Possible hidden phases in photo-doped Mott insulators

Yuta Murakami (RIKEN CEMS)

Ref

YM, S. Takayoshi, T. Kaneko, Z. Sun, D. Golež , A. J. Millis and P. Werner, Comm. Phys. **5**, 23 (2022).

YM, S. Takayoshi, T. Kaneko, A. Läuchli and P. Werner, Phys. Rev. Lett. **130**, 106501 (2023).

Review: YM, D Golež, M Eckstein, P Werner, arXiv:2310.05201.

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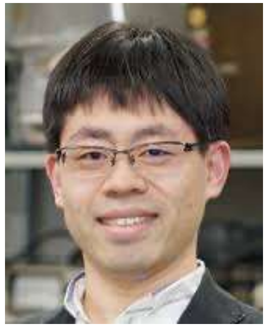


S. Takayoshi

Osaka University

T. Kaneko

JST

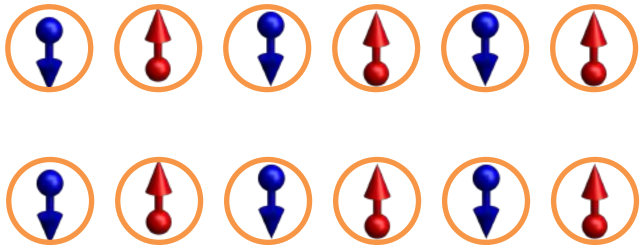
科研費
KAKENHI

Doping charge carriers into Mott insulators: Equilibrium

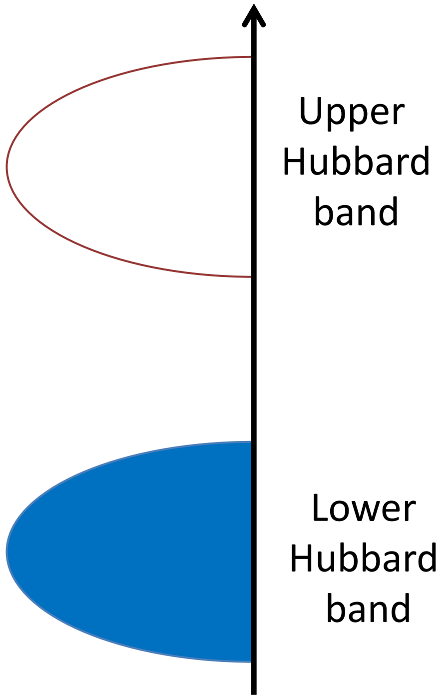
Ex) Hubbard model

$$\hat{H} = -v \sum_{\langle i,j \rangle,\sigma} \hat{c}_i^\dagger \hat{c}_j + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

