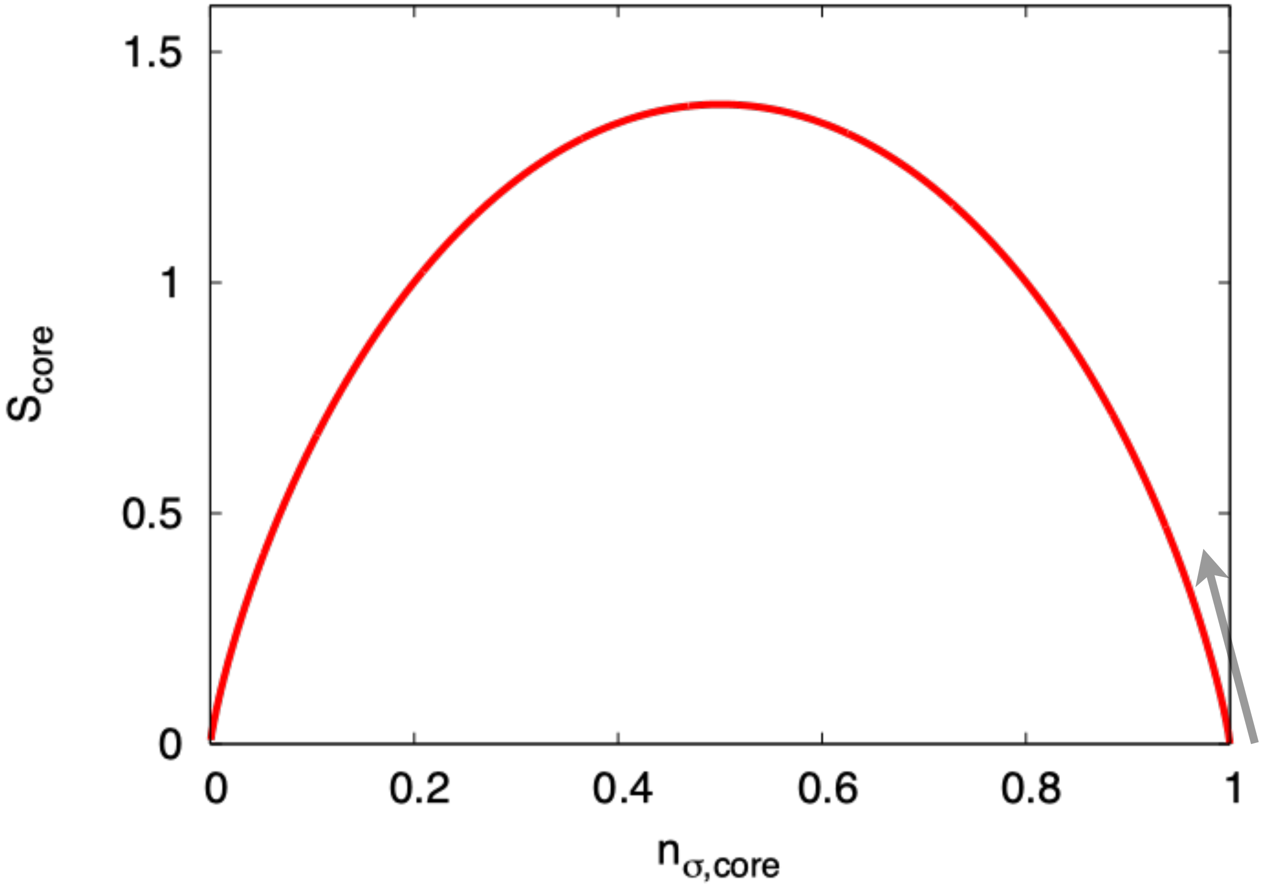


Entropy cooling (“evaporative cooling”)

- Photo-doping from/to flat bands *Werner, Eckstein, Mueller & Refael, Nat. Comm. (2019)*
  - Entropy of the core band in the narrow band (atomic) limit:

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



rapid increase of entropy of the core upon hole doping

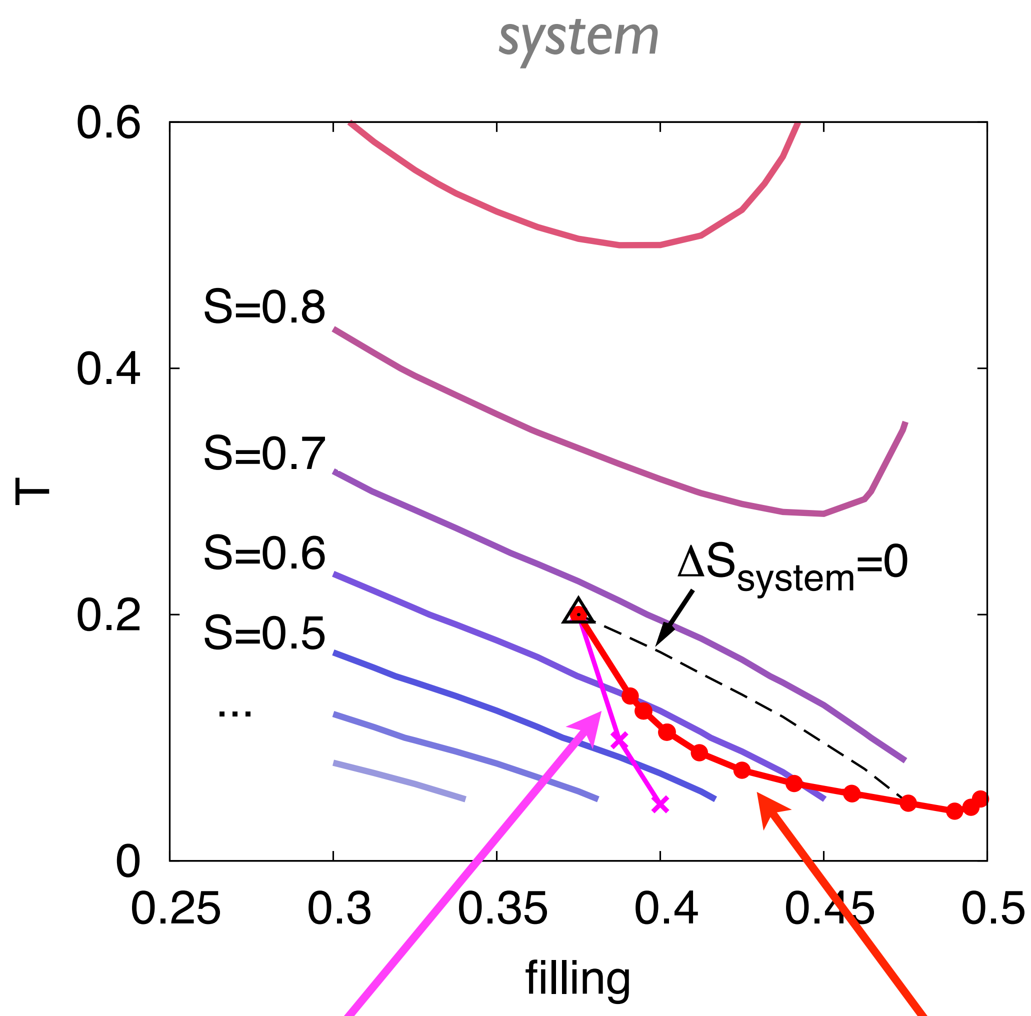
  - In case of isentropic doping process:

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

cooling of system due to entropy reshuffling

Entropy cooling ("evaporative cooling")

- **Photo-doping from/to flat bands** *Werner, Eckstein, Mueller & Refael, Nat. Comm. (2019)*
  - Constant entropy contours in the filling-temperature plane



isentropic case

quasi-particle temperature and fillings realized by chirped pulses

Entropy cooling (“evaporative cooling”)

