Spin and Charge Excitations in Stripe-Ordered Cuprates

Takami Tohyama

Department of Applied Physics
Tokyo University of Science

Tokyo University of Science, Japan

Kenji Tsutsui QST

Shigetoshi Sota RIKEN

Michiyasu Mori JAEA

Outline

- Charge stripes in hole-doped cuprates

- Dynamical density-matrix renormalization group (DDMRG) calculations of dynamical spin and charge structure factors for a 24x4 *t*-*t'*-*J* ladder

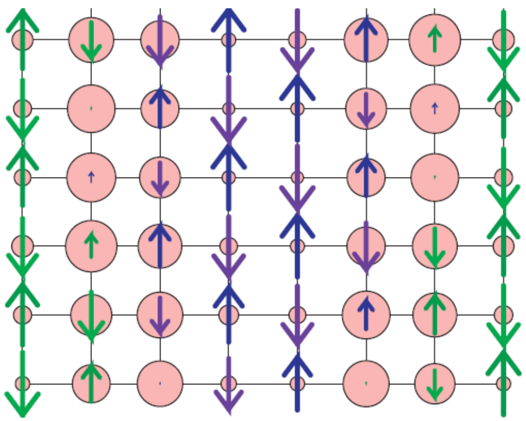
- Comparison with RIXS experiments and some implication for electron-doped cuprates

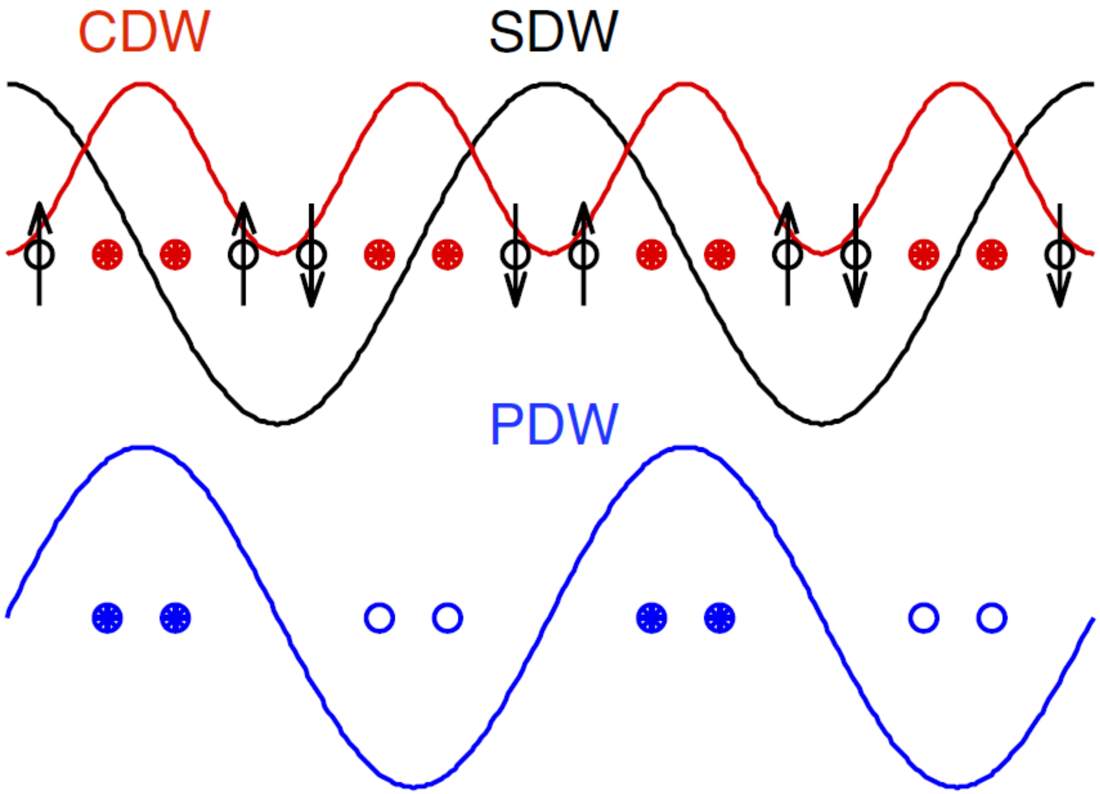
T.T., M. Mori, and S. Sota, Phys. Rev. B **97**, 235137 (2018)