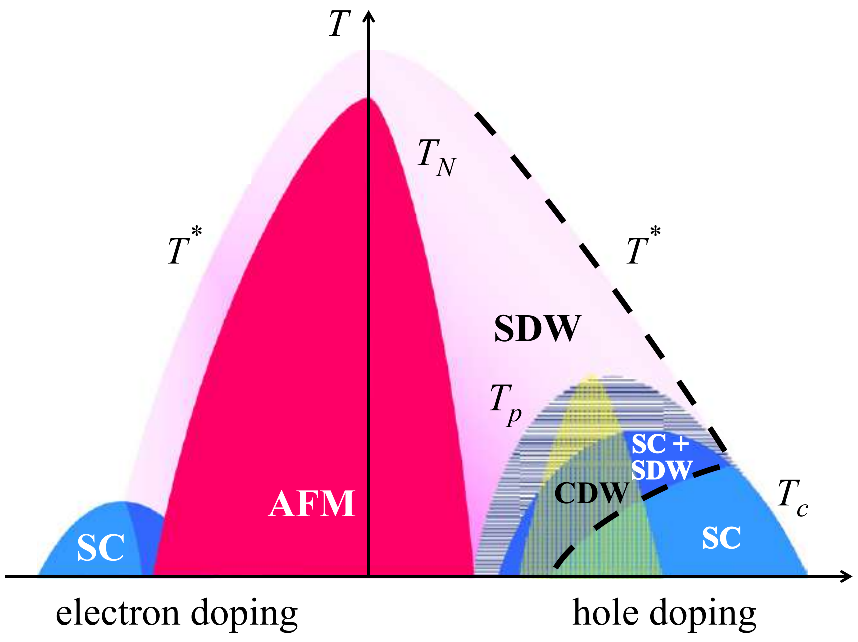
Mott Insulator@$U >> v$



Half filling: # electrons= # sites



Phase diagram of cuprate

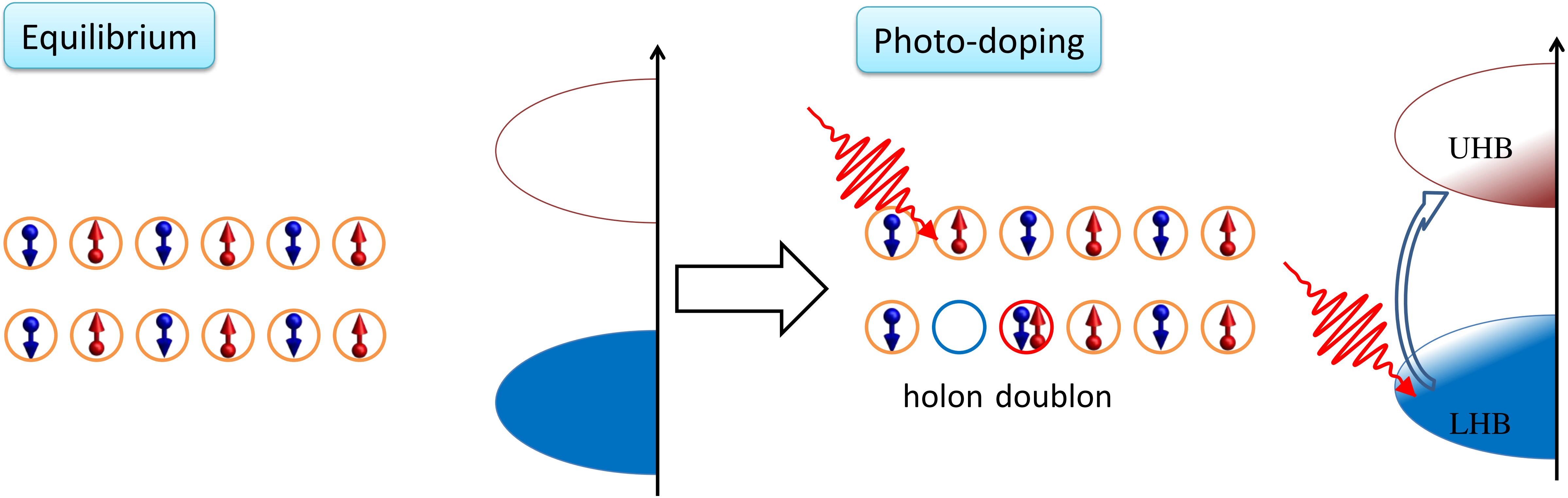


A. Kordyuk, Low. Temp. Phys. **41**, 319 (2015)

Doping activates correlations between spin, orbital and charge

⇨ Emergence of rich phases

Doping charge carriers into Mott insulators



Various types of charge carriers are activated at the same time

cf. Equilibrium doping → holon **or** doublon

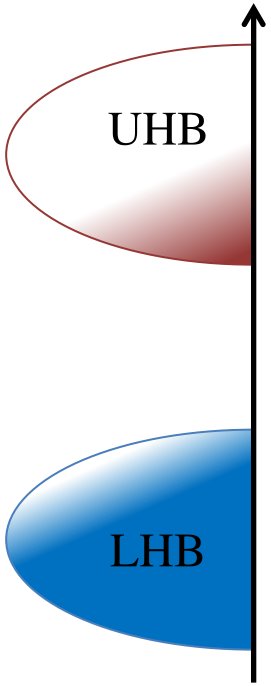
Long-life time of photo-carriers and metastable states

Life-time of doublon・holon

$U \gg v \quad \Rightarrow \quad \tau_{\mathrm{rec}} \gg 1/v$ (Exponential with U/v)

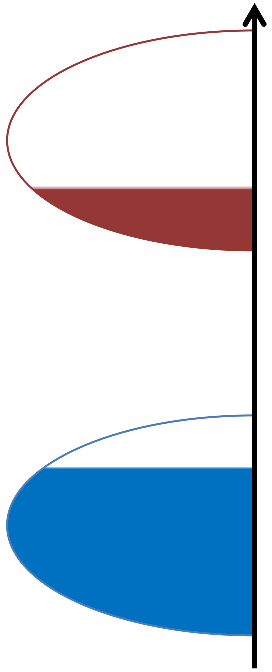
N. Strohmaiser, et. al., PRL **104**, 080401 (2010).
R. Sensarma, et. al., PRB **82**, 224302 (2010).
A. Rosch, et. al., PRL **101**, 265301 (2008).

Just after excitation



- (Approximate) conservation of doublons and holons
- Intraband relaxation + Cooling via environment

Metastable steady state



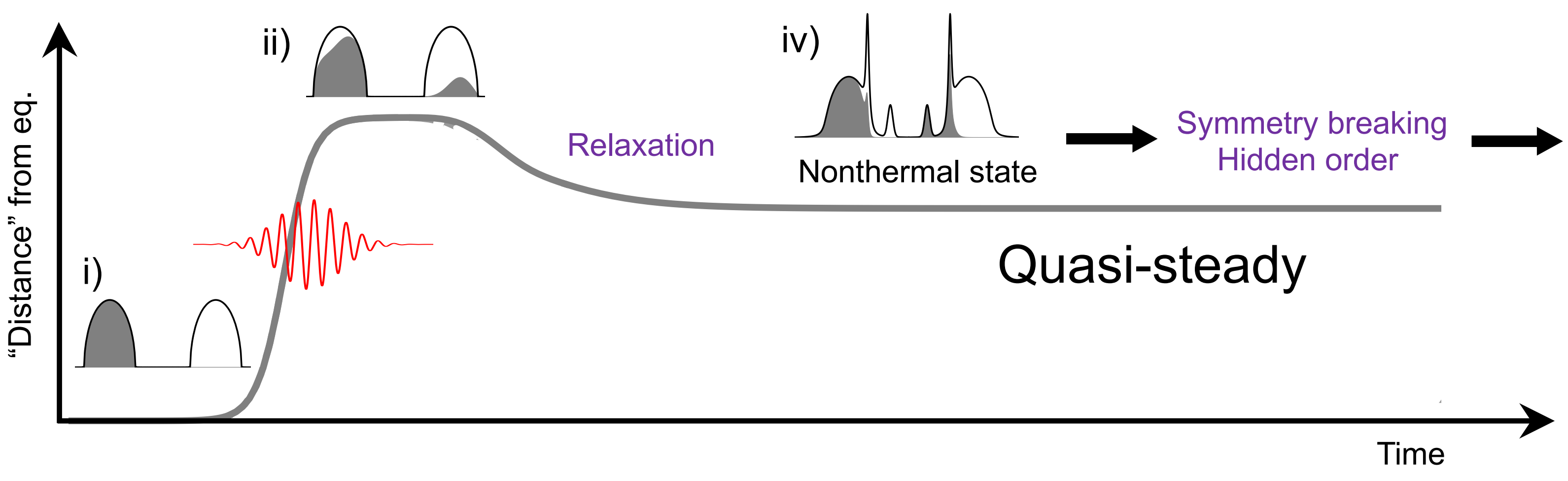
General question & three complementary approaches

What kinds of metastable states emerge in photo-doped Mott insulators?

Review: YM, D Golež, M Eckstein, P Werner, arXiv:2310.05201

1) Direct time-evolution

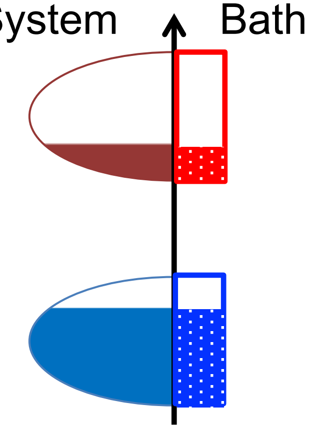
Methods:
Exact Diagonalization,
Tensor network,
Dynamical mean-field theory,
etc…



2) Quasi-NESS approach

Approximate quasi-steady state with a true steady state supported by external bath