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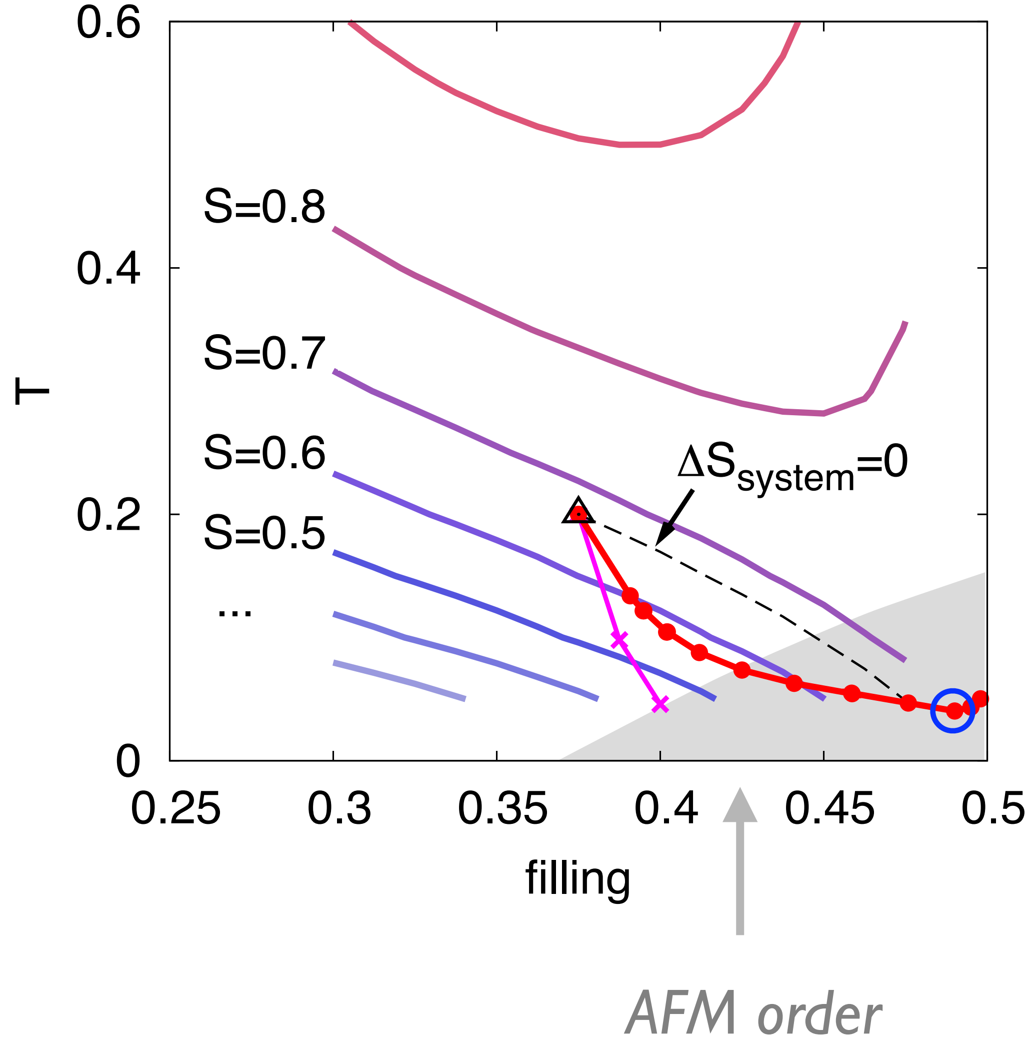
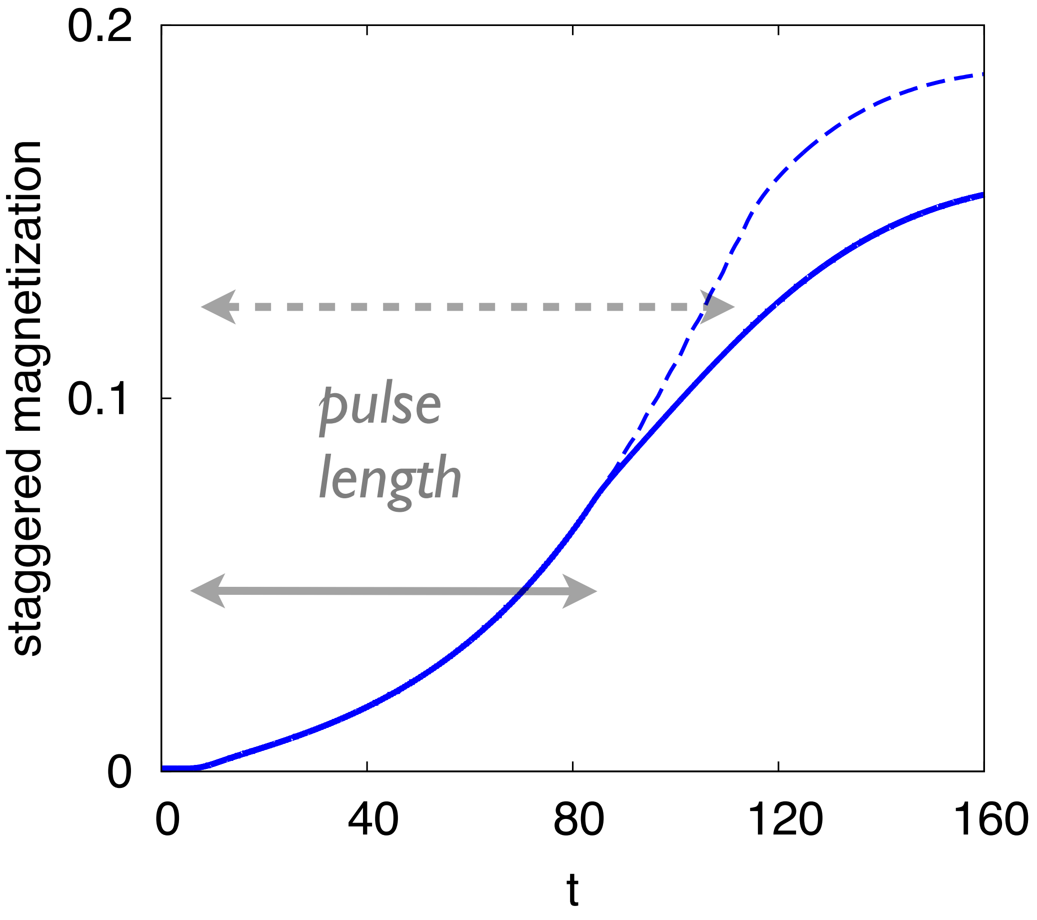
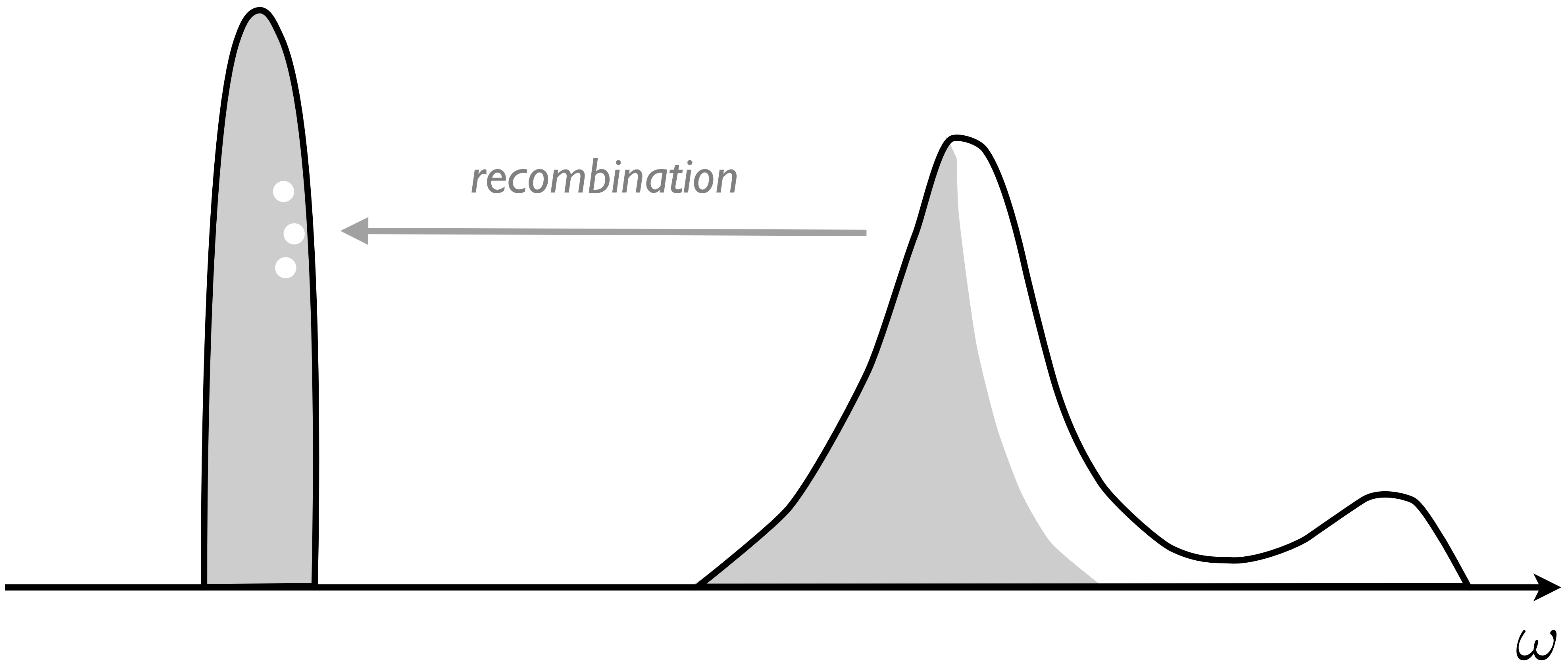




Entropy trapping

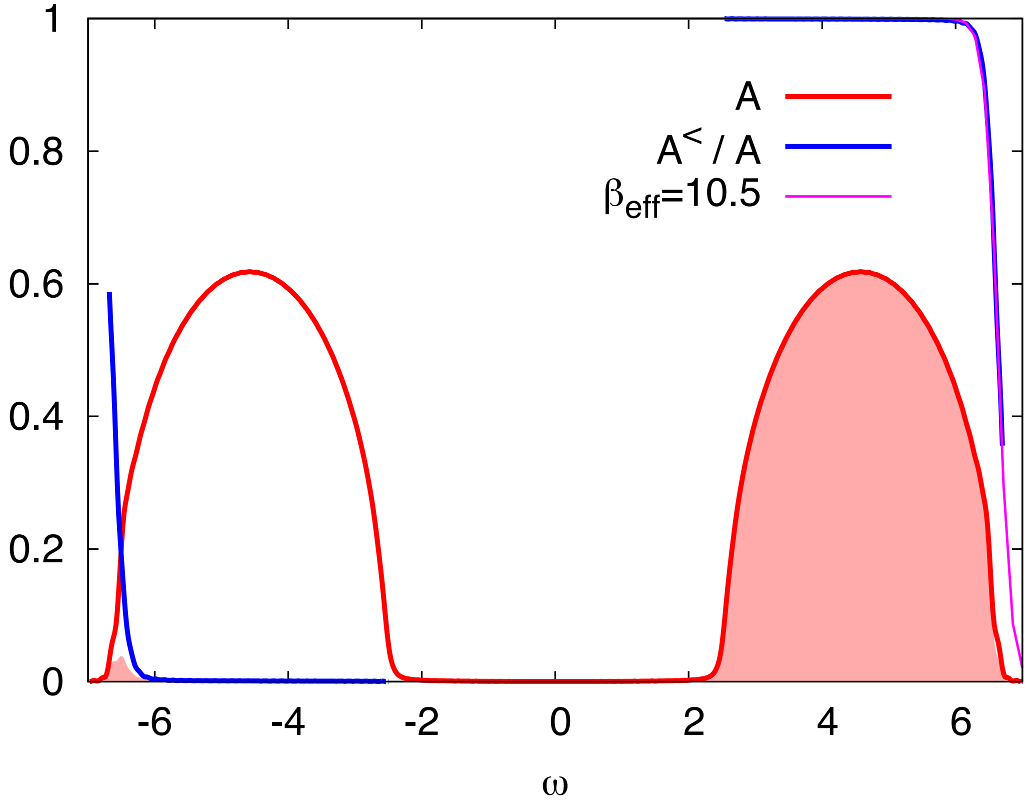
- Thermalization bottleneck prevents system from heating
    - e. g. recombination of electrons and holes can be very slow if the gap size is large



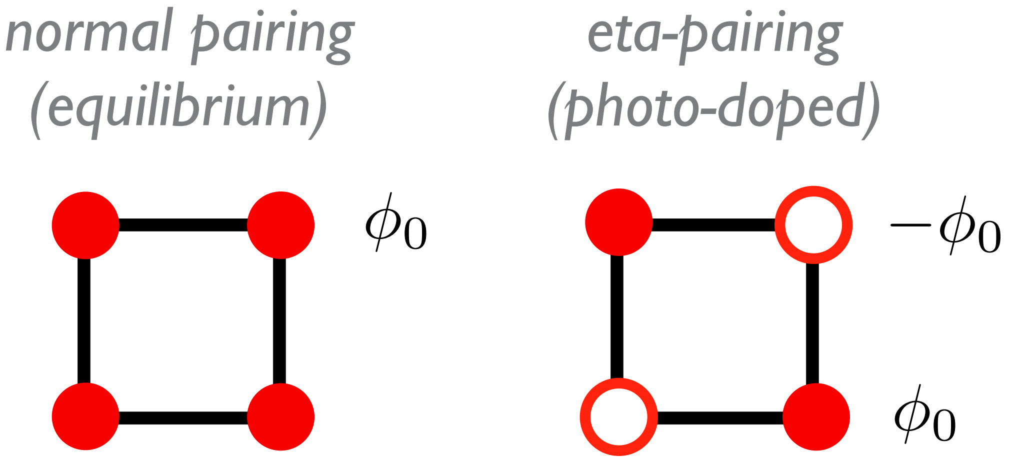
Superconductivity

- Nonthermal superconductivity in entropy-cooled systems
  - η pairing in a repulsive Hubbard model with inverted population and positive effective doublon/holon temperature