- Effect of dimensionality on dynamical spin and charge structure factors

- RIXS in one-dimensional extended Hubbard model

Schematic diagram of stripe order in 1/8-doped $La_{1.875}La_{0.125}CuO_4$



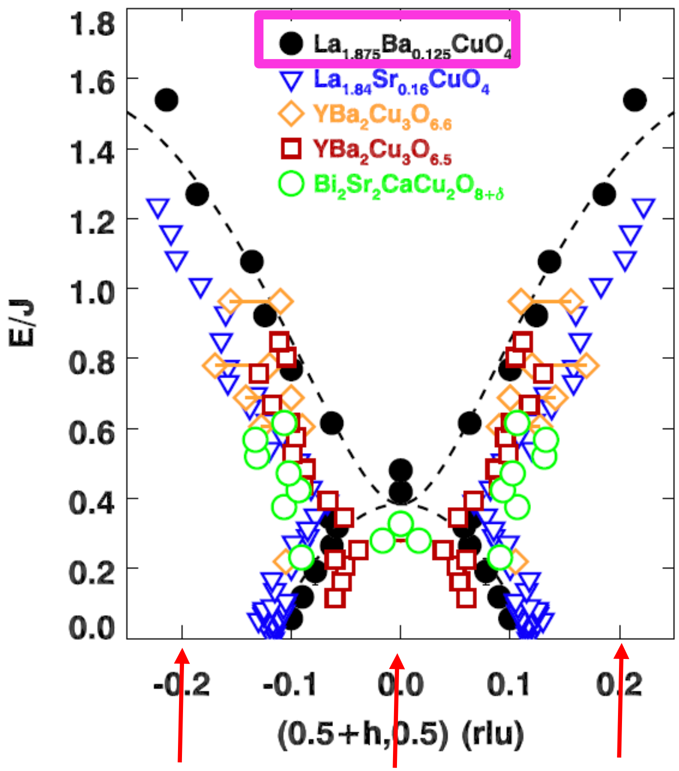


Review: M. Fujita *et al*., J. Phys. Soc. Jpn. **81**, 011007 (2012)

Spin dynamics in stripe-ordered hole-doped cuprates: experiments

Inelastic neutron scattering

"hourglass" around (π,π)