J. Li, et. al., PRB **102**, 165136 (2020).
J. Li and M. Eckstein, PRB **103** 045133 (2021).



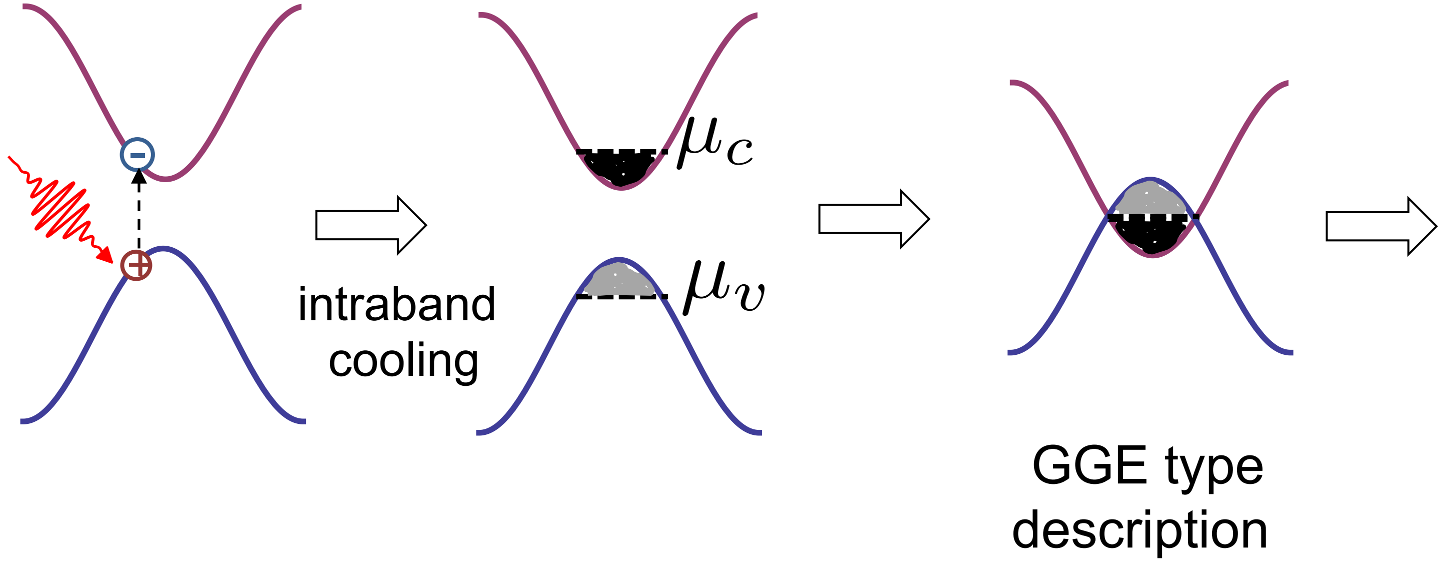
3) Quasi-equilibrium approach

- ▷ Analogous to photo-doped semiconductor
- ▷ Mainly used in this talk

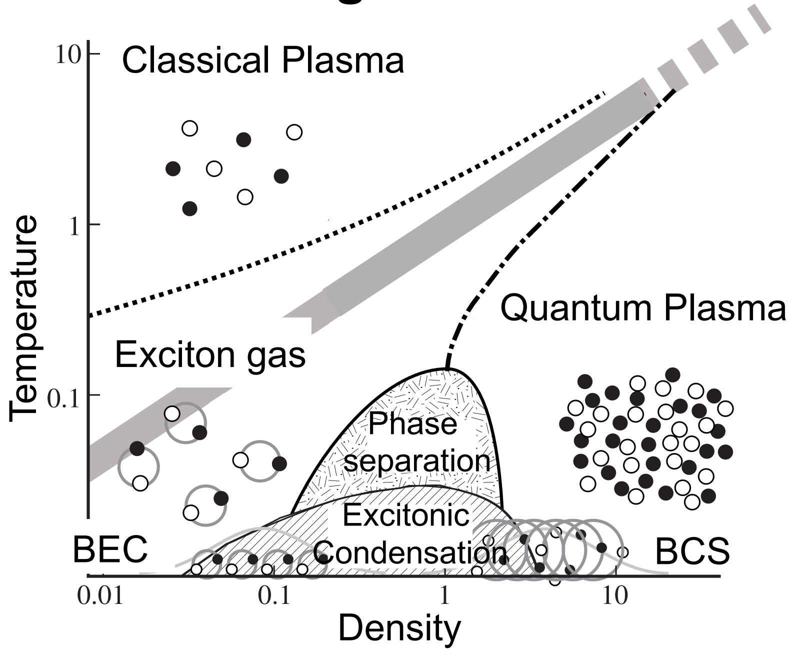
A. Rosch, et. al., PRL **101**, 265301 (2008).
Y. Kanamori, et al., PRL 107, 167403 (2011).
YM, et. al., Comm. Phys. 5, 23 (2022).

Quasi-equilibrium approach for photo-doped semiconductors

K. Asano, Bussei Kenkyu (2013).
L. V. Keldysh, *Contemporary Phys.* **27**, 395 (1986).



Phase diagram



Conservation of electrons and holes ⇒ Effective equilibrium problem

Effective chemical potential & temperature
"μ_c, μ_v, T_{eff}"

Strongly correlated systems?

Quasi-equilibrium description for strongly correlated systems

YM, et. al., Comm. Phys. **5**, 23 (2022).

Step1

Apply the Schrieffer-Wolff transformation (1/U expansion)

Original Hamiltonian: $\hat{H}$

⇩

Effective model with conserved local multiplets dressed with virtual fluctuation

Effective Hamiltonian: $\hat{H}_{\mathrm{eff}}$

ex) doublons, holons

Step2

Introducing **chemical potential** for local multiplets and effective temperature

$$\hat{K}_{\mathrm{eff}} = \hat{H}_{\mathrm{eff}} - \sum_{g \in \mathrm{ps}} \mu_g \hat{n}_g \qquad \hat{\rho}_{\mathrm{eff}} = \exp(-\beta_{\mathrm{eff}} \hat{K}_{\mathrm{eff}})$$