Rosch, Rasch, Binz & Vojta, PRL (2008); Werner, Li, Golez & Eckstein, PRB (2019)



state with almost complete population inversion and "cold" effective T>0 prepared by entropy-cooling protocol



$$\phi_0 = \langle c_\uparrow c_\downarrow \rangle$$

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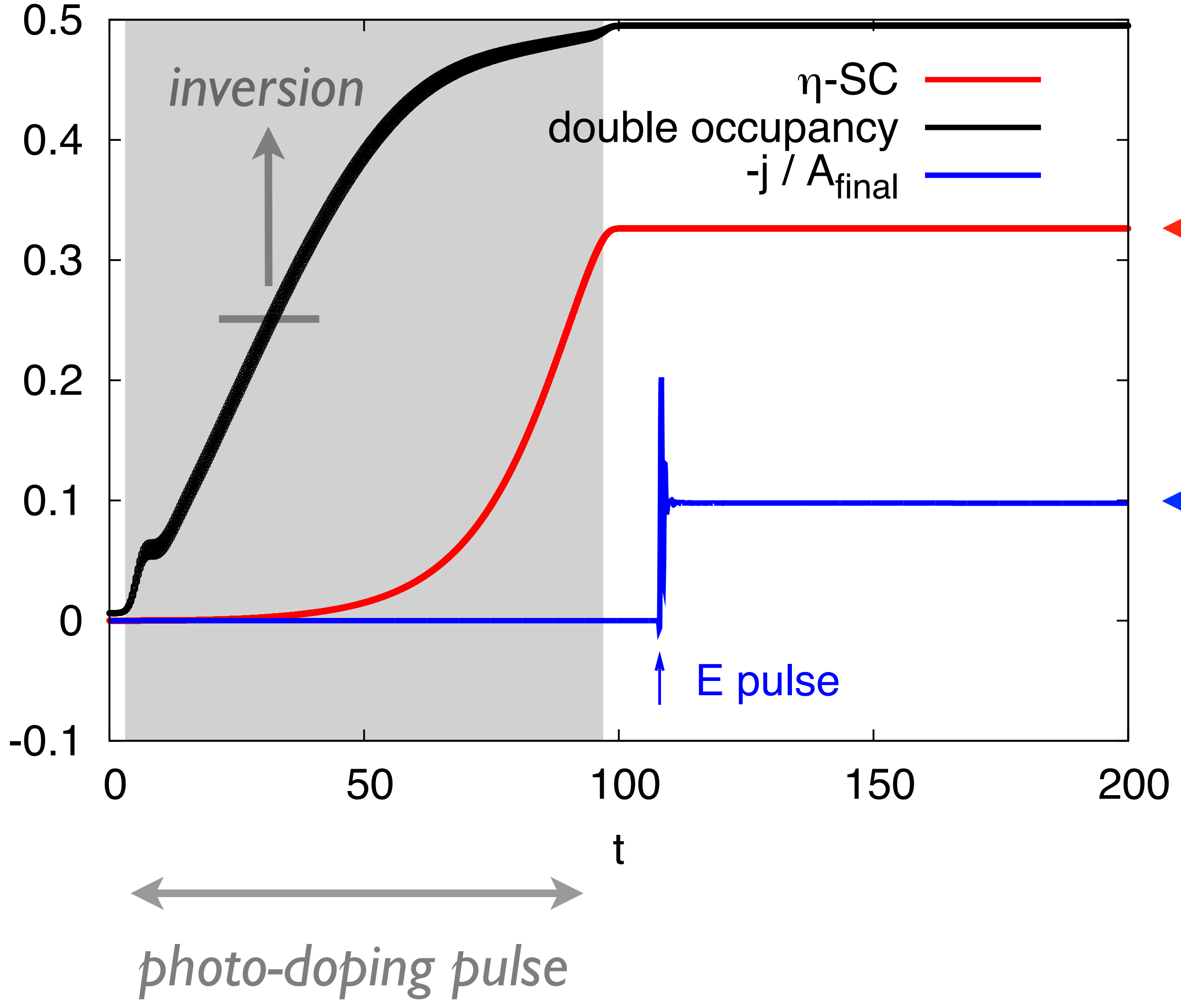


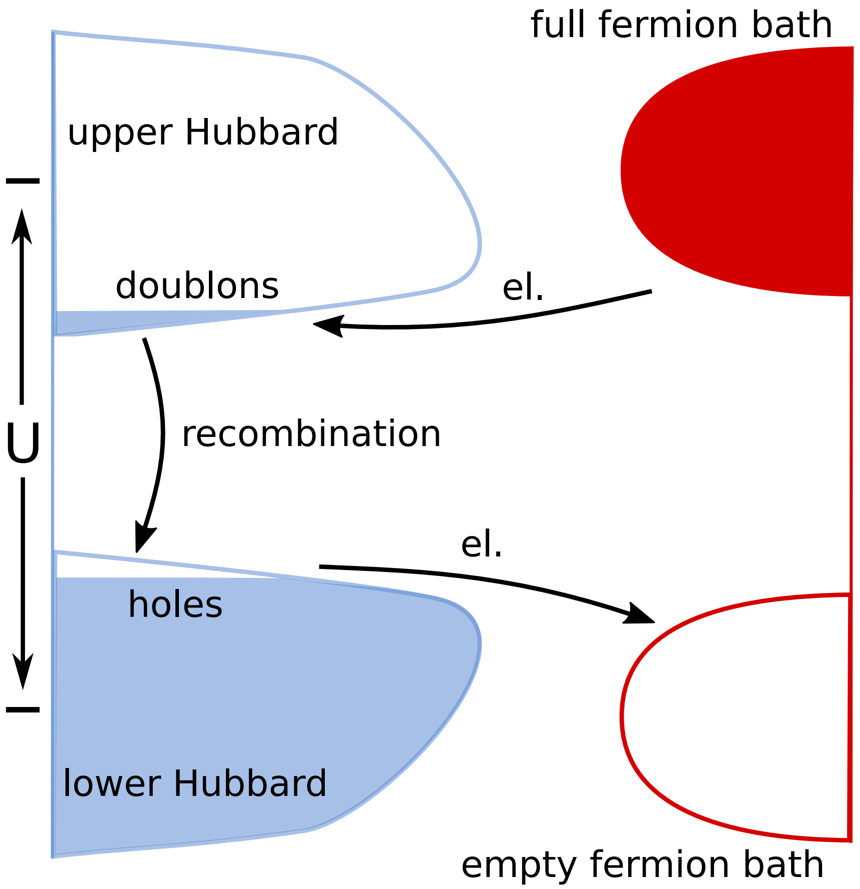
light-induced η-pairing

non-decaying current consistent with superconductivity

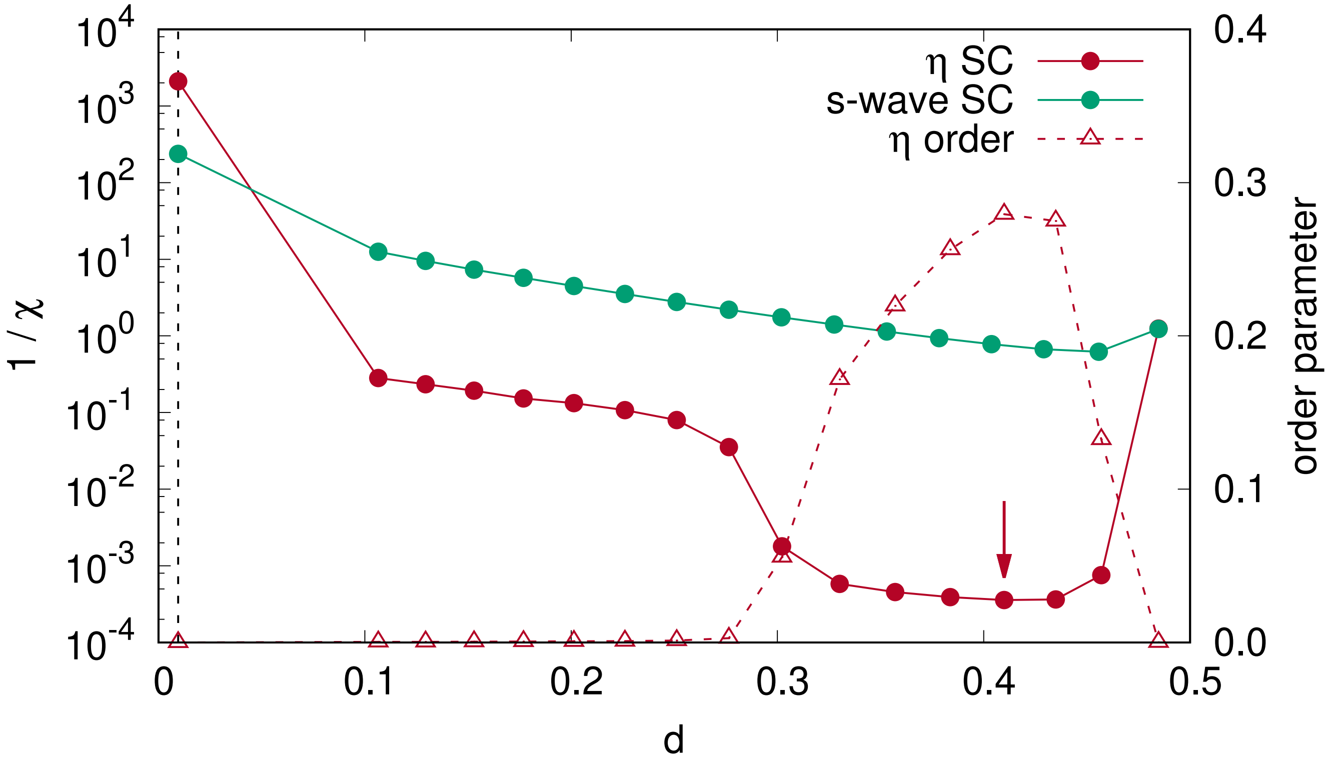
Superconductivity

- Nonthermal superconductivity in entropy-cooled systems
  - Nonequilibrium phase diagram of photo-doped Mott insulators
  - Use steady-state DMFT to control doublon concentration and T_{eff}