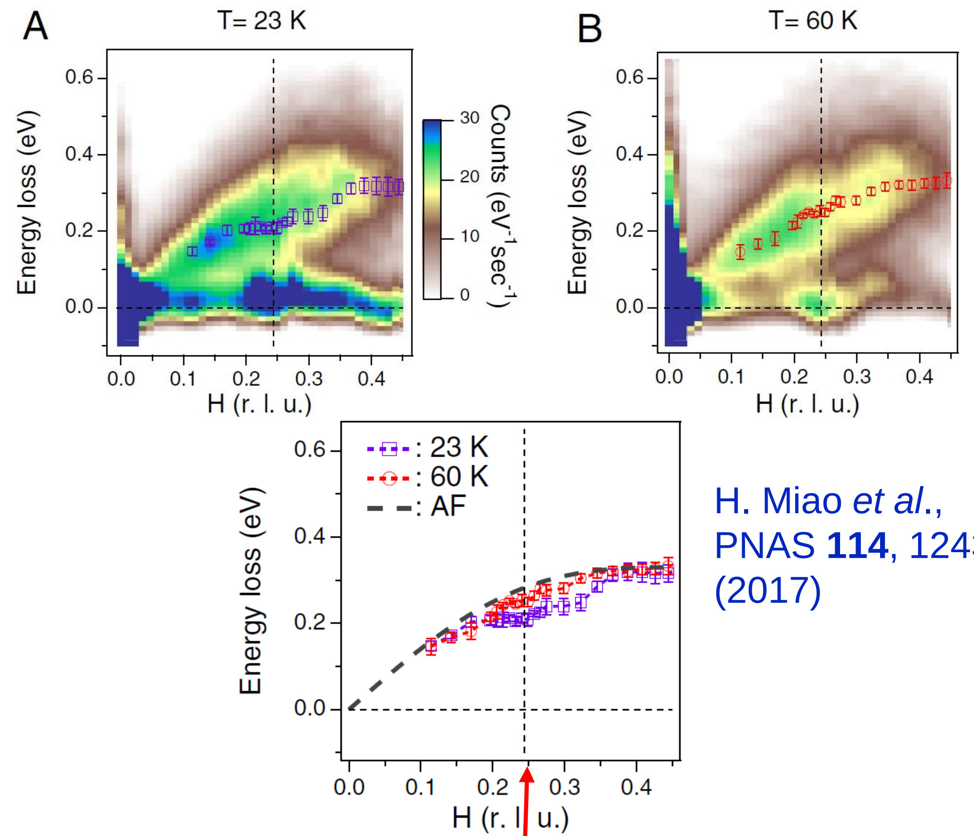
$(0.6\pi,\pi)$ (π,π) $(1.4\pi,\pi)$

M. Fujita *et al*., J. Phys. Soc. Jpn. **81**, 011007 (2012)

Resonant inelastic x-ray scattering

"plateau" around $(0.5\pi,0)$

stripe-ordered $La_{1.875}Ba_{0.125}CuO_4$

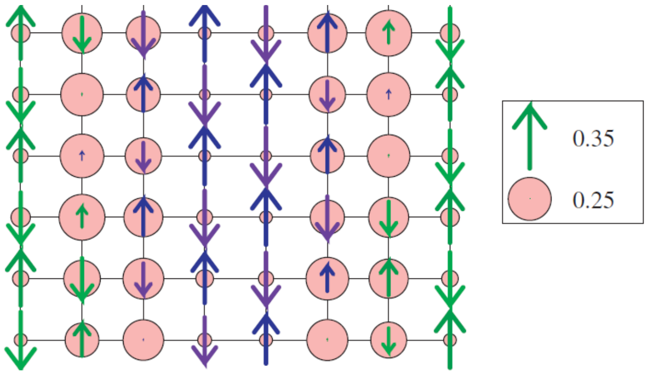


$(0.5\pi,0)$

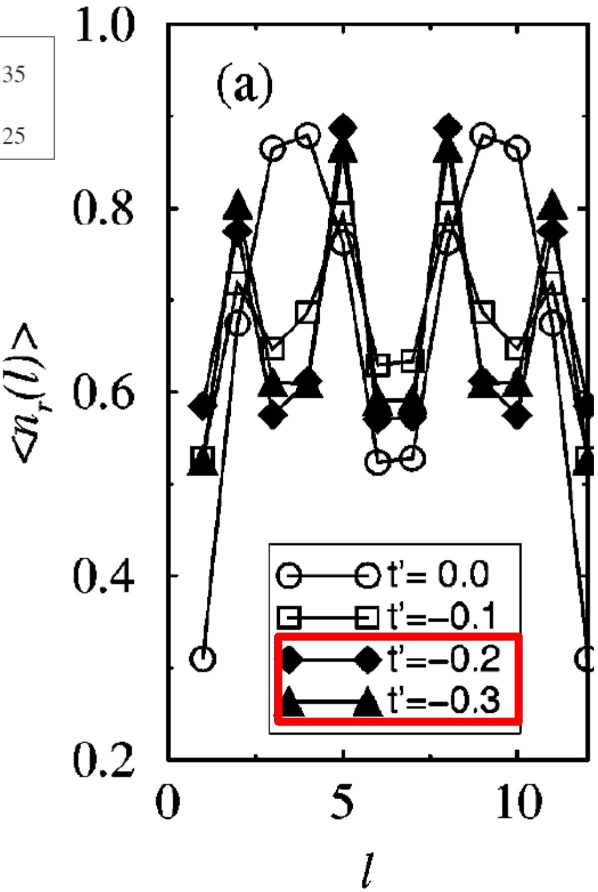
H. Miao *et al*., PNAS **114**, 12430 (2017)