GGE type description

Step3

Solve the effective problem with existing **equilibrium** methods

Example : Extended Hubbard model

$$\hat{H} = -v \sum_{\langle i,j \rangle,\sigma} \hat{c}_i^\dagger \hat{c}_j + \hat{H}_U + \hat{H}_V$$

with

$$\hat{H}_U = U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

$$\hat{H}_V = V \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

$$U \gg v, V$$

Effective model with conserved local multiplets and effects of virtual fluctuation

$$\hat{H}_{\mathrm{eff}} = \hat{H}_U \quad \leftarrow \quad \mathcal{O}(U)$$

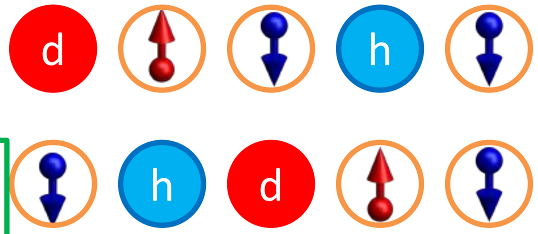
$$+ \hat{H}_{\mathrm{kin,LHB}} + \hat{H}_{\mathrm{kin,UHB}} \quad \leftarrow \quad \mathcal{O}(v)$$

$$+ \hat{H}^{(2)}_{U,\mathrm{shift}} + \boxed{\hat{H}_{\mathrm{spin,ex}}} + \boxed{\hat{H}_{\mathrm{dh,ex}}} + \boxed{\hat{H}^{(2)}_{\mathrm{kin,LHB}} + \hat{H}^{(2)}_{\mathrm{kin,UHB}} + \hat{H}^{(2)}_{\mathrm{dh,slide}}} + \boxed{\hat{H}_V}$$

$\mathcal{O}(J_{\mathrm{ex}})$ $\quad J_{\mathrm{ex}} = \frac{4v^2}{U}$

3 site terms

4 types of pseudo-particles



Exchange coupling for spins

$$\hat{H}_{\mathrm{spin,ex}} = J_{\mathrm{ex}} \sum_{\langle i,j \rangle} \hat{\mathbf{s}}_i \cdot \hat{\mathbf{s}}_j$$

Exchange coupling for doublon-holon

$$\hat{H}_{\mathrm{dh,ex}} = -J_{\mathrm{ex}} \sum_{\langle i,j \rangle} \hat{\boldsymbol{\eta}}_i \cdot \hat{\boldsymbol{\eta}}_j$$

$$\hat{\eta}_i^+ = (-)^i \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow}^\dagger$$

$$\hat{\eta}_i^z = \frac{1}{2}(\hat{n}_i - 1)$$

Previous analysis : metastable η pairing phase

Cold atom with extreme doping

A. Rosch, et. al., PRL **101**, 265301 (2008).

Metastable state with doublon or holon

$$\hat{H}_{\mathrm{dh,ex}} = -J_{\mathrm{ex}} \sum_{\langle i,j \rangle} \hat{\boldsymbol{\eta}}_i \cdot \hat{\boldsymbol{\eta}}_j \qquad \hat{\eta}_i^+ = (-)^i \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow}^\dagger, \quad \hat{\eta}_i^z = \frac{1}{2}(\hat{n}_i - 1)$$

$SU_c(2)$ Symmetry

⇒

$$|\Psi\rangle = e^{-i\theta \sum_i S_i^x} |\Uparrow\Uparrow\ldots\rangle = e^{-i\frac{\theta}{2}\sum_i (-1)^i (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \mathrm{H.c.})} |0\rangle,$$

$$\cos\theta = 1 - 2n_d \qquad \langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle = \frac{(-1)^i}{2} \sin\theta$$

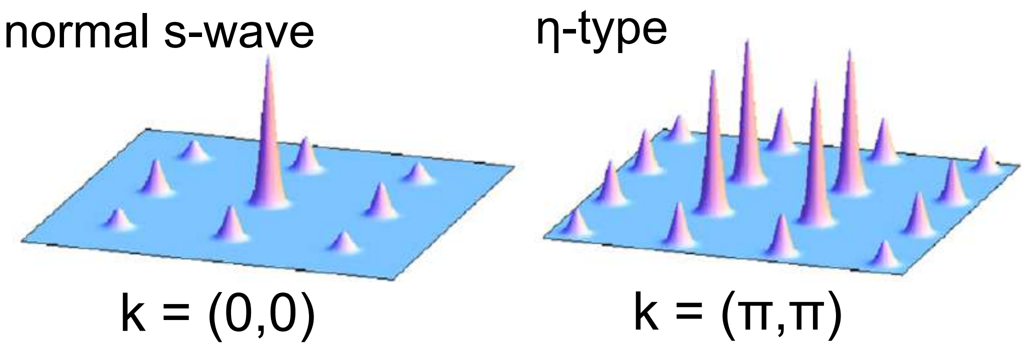
η paring state

Yang's η-pairing state

$$|\phi_{N_\eta}\rangle = \frac{1}{\sqrt{C_{N_\eta}}} (\hat{\eta}^+)^{N_\eta} |0\rangle$$

$$\hat{\eta}^+ = \sum_j (-1)^j \hat{c}_{j,\downarrow}^\dagger \hat{c}_{j,\uparrow}^\dagger = \sum_k \hat{c}_{\pi-k,\downarrow}^\dagger \hat{c}_{k,\uparrow}^\dagger$$

C. N. Yang, Phys. Rev. Lett. 63, 2144 (1989).



Momentum distribution of fermion pair

Photo-doped metastable states in 1D ?

Quasi-equilibrium approach for 1D extended Hubbard model

- ▷ Numerical analysis (A tensor network: iTEBD) — YM, et al., Comm. Phys. **5**, 23 (2022).
- ▷ Analytical discussion — YM, et al., Phys. Rev. Lett. **130**, 106501 (2023).

⇩

Main points

- ▷ Exact from of wave function of photo-doped states: $|\Psi\rangle = |\Psi^{\mathrm{GS}}_{\mathrm{SF}}\rangle|\Psi^{\mathrm{GS}}_{\mathrm{spin}}\rangle|\Psi^{\mathrm{GS}}_{\eta-\mathrm{spin}}\rangle$
- ▷ Spin, charge and η-spin separation
- ▷ Intuitive insight into physics of metastable states

Emergent degrees of freedoms by photo-doping lead to intriguing nonequilibrium phases!

Exact wave function of photo-doped metastable states

YM, et al., PRL. **130**, 106501 (2023).