Li, Golez, Werner & Eckstein, PRB (2020)



steady-state formalism



inverse susceptibility for uniform and staggered superconductivity

Superconductivity

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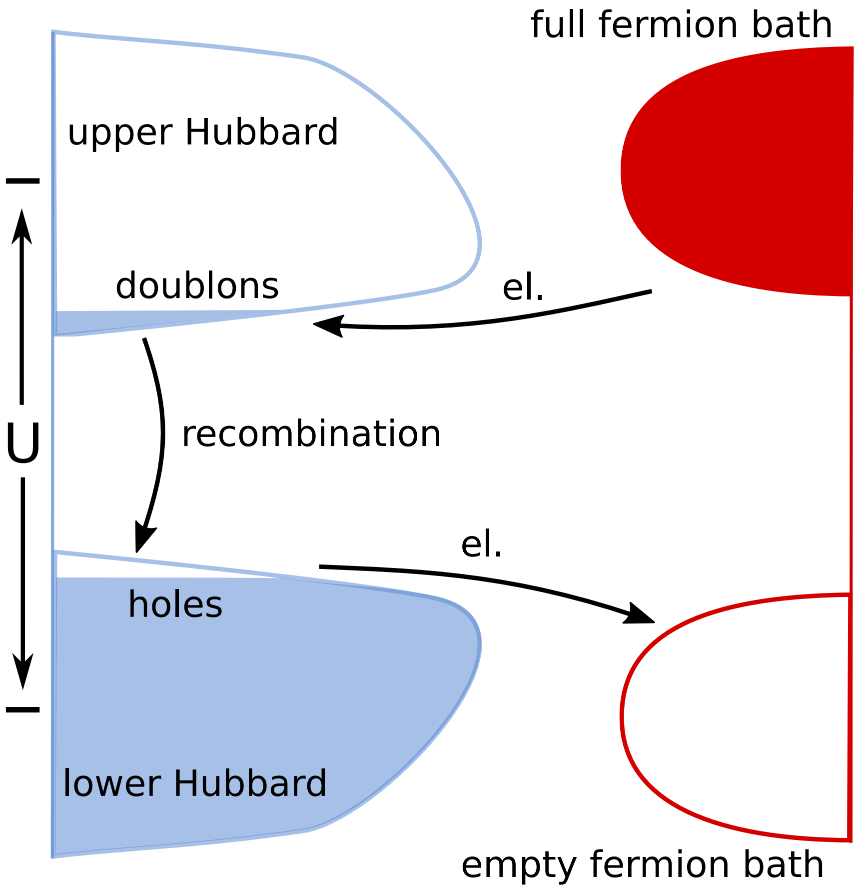

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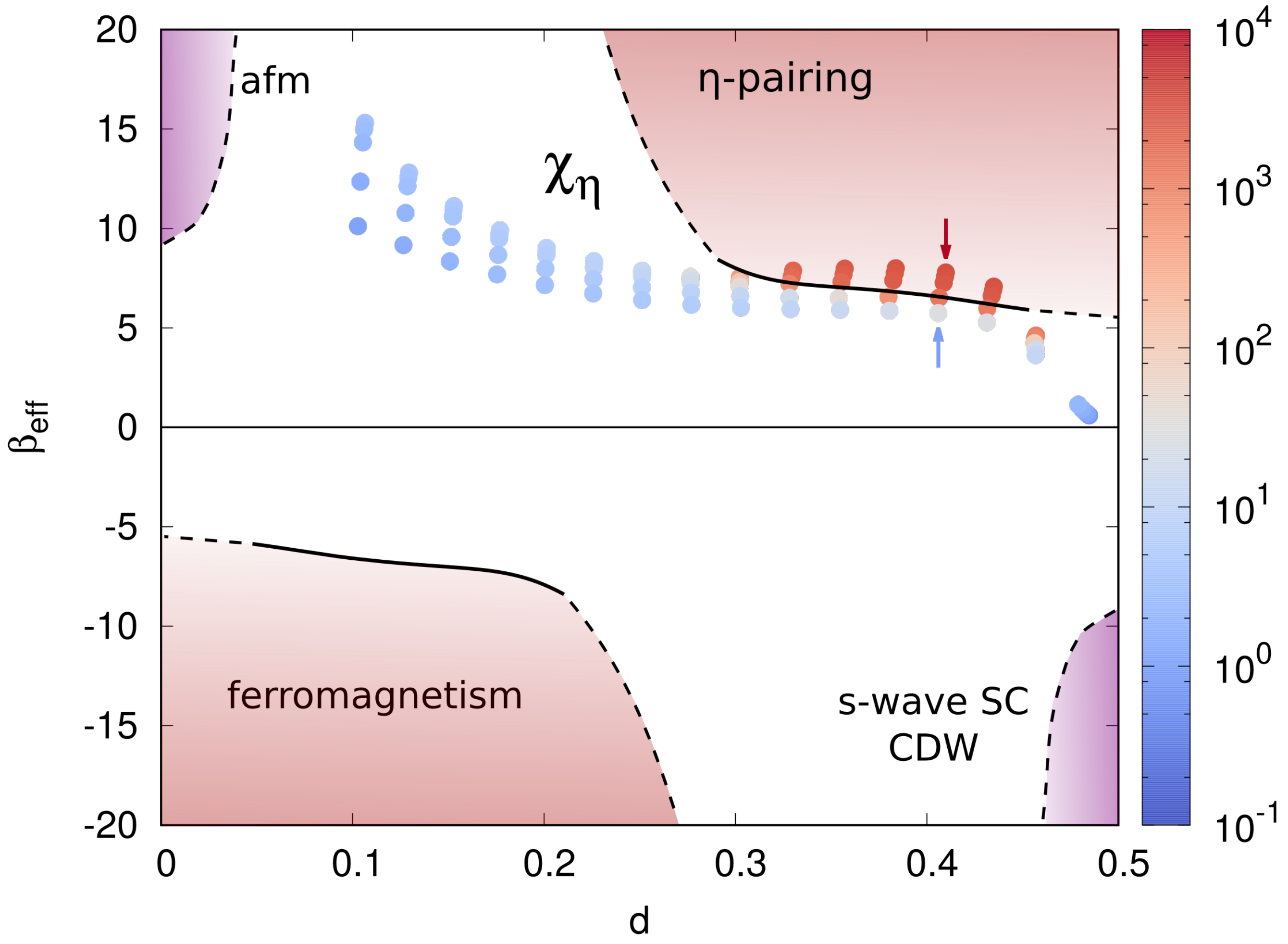
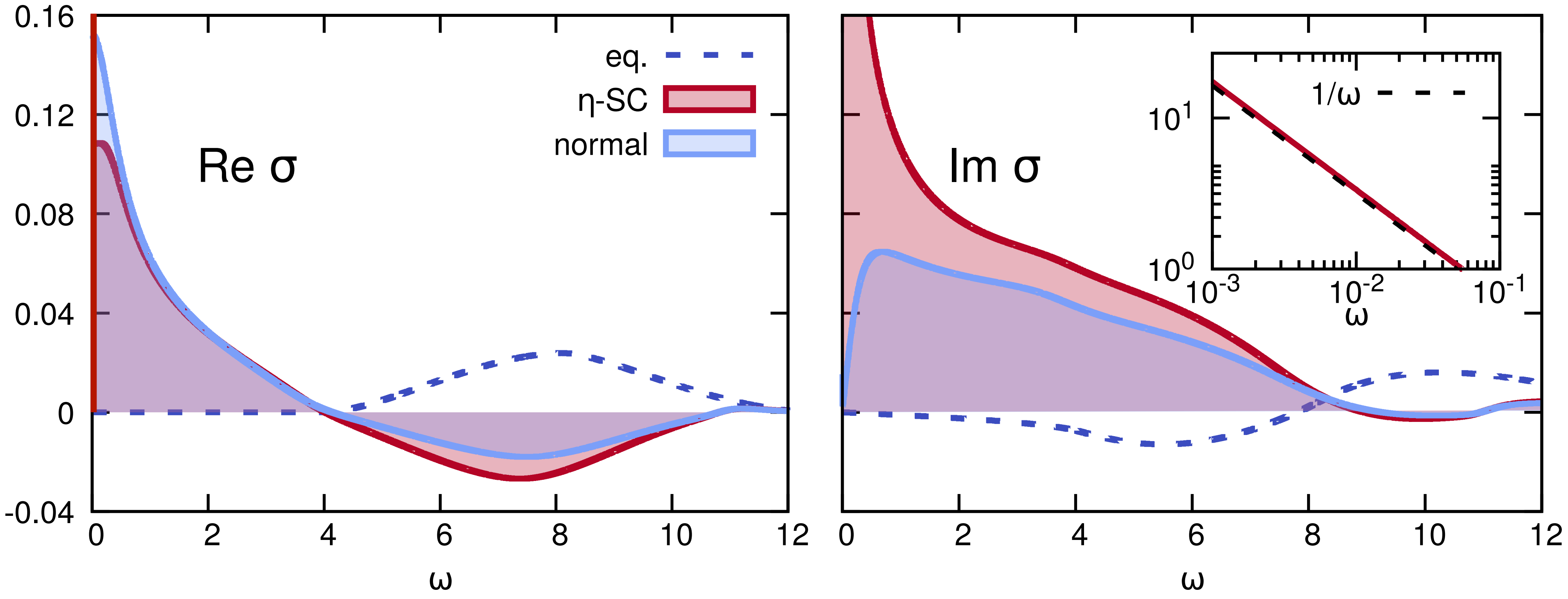


phase diagram

Superconductivity

- Nonthermal superconductivity in entropy-cooled systems
  - Optical conductivity of the η pairing state

    Li, Golez, Werner & Eckstein, PRB (2020)

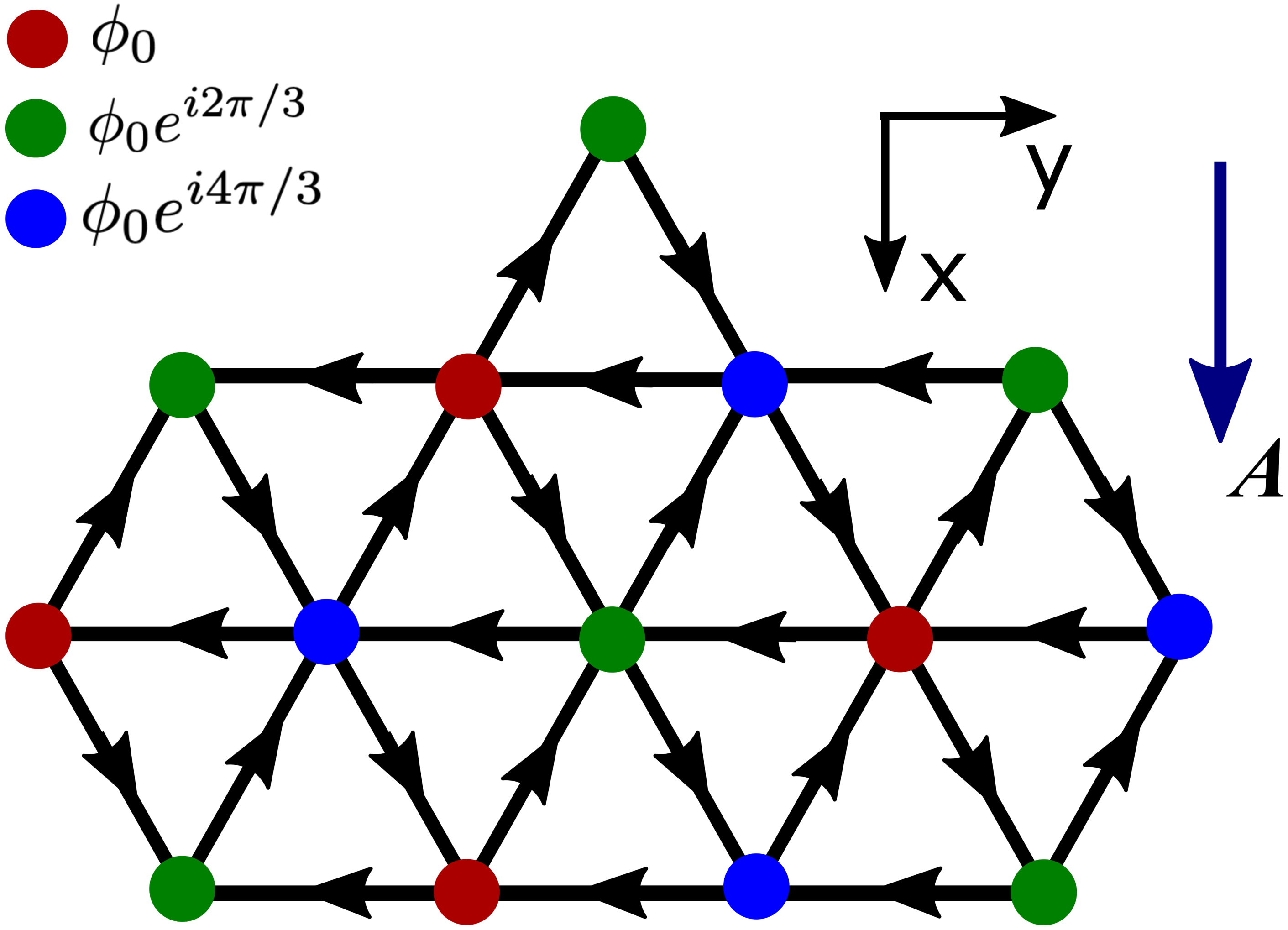


  - No gap in the real part (in contrast to s-wave SC)
  - two-fluid picture: condensed doublons/holons coexist with normal singlons

Superconductivity

- Nonthermal superconductivity in entropy-cooled systems
  - What happens in photo-doped systems on frustrated lattices?
  - Can we realize an analogue of 120-degree order?

Li, Mueller, Kim, Laeuchli & Werner, arXiv (2022)



chiral superconducting state with loop currents

experimental signature:

second-order transverse supercurrent response for A along x

Superconductivity

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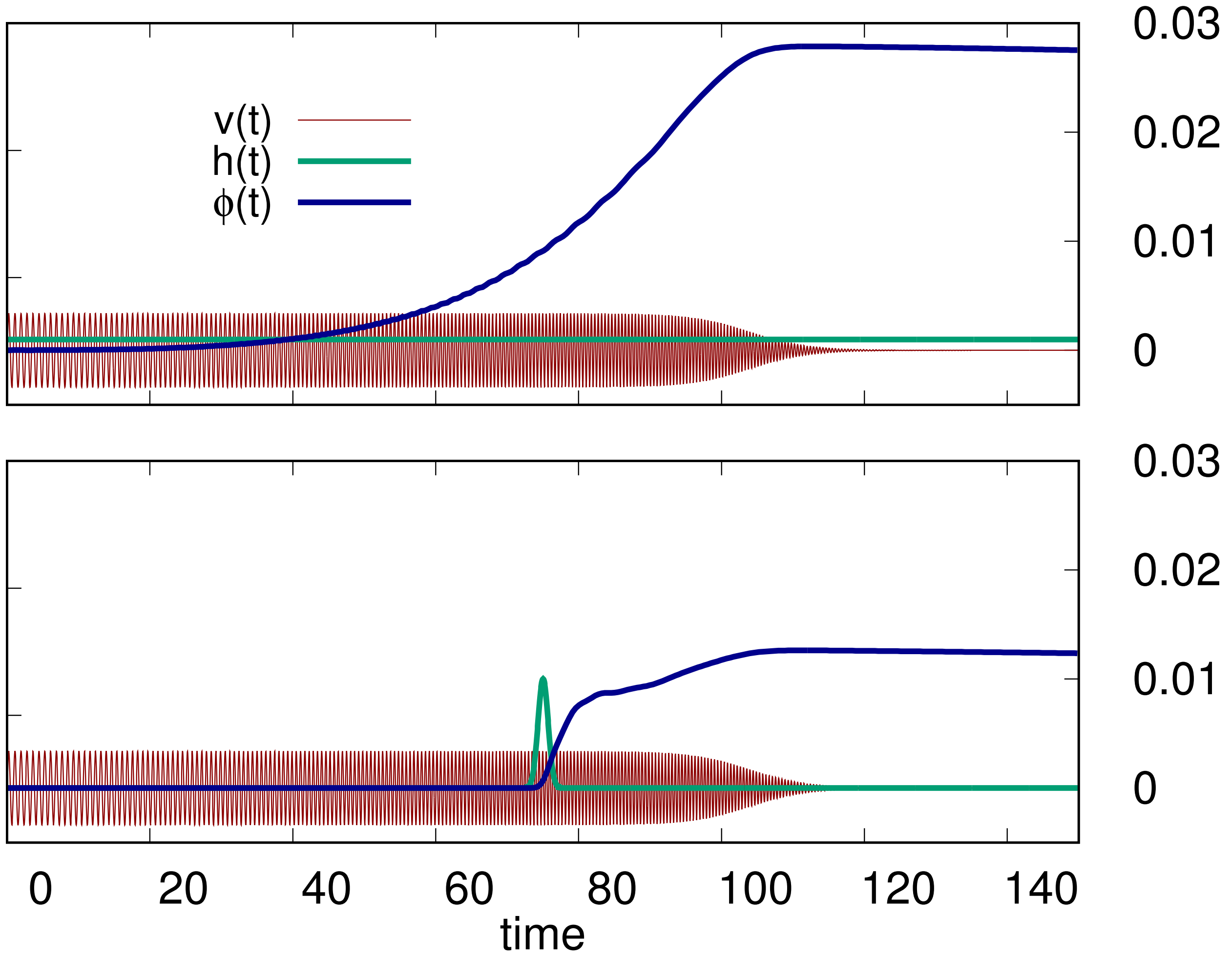
  Li, Mueller, Kim, Laeuchli & Werner, arXiv (2022)

  - Evidence from entropy-cooling protocol (for $\varphi = 0$)



with constant applied seed field

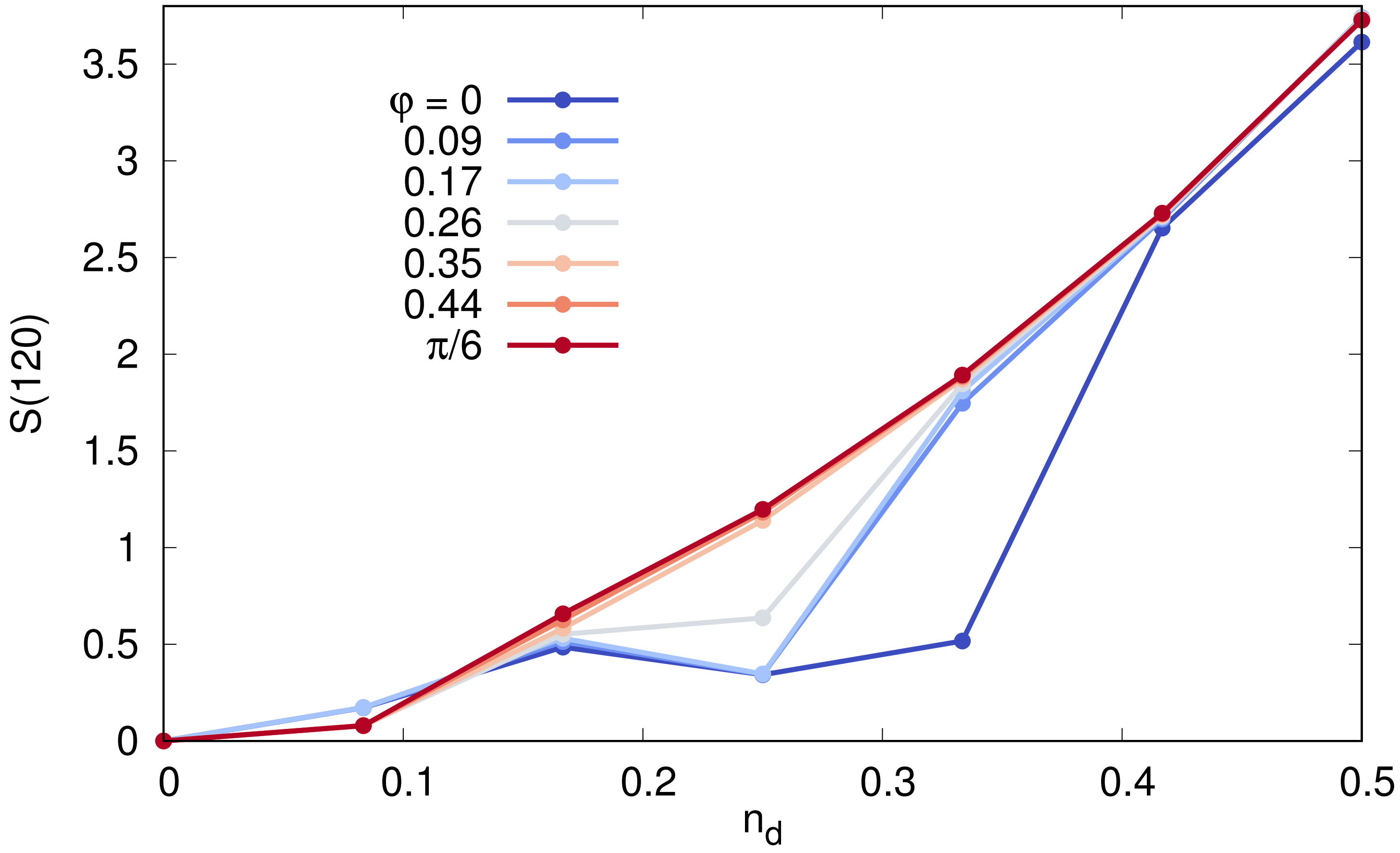
with short seed-field pulse

Superconductivity

- Nonthermal superconductivity in entropy-cooled systems
  - What happens in photo-doped systems on frustrated lattices?
  - Can we realize an analogue of 120-degree order?