Wave function @ $U \to \infty$, V/J_{ex} = const, $T_{eff}=0$

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

Spinless fermion (Position of Singlons)	Squeezed spin space	Squeezed η -spin space
$H_{\rm SF,free}$	$H^{\rm (SQ)}_{\rm spin}$	$H^{\rm (SQ)}_{\eta-{\rm spin}}$

- ▷ Extension of Ogata-Shiba state in equilibrium $|\Psi\rangle = |\Psi^{\rm GS}_{\rm SF}\rangle|\Psi^{\rm GS}_{\rm spin}\rangle$

M. Ogata & H. Shiba, PRB 41 2326 (1990).

- ▷ Spin, charge and η-spin separation
- ▷ Useful insight into physics

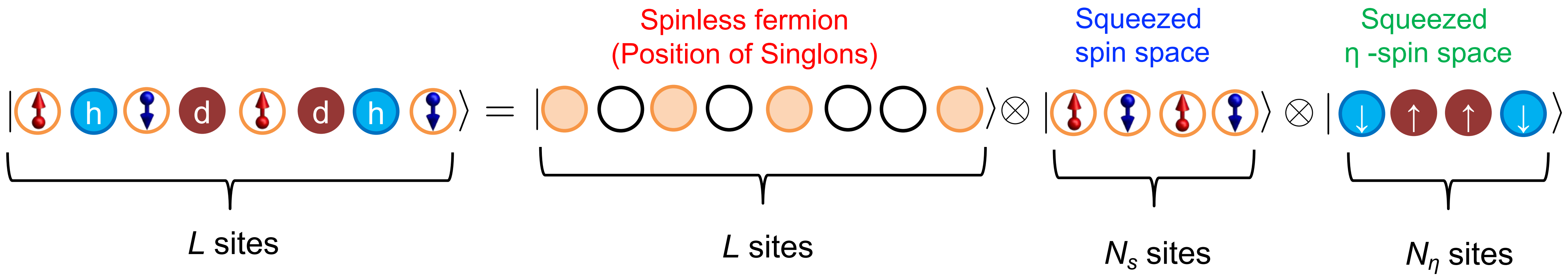
cf. V=0 limit
F Woynarovich,
J. Phys. C 15 97 (1982)

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

New expression of states: $\hat{U}$

L: System size
N_s: Number of singly occupied sites
N_η: Number of doublons and holons

YM, et al., PRL. **130**, 106501 (2023).



Hamiltonian for J_{ex} = 0 in the new expression

0 th order wave function

$$\hat{U}\hat{H}_{\mathrm{kin}}\hat{U}^{\dagger} = -t_{\mathrm{hop}}\sum_{\langle i,j\rangle}(\hat{c}_i^{\dagger}\hat{c}_j + \mathrm{h.c.})(\equiv \hat{H}_{\mathrm{SF,free}}) \Rightarrow |\Psi_{\mathrm{SF}}^{\mathrm{GS}}\rangle|\Psi_{\sigma,\eta}\rangle$$

i.e. Degeneracy of $2^{N_s}\cdot 2^{N_\eta}$

$|\Psi_{\sigma,\eta}\rangle$ is determined by degenerate perturbation theory

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

$\mathcal{O}(J_{\mathrm{ex}})$ terms projected to $|\Psi_{\mathrm{SF}}^{\mathrm{GS}}\rangle|\boldsymbol{\sigma}\rangle|\boldsymbol{\eta}\rangle$

YM, et al., PRL. **130**, 106501 (2023).

$$\hat{H}_{\mathrm{spin}}^{(\mathrm{SQ})} = J_{\mathrm{ex}}^{s}\sum_i \hat{\mathbf{s}}_{i+1}\cdot\hat{\mathbf{s}}_i,$$

$$\hat{H}_{\eta-\mathrm{spin}}^{(\mathrm{SQ})} = -J_X^{\eta}\sum_j(\hat{\eta}_{j+1}^{x}\hat{\eta}_j^{x}+\hat{\eta}_{j+1}^{y}\hat{\eta}_j^{y}) + J_Z^{\eta}\sum_j \hat{\eta}_{j+1}^{z}\hat{\eta}_j^{z},$$

with

$$J_{\mathrm{ex}}^{\mathrm{s}} = (\tilde{x}-\tilde{x}')J_{\mathrm{ex}}$$

$$J_X^{\eta} = (\tilde{y}-\tilde{y}')J_{\mathrm{ex}}$$

$$J_Z^{\eta} = -(\tilde{y}-\tilde{y}')J_{\mathrm{ex}} + 4\tilde{y}V$$

2-site terms

$$\tilde{x} = n_s - \frac{\sin^2(\pi n_s)}{\pi^2 n_s},$$

$$\tilde{y} = n_\eta - \frac{\sin^2(\pi n_\eta)}{\pi^2 n_\eta};$$

3-site terms

$$\tilde{x}' = \frac{\sin(2\pi n_s)}{2\pi} - \frac{\sin^2(\pi n_s)}{\pi^2 n_s},$$

$$\tilde{y}' = \frac{\sin(2\pi n_\eta)}{2\pi} - \frac{\sin^2(\pi n_\eta)}{\pi^2 n_\eta}.$$

n_s: Density of singly occupied sites
n_η: Density of doublons and holons

- ▷ spin and η-spin are separated
- ▷ Exchange couplings are renormalized

Summary

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

$H_{\mathrm{SF,free}}$ $\quad H_{\mathrm{spin}}^{(\mathrm{SQ})}$ $\quad H_{\eta-\mathrm{spin}}^{(\mathrm{SQ})}$

Indication to nonequilibrium phases

YM, et al., PRL. **130**, 106501 (2023).

η-spin sectors — Described by the XXZ model ⇨ Two types of phases

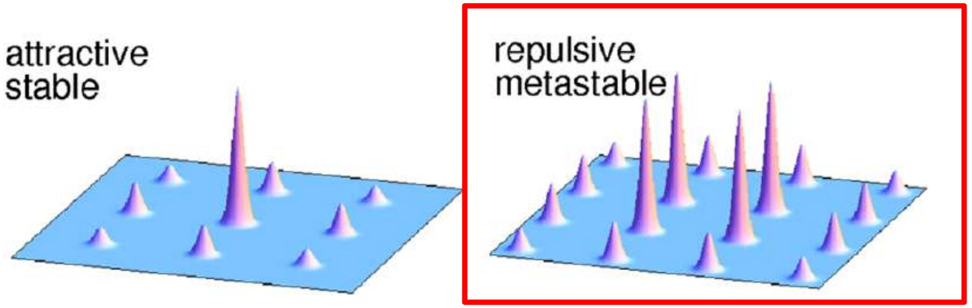
$J_Z < J_X$: Gapless phase of the XXZ model