    Li, Mueller, Kim, Laeuchli & Werner, arXiv (2022)

  - Evidence from exact diagonalization (12 sites)



pairing structure factor

$$S(120) \sim \sum_{ij} \theta_i \theta_j^* \langle \phi_i^+ \phi_j^- \rangle$$

$$\theta_{i=R,G,B} = 1, e^{i2\pi/3}, e^{i4\pi/3}$$

GGE description of photo-doped states

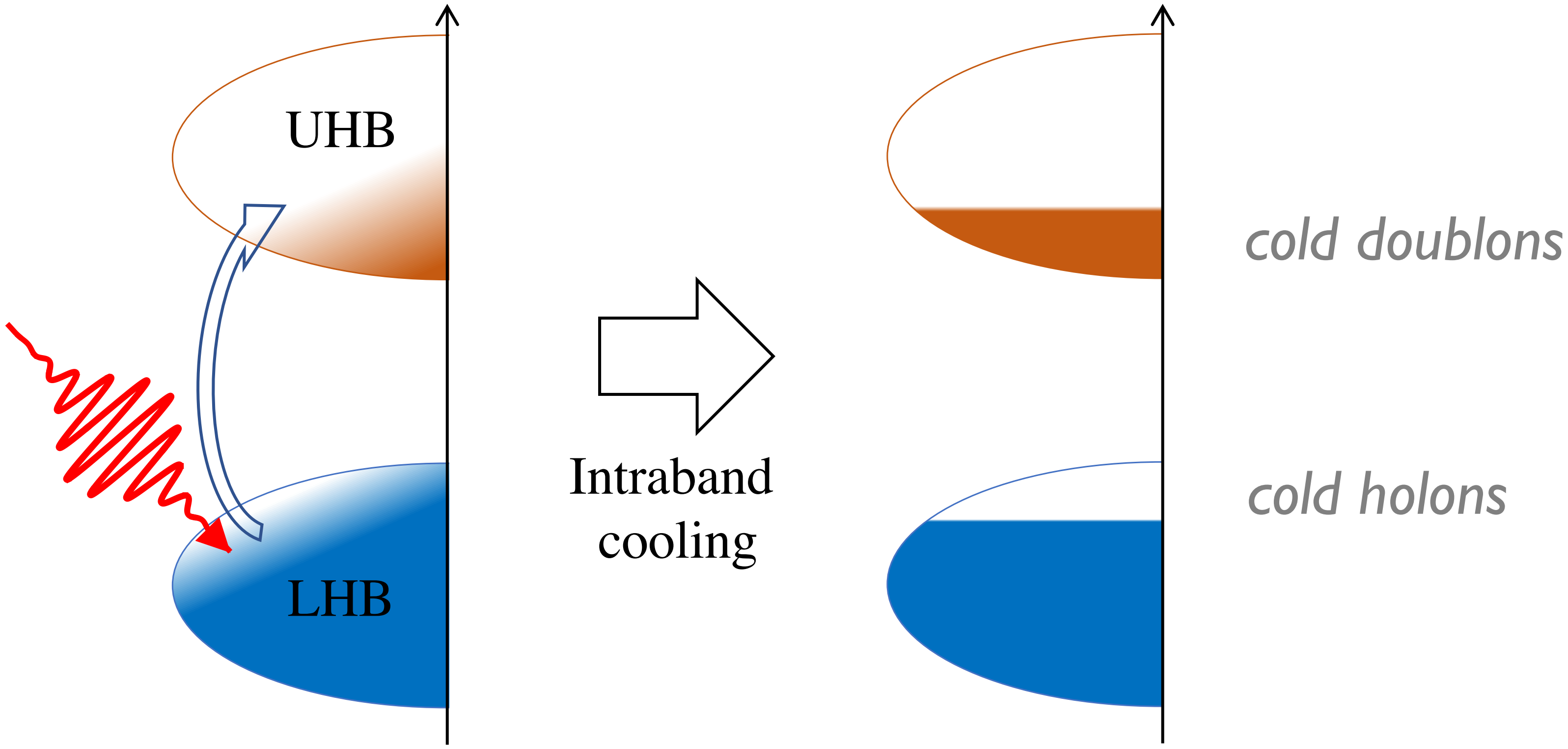
- Compute effective Hamiltonian by Schrieffer-Wolff transformation

  Murakami et al., Comm. Physics (2022)

  - U-V Hubbard model

$$H = -t_{\text{hop}} \sum_{\langle i,j \rangle,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + H_U + H_V$$

  - Photo-doping leads to steady-state with "cold" doublons/holons



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$$H = -t_{\mathrm{hop}} \sum_{\langle i,j \rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + H_U + H_V$$

  - Eliminate terms which change number of doublons/holons/singlons

$$H_{\mathrm{eff}} = H_U + H_{\text{kin,doublon}} + H_{\text{kin,holon}} + H_V \\ + H_{\text{spin-ex}} + H_{\text{dh-ex}} + H_{\text{U-shift}} + H_{\text{3-site}}$$

$$H_{\text{spin-ex}} = J_{\mathrm{ex}} \sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j$$

spin exchange term determines correlations between neighobring singlons

$$H_{\text{dh-ex}} = -J_{\mathrm{ex}} \sum_{\langle i,j \rangle} \vec{\eta}_i \cdot \vec{\eta}_j$$

doublon-holon exchange term determines correlations between neighboring doublon-holon pairs

GGE description of photo-doped states

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  Murakami et al., Comm. Physics (2022)

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  - Eliminate terms which change number of doublons/holons/singlons

$$\begin{aligned} H_{\text{eff}} = &\, H_U + H_{\text{kin,doublon}} + H_{\text{kin,holon}} + H_V \\ &+ H_{\text{spin-ex}} + H_{\text{dh-ex}} + H_{\text{U-shift}} + H_{\text{3-site}} \end{aligned}$$

$$H_{\text{spin-ex}} = J_{\text{ex}} \textstyle\sum_{\langle i,j \rangle} \vec{s}_i \cdot \vec{s}_j$$

$$H_{\text{dh-ex}} = -J_{\text{ex}} \textstyle\sum_{\langle i,j \rangle} \vec{\eta}_i \cdot \vec{\eta}_j$$

$$\begin{aligned} \eta_i^+ &= (-1)^i c_{i\downarrow}^{\dagger} c_{i\uparrow}^{\dagger} \\ \eta_i^- &= (-1)^i c_{i\uparrow} c_{i\downarrow} \\ \eta_i^z &= \tfrac{1}{2}(n_i - 1) \end{aligned}$$

GGE description of photo-doped states

- Compute effective Hamiltonian by Schrieffer-Wolff transformation

  Murakami et al., Comm. Physics (2022)

  - U-V Hubbard model

$$H = -t_{\mathrm{hop}} \sum_{\langle i,j \rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) + H_U + H_V$$

  - Eliminate terms which change number of doublons/holons/singlons

$$J_{\mathrm{ex}} = \frac{4t^2_{\mathrm{hop}}}{U}$$

$$(\uparrow, \downarrow) \rightarrow \underbrace{(\uparrow\downarrow, 0)}_{\Delta E = U} \rightarrow (\downarrow\uparrow)$$

spin exchange is antiferro

$$(\uparrow\downarrow, 0) \rightarrow \underbrace{(\uparrow, \downarrow)}_{\Delta E = -U} \rightarrow (0, \uparrow\downarrow)$$

doublon-holon exchange is ferro

GGE description of photo-doped states

- Compute effective Hamiltonian by Schrieffer-Wolff transformation

  Murakami et al., Comm. Physics (2022)

  - Introduce separate chemical potentials for doublons and holons

$$N_h = \sum_i n_i^h, \quad n_i^h = (1 - n_{i\uparrow})(1 - n_{i\downarrow})$$

$$N_d = \sum_i n_i^d, \quad n_i^d = n_{i\uparrow} n_{i\downarrow}$$

  - Introduce grand-canonical Hamiltonian for photo-doped state

$$K_{\text{eff}} = H_{\text{eff}} - \mu_d N_d - \mu_h N_h \qquad \rho_{\text{eff}} = e^{-\beta_{\text{eff}} K_{\text{eff}}}$$

controls density of doublons *controls density of holons*

  - Then use favorite equilibrium method to solve this problem

GGE description of photo-doped states

- Compute effective Hamiltonian by Schrieffer-Wolff transformation

  Murakami et al., Comm. Physics (2022)

  - Static observables can be computed directly from $\rho_{\text{eff}} = e^{-\beta_{\text{eff}} K_{\text{eff}}}$
  - Response functions $-i\langle[A(t), B(0)]_{\pm}\rangle$ can also be computed, but
    - initial state described by K_{eff}
    - time propagation determined by H_{eff}

    must split the operators A and B into terms which change the doublon number by +1, 0, -1 and multiply these terms with appropriate phase factors

    $$A = \sum_\alpha A_\alpha \quad H_\mu = -\sum_G \mu_G N_G$$

    $$\lambda_\alpha = -\sum_G \mu_G \Delta N_{G,\alpha}$$

    $$e^{-iH_\mu t} A_\alpha e^{iH_\mu t} = e^{-i\lambda_\alpha t} A_\alpha$$

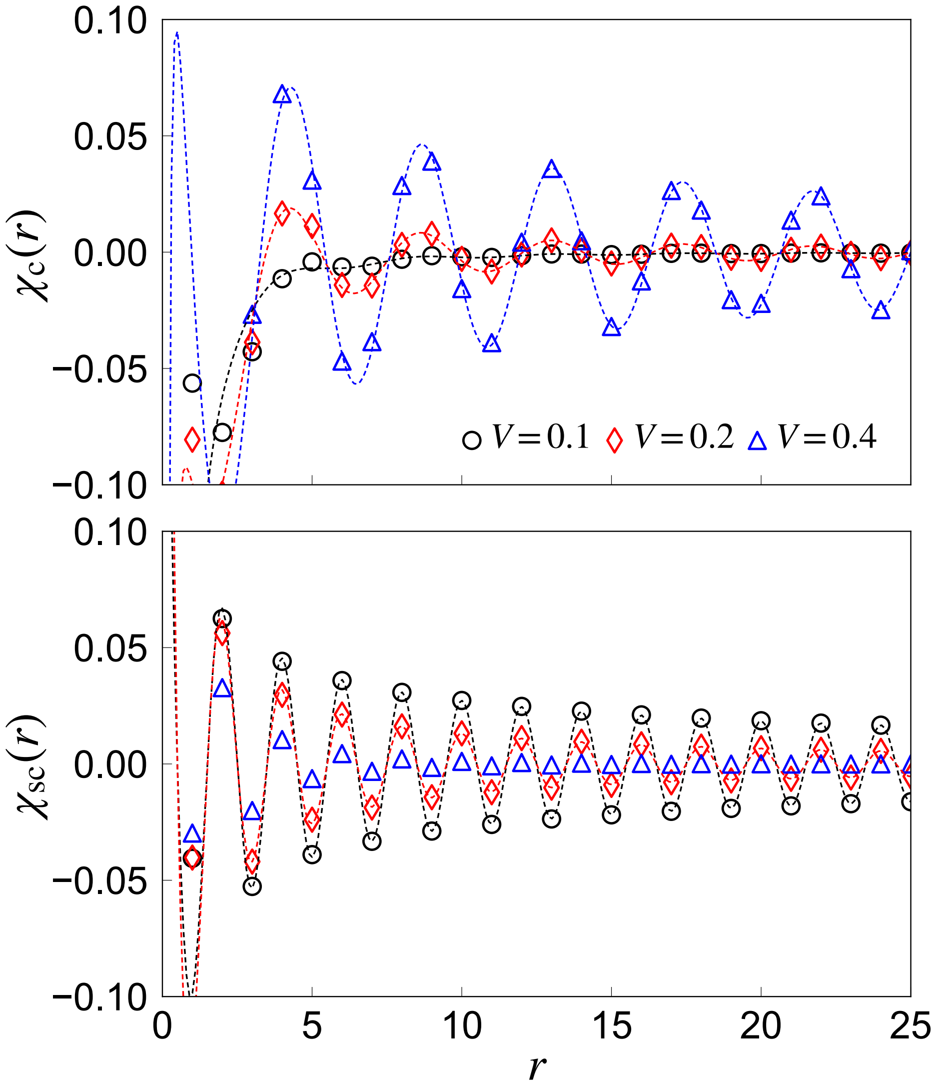
  - To determine the nonequilibrium phase diagram, measure the decay of spin, charge and eta-spin correlations, e. g. using iTEBD

GGE description of photo-doped states

- Compute effective Hamiltonian by Schrieffer-Wolff transformation

  Murakami et al., Comm. Physics (2022)

  - Charge and eta-pairing correlations in the photo-doped 1D U-V Hubbard model ($H_{\rm eff}$ without 3-site terms) at $n_d = n_h = 0.23$



charge correlations dominate for V=0.4

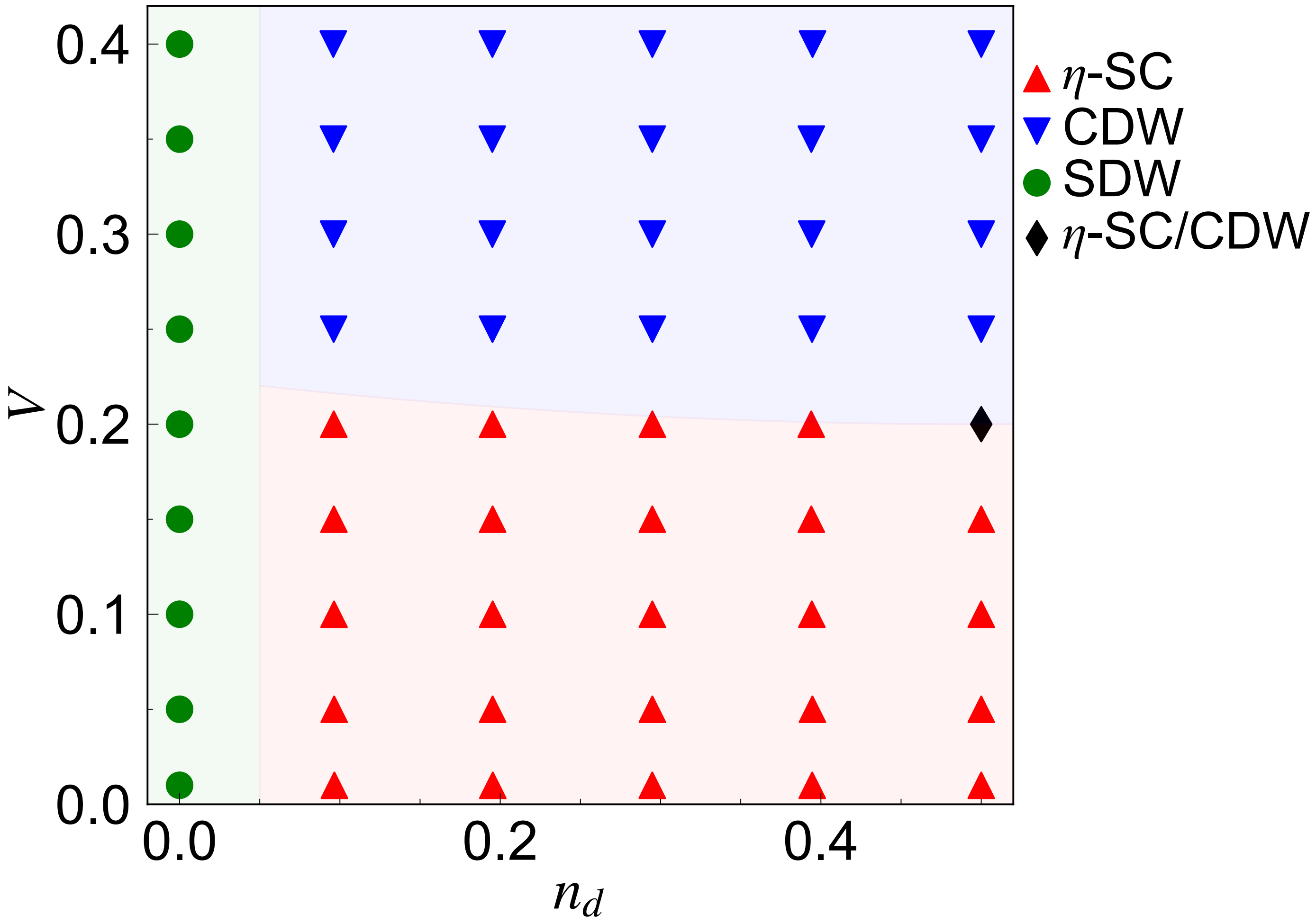
eta pairing correlations dominate for V=0.1, 0.2

GGE description of photo-doped states

- Compute effective Hamiltonian by Schrieffer-Wolff transformation

  Murakami et al., Comm. Physics (2022)

  - "Zero effective temperature" phase diagram of photo-doped 1D U-V Hubbard model (H_{eff} without 3-site terms)

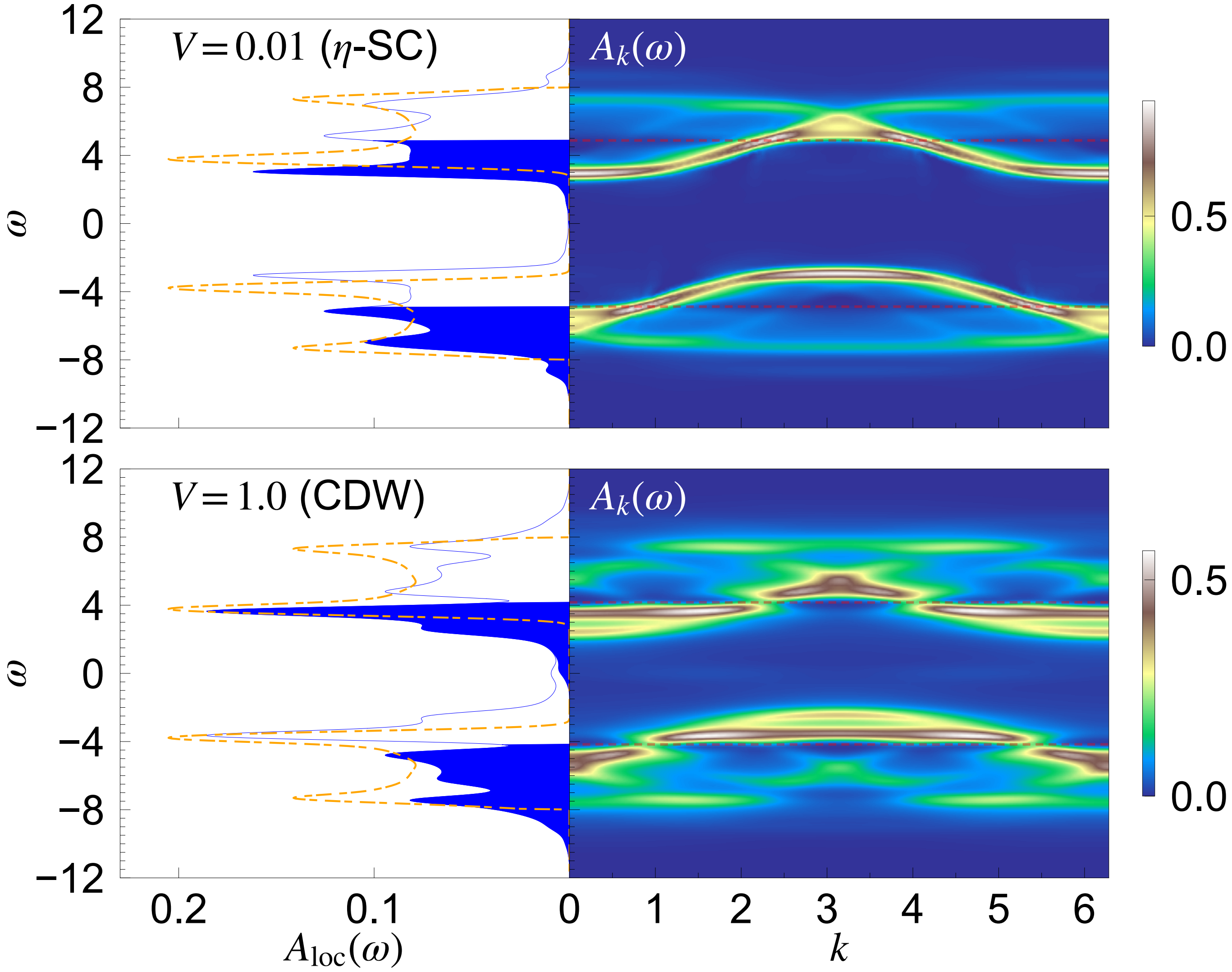


GGE description of photo-doped states

- Compute effective Hamiltonian by Schrieffer-Wolff transformation

  Murakami et al., Comm. Physics (2022)

  - Spectral functions of the photo-doped 1D U-V Hubbard model (H_{eff} without 3-site terms)



not gapped for the eta-pairing phase

Spin, charge and eta-spin separation in 1D

- Exact wave function in the limit of large on-site repulsion

  Murakami et al., arxiv:2212.06263 (2022)

  - Consider $H_{\rm eff}$ with fixed number of doublons and holons
  - Wave function in the limit $J_{\rm ex} \to 0,\ V/J_{\rm ex} = \mathrm{const}$ is a generalization of the Ogata-Shiba state

    Ogata & Shiba, PRB 41, 2326 (1990) *(doped equilibrium model)*

    - For $J_{\rm ex} = V = 0$: Eigenstates of $H_{\rm eff}$ are degenerate w. r. t. spin and eta-spin configurations

      $H_{\rm kin,doublon} + H_{\rm kin,holon}$ *does not flip spins or exchange d-h pairs*

      $$|\Psi\rangle = |\Psi_{\rm SF}^{\rm GS}\rangle|\Psi_{\sigma,\eta}\rangle$$

      ground state of spinless Fermions

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      $H_{\text{kin,doublon}} + H_{\text{kin,holon}}$ *does not flip spins or exchange d-h pairs*

$$|\Psi\rangle = |\Psi^{\text{GS}}_{\text{SF}}\rangle|\Psi_{\sigma,\eta}\rangle$$