η-pairing state with slowly decaying

$$\chi_{\mathrm{pair}}(r) \equiv \langle \hat{\eta}^x(r)\hat{\eta}^x(0)\rangle$$

※ Alternating sign in definition of $\hat{\eta}_i^+ = (-)^i \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow}^\dagger$

⇨ **usual pair correlations are staggered**



A. Rosch, et. al., PRL **101**, 265301 (2008).

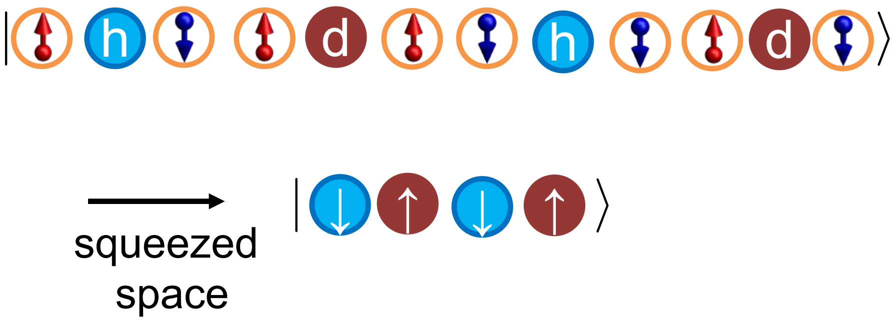
$J_Z > J_X$: Gapful phase of the XXZ model

CDW state with slowly decaying

$$\chi_{\mathrm{charge}}(r) \equiv \langle \hat{\eta}^z(r)\hat{\eta}^z(0)\rangle$$

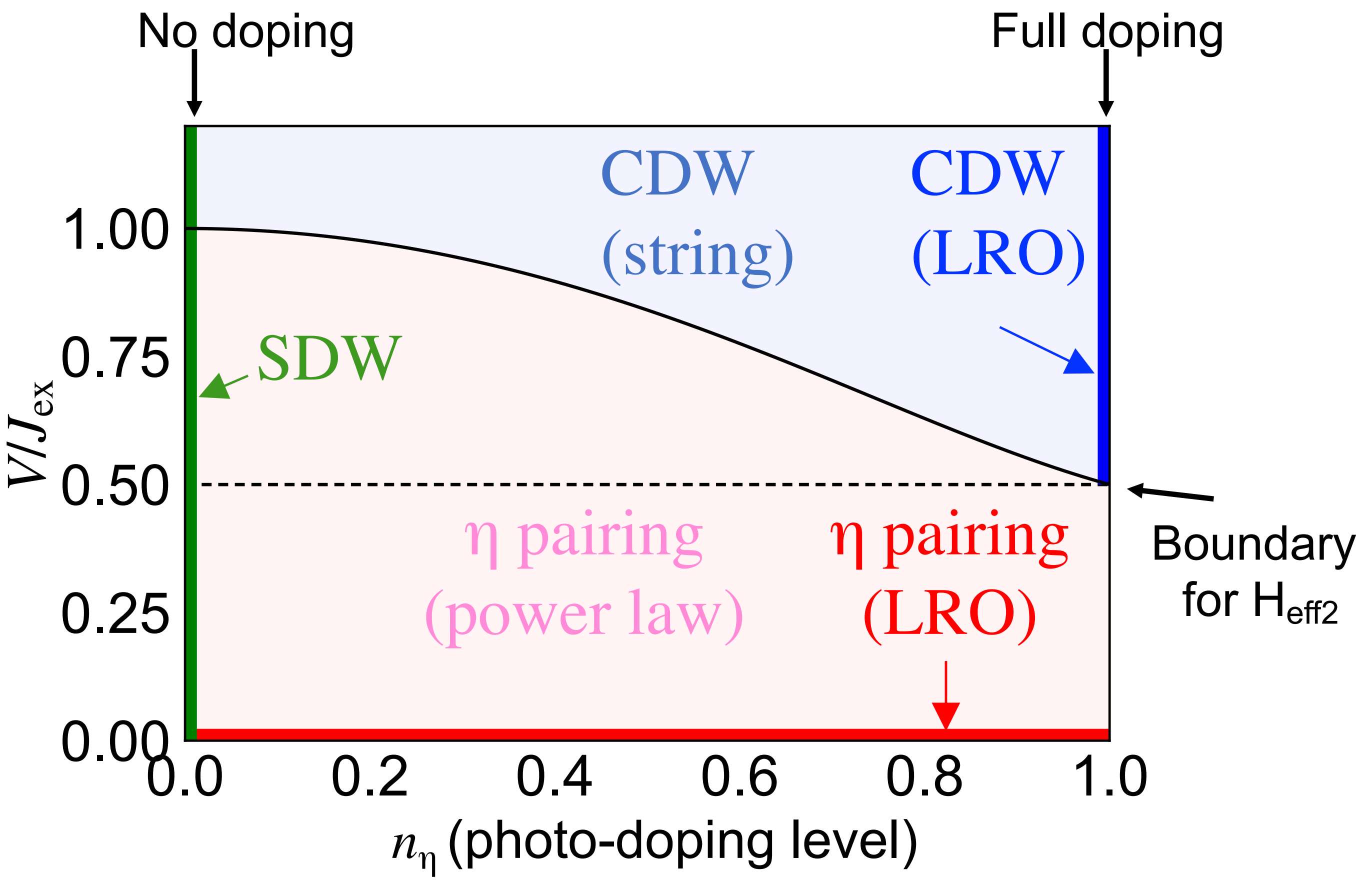
※ Long range order in the squeezed η spin space