← *degeneracy of $2^{N_s}2^{N_\eta}$ lifted by $\mathcal{O}(J_{\text{ex}})$ terms*

↑ *ground state of spinless Fermions*

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  - Consider H_{eff} with fixed number of doublons and holons
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    Ogata & Shiba, PRB 41, 2326 (1990) *(doped equilibrium model)*

    - After taking into account the $\mathcal{O}(J_{\text{ex}})$ terms, the squeezed spin and eta-spin spaces get decoupled

$$H^{\text{squeezed}}_{\text{spin}} = J^s_{\text{ex}} \sum_i \vec{s}_{i+1} \cdot \vec{s}_i$$

$$H^{\text{squeezed}}_{\eta-\text{spin}} = -J^s_X \sum_j (\eta^x_{j+1}\eta^x_j + \eta^y_{j+1}\eta^y_j) + J^s_Z \sum_j \eta^z_{j+1}\eta^z_j$$

Spin, charge and eta-spin separation in 1D

- Exact wave function in the limit of large on-site repulsion

  Murakami et al., arxiv:2212.06263 (2022)

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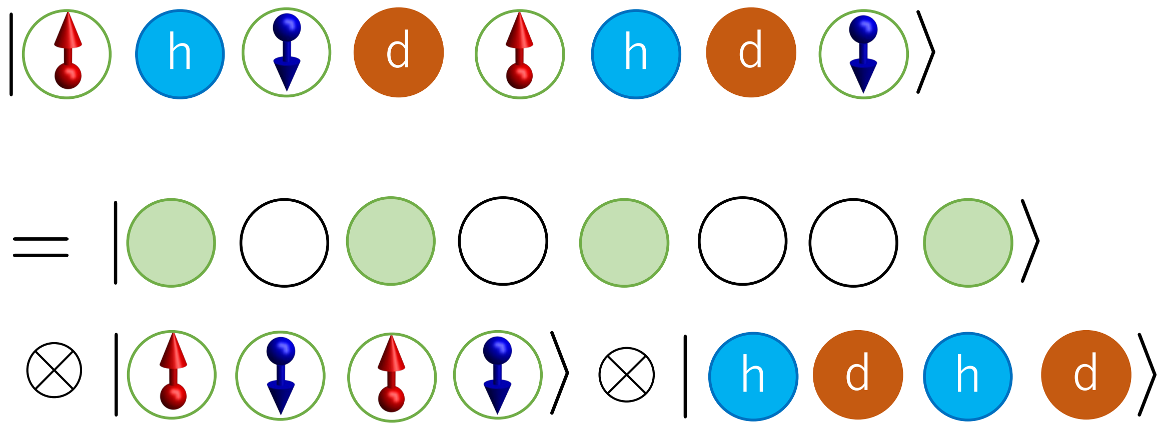
$$|\Psi\rangle = |\Psi^{\rm GS}_{\rm SF}\rangle|\Psi^{\rm GS}_{\sigma}\rangle|\Psi^{\rm GS}_{\eta}\rangle$$

ground state of $H^{\rm squeezed}_{\rm spin}$

ground state of $H^{\rm squeezed}_{\eta-{\rm spin}}$



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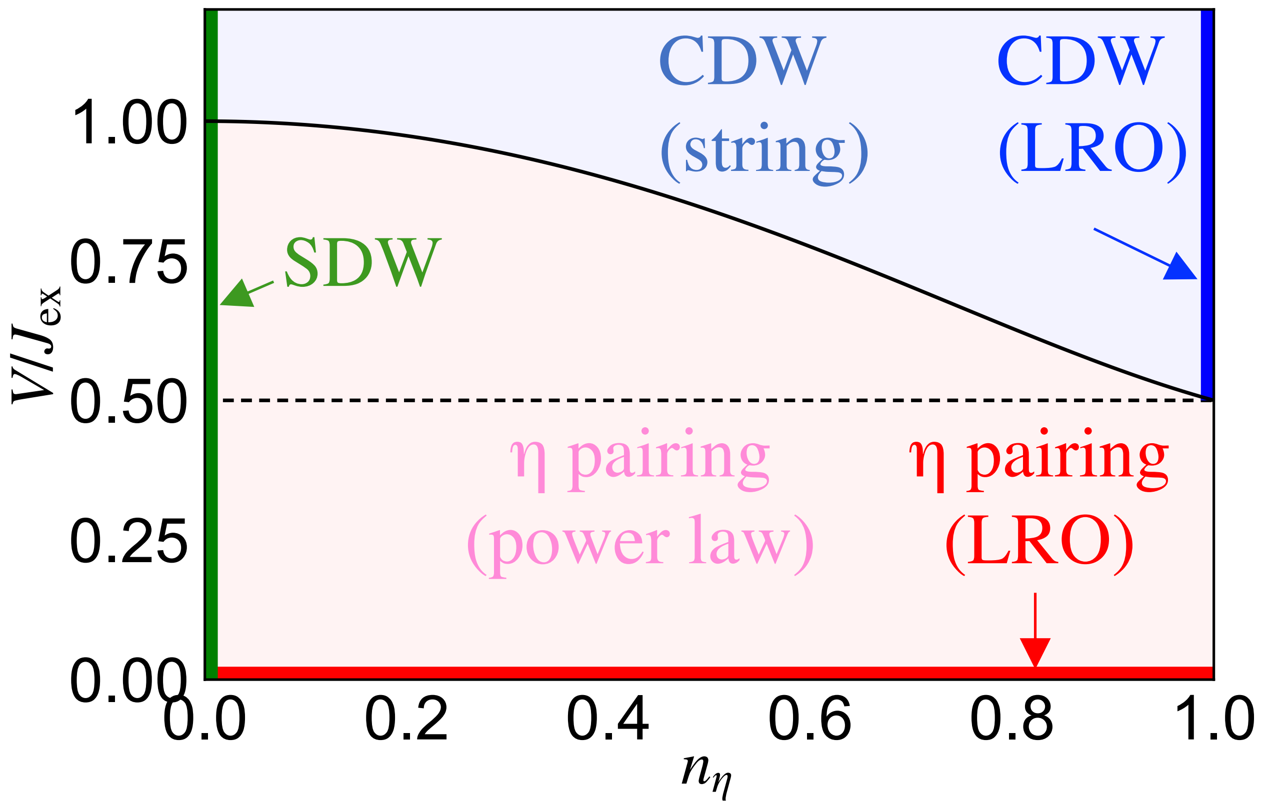
phase diagram (including 3-site terms)



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$$|\Psi\rangle = |\Psi_{\mathrm{SF}}^{\mathrm{GS}}\rangle|\Psi_{\sigma}^{\mathrm{GS}}\rangle|\Psi_{\eta}^{\mathrm{GS}}\rangle$$

allows to calculate the central charge *C*

measures the number of gapless modes

free fermions
(gapless)

AFM Heisenberg
(gapless)

XXZ model
small V/J$_{\mathrm{ex}}$: gapless (eta-pairing)
large V/J$_{\mathrm{ex}}$: gapful (CDW)

Spin, charge and eta-spin separation in 1D

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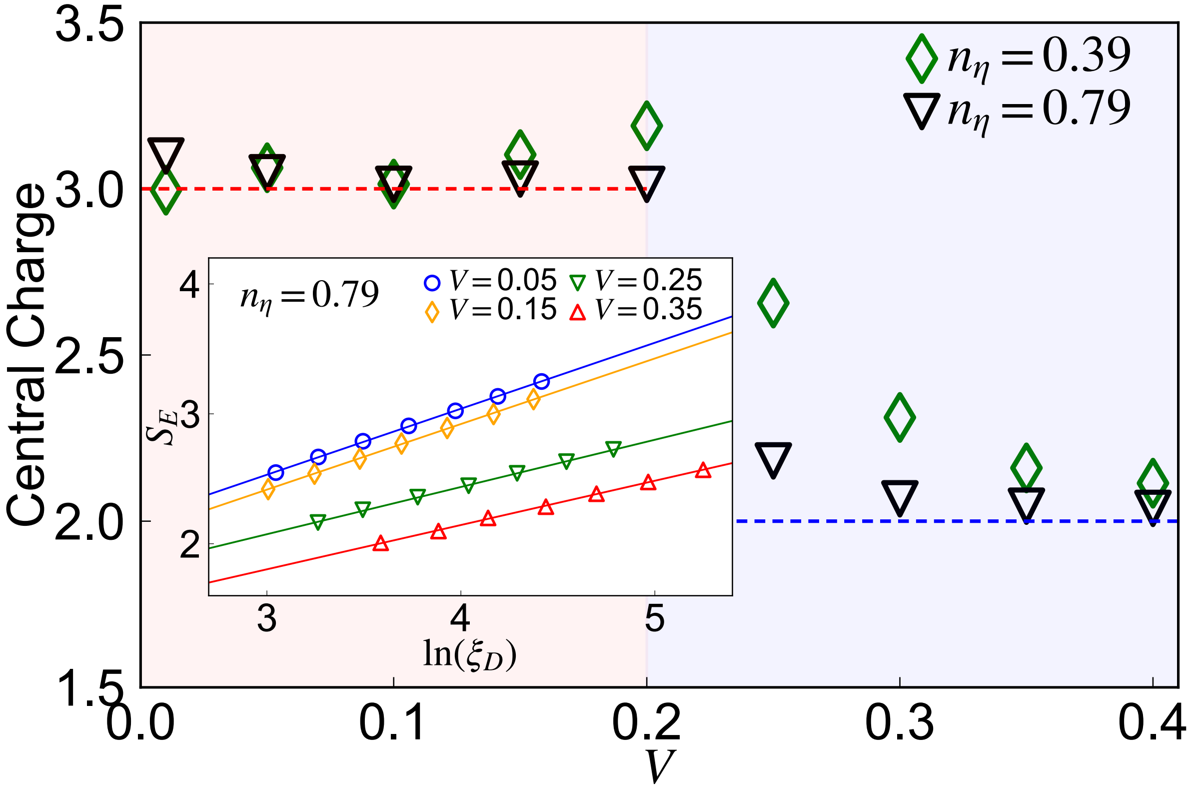
$$|\Psi\rangle = |\Psi^{\mathrm{GS}}_{\mathrm{SF}}\rangle|\Psi^{\mathrm{GS}}_{\sigma}\rangle|\Psi^{\mathrm{GS}}_{\eta}\rangle$$

eta-pairing phase has *C*=3

CDW phase has *C*=2

confirmed by iTEBD analysis of the entanglement entropy



Conclusions

- Nonthermal superconducting states in the Hubbard model
  - Mechanisms for realizing cold photo-doped Mott states
    - *Entropy cooling*: photo-doping from flat bands
    - *Coupling to baths*: injection of "cold" doublons and holes
  - Examples
    - *eta-pairing* on bipartite lattices
    - *chiral superconductivity* on geometrically frustrated lattices
  - *Spin, charge and eta-spin separation* in photo-doped 1D Mott systems

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arXiv:2202.10176 (2022)
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