⇨ **String type order** cf. Haldane phase

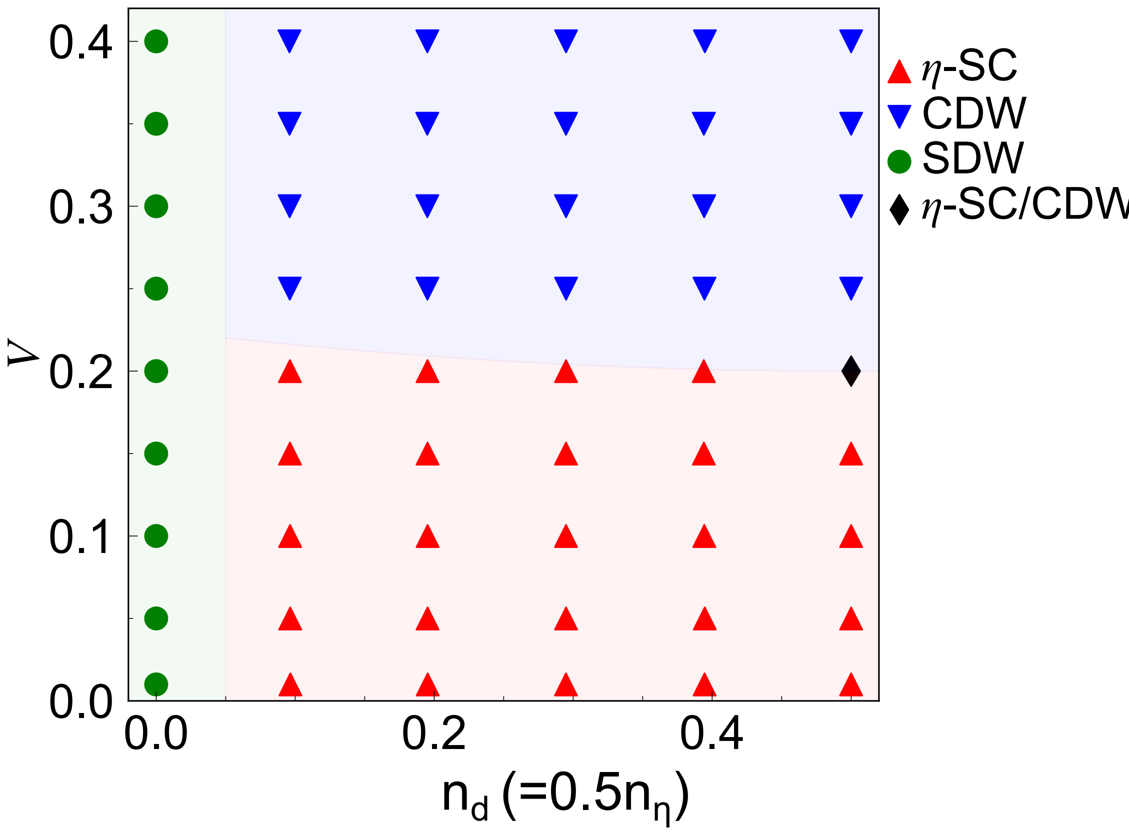


Phase diagram of the photo-doped states at $T_{eff} = 0$

U→∞ phase diagram @ half-filling



iTEBD results for H_{eff2} with $J_{ex} = 0.4$



- ▹ 3 site terms favor η pairing phase
- ▹ Analytic argument well explains numerically obtained phase diagram for H_{eff2} (no 3 site terms)
- ▹ Picture at U→∞ works well even for finite U

Insight into total central charge

Total central charge (**c**) ~ Number of massless modes

$$|\Psi\rangle = \underbrace{|\Psi^{\mathrm{GS}}_{\mathrm{SF}}\rangle}_{H_{\mathrm{SF,free}}} \underbrace{|\Psi^{\mathrm{GS}}_{\mathrm{spin}}\rangle}_{H^{(\mathrm{SQ})}_{\mathrm{spin}}} \underbrace{|\Psi^{\mathrm{GS}}_{\eta-\mathrm{spin}}\rangle}_{H^{(\mathrm{SQ})}_{\eta-\mathrm{spin}}}$$

- ▹ **Charge (SF) sector**: gapless
- ▹ **Spin sector**: gapless
- ▹ **η-spin sector:** { η pairing → gapless; CDW → gapful

⇒ **η pairing: c=3 ? & CDW: c=2 ?**

Total central charge: iTEBD analysis for H_{eff2}

Scaling analysis

J. A. Kjäll, et al., PRB **87**, 235106 (2013).

$$S_E = \frac{c}{6}\ln(\xi_D) + s_0$$

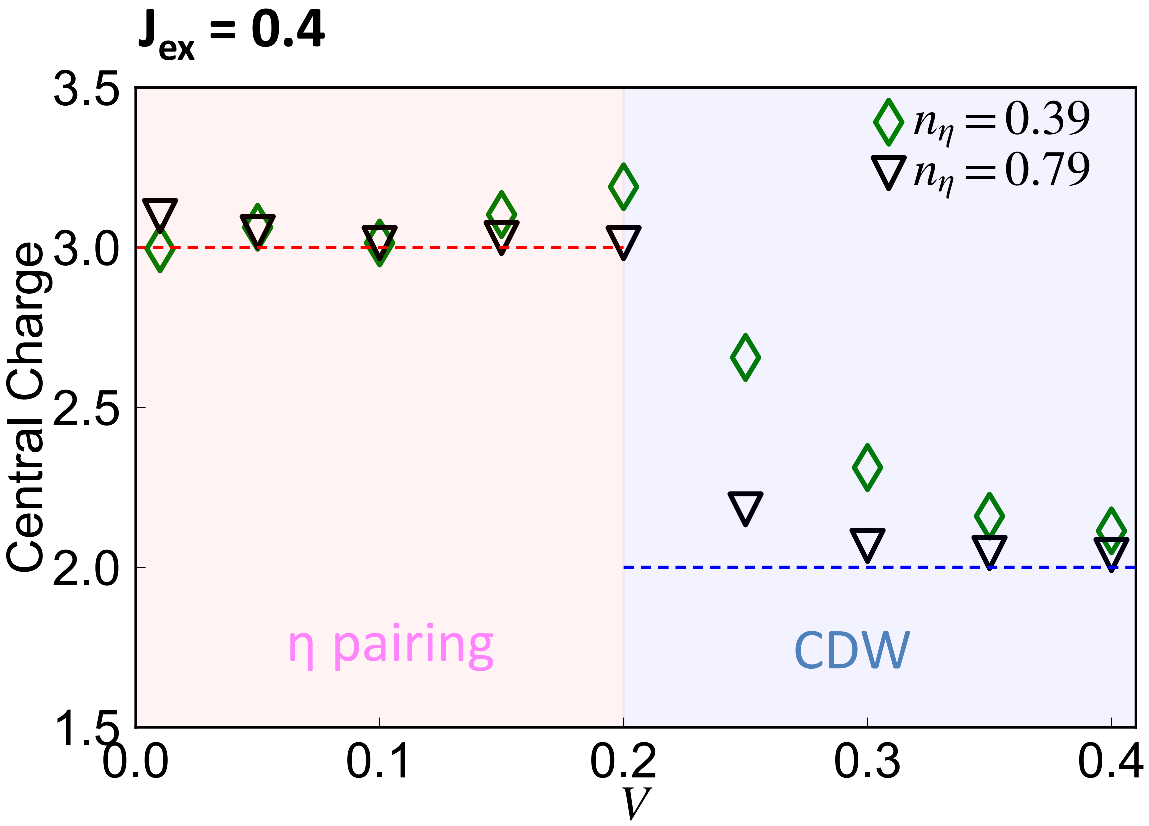
c: central charge

D: cut-off dimension

ξ_D: correlation length at D

S_E: entanglement entropy at D

η pairing: c=3 & CDW: c=2



c=3 in single-band Hubbard model is not expected in equilibrium

⇩

Emergence of extra degrees of freedom by photo-doping!

Naïve expectation of single-particle spectrum

$$A_k(\omega) = -\frac{1}{\pi}\mathrm{Im}G_k^R(\omega) \quad \text{with} \quad G_k(t,t') = -i\langle \mathcal{T} c_k(t) c_k^\dagger(t') \rangle$$

Equilibrium doped system

Electron = charge (SF) degree + spin degree

gapless gapless

⇨ **Gapless** around Fermi level

Photo-doped system

Electron = charge (SF) degree + spin degree + η spin degree

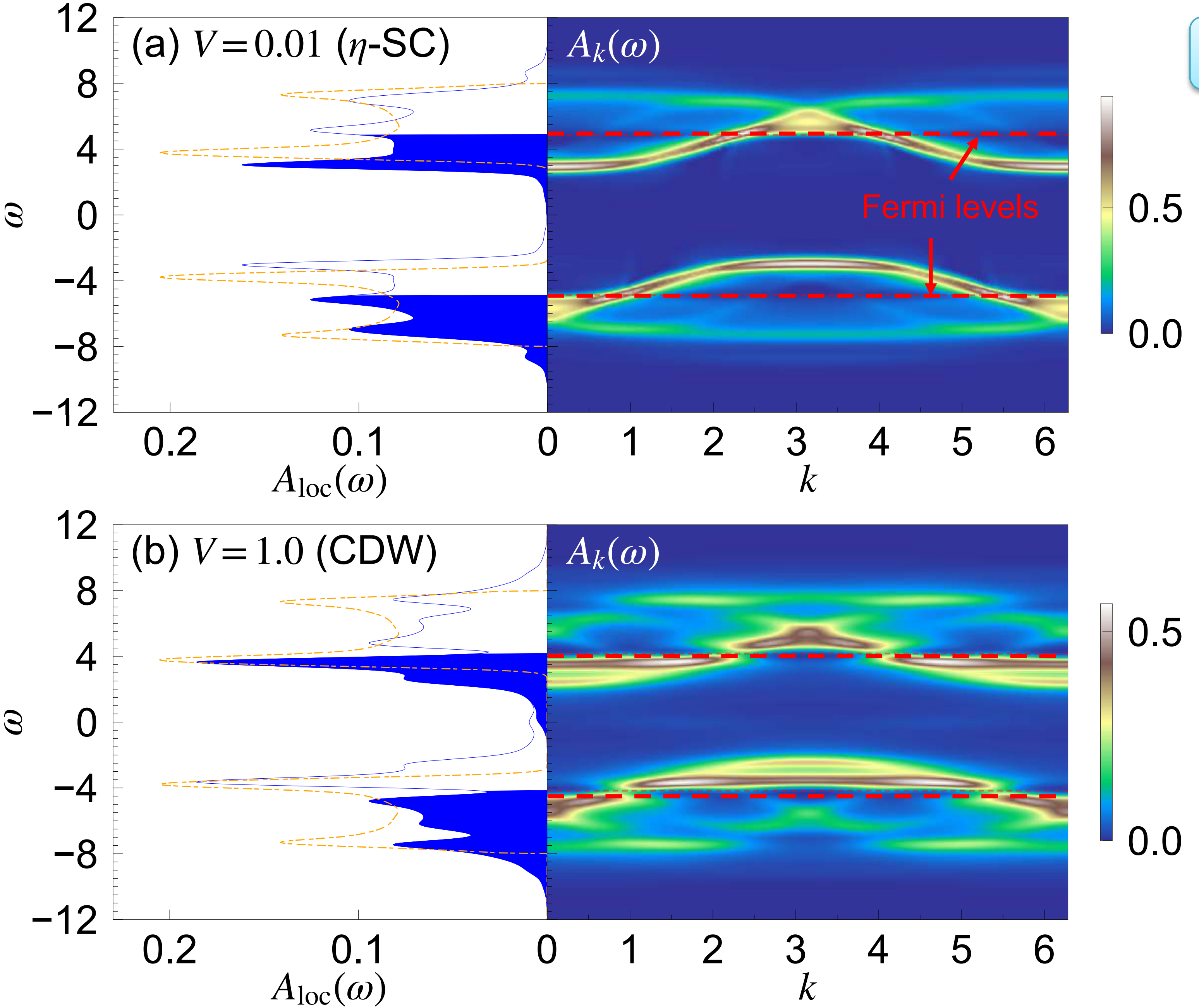
gapless gapless η pairing: gapless

CDW: gapful

⇨ η pairing phase : **Gapless** around Fermi level ?

CDW phase : **Gapful** around Fermi level ?

Single particle spectra for η pairing state and CDW state



η pairing state

No gap close to the Fermi level

⇨ Gapless SC

cf. DMFT J. Li et al, Mod. Phys. Lett B (2022)

CDW

Finite Gap at the Fermi level

Summary

Large gap Mott system ⇨ Approximate conservation of charge carriers ⇨ Quasi steady states

Photo-doped states in 1D extended Hubbard model

- ▹ Extension of Ogata-Shiba state in equilibrium : $|\Psi\rangle = |\Psi_{\mathrm{SF}}^{\mathrm{GS}}\rangle|\Psi_{\mathrm{spin}}^{\mathrm{GS}}\rangle|\Psi_{\eta-\mathrm{spin}}^{\mathrm{GS}}\rangle$
- ▹ Spin, charge and η-spin separation
- ▹ Intuitive insight into physics of metastable states

YM, et al., Comm. Phys. **5**, 23 (2022):

YM, et al., PRL. **130**, 106501 (2023).

Emergent degrees of freedoms by photo-doping lead to intriguing nonequilibrium phases!

Review on nonequilibrium Mott insulators: YM, D Golež, M Eckstein, P Werner, arXiv:2310.05201