Ground-state properties in the 1/8-hole-doped 12x4 *t-t′-J* ladder

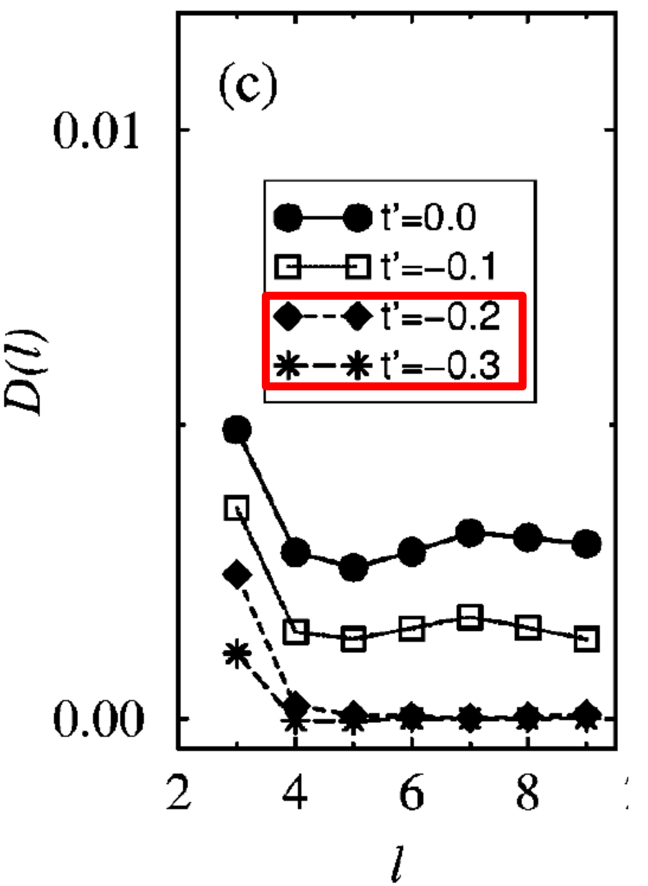
J/*t* = 0.35



charge density



d-wave paring correlation



S. White and D. J. Scalapino, PRB **60**, R753 (1999)

t-t'-J model

$$H_{tJ} = -t \sum_{<i,j>_1,\sigma} \tilde{c}^{+}_{i,\sigma}\tilde{c}_{j,\sigma} - t' \sum_{<i,j>_2,\sigma} \tilde{c}^{+}_{i,\sigma}\tilde{c}_{j,\sigma} + \text{h.c.} + J \sum_{<i,j>_1} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j \right)$$

Hole-doped four-leg *t-t'-J* ladder gives a charge-stripe order

S. White and D. J. Scalapino, PRB **60**, R753 (1999)

We calculate dynamical spin and charge structure factors

$$S(\mathbf{q},\omega) = -\frac{1}{\pi} \operatorname{Im} \langle 0 | S^{z}_{-\mathbf{q}} \frac{1}{\omega - H_{tJ} + E_0 + i\gamma} S^{z}_{\mathbf{q}} | 0 \rangle$$

$$N(\mathbf{q},\omega) = -\frac{1}{\pi} \operatorname{Im} \langle 0 | N_{-\mathbf{q}} \frac{1}{\omega - H_{tJ} + E_0 + i\gamma} N_{\mathbf{q}} | 0 \rangle$$

24x4 *t-t'-J* ladder

x (leg) direction → open boundary

y (rung) direction → periodic boundary

J/*t* = 0.4

t'/*t* = -0.25

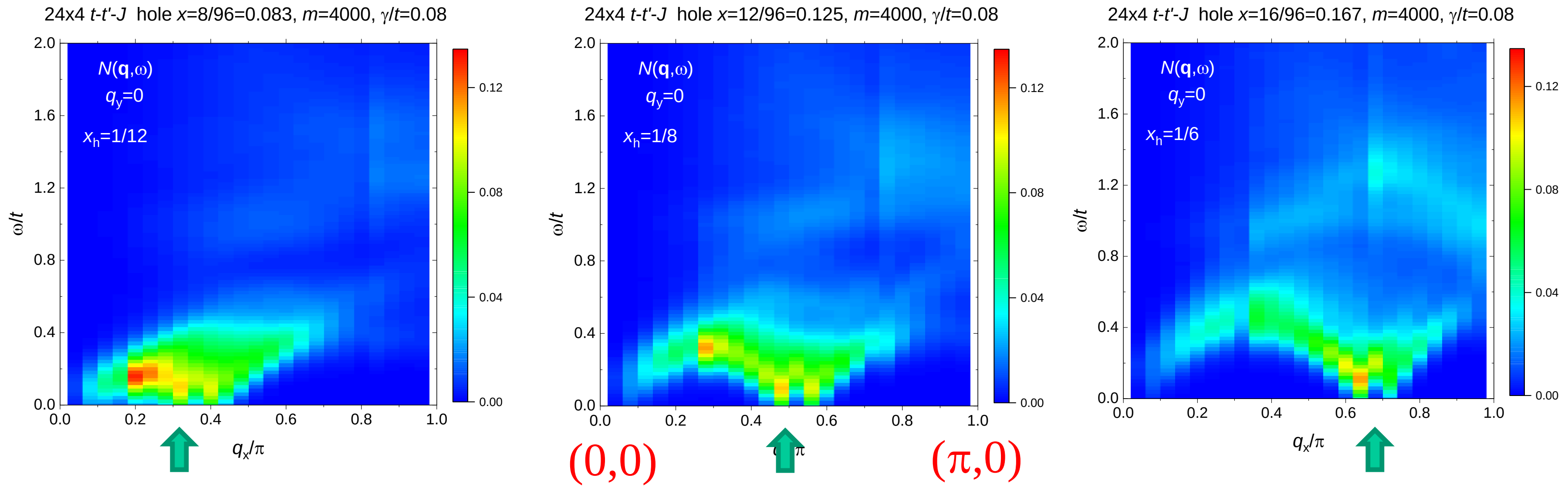
Dynamical density-matrix renormalization group (DDMRG)

T.T., M. Mori, and S. Sota, Phys. Rev. B **97**, 235137 (2018)

Dynamical charge structure factor in the 24x4 *t-t'-J* ladder

hole doping

x=1/12 *x*=1/8 *x*=1/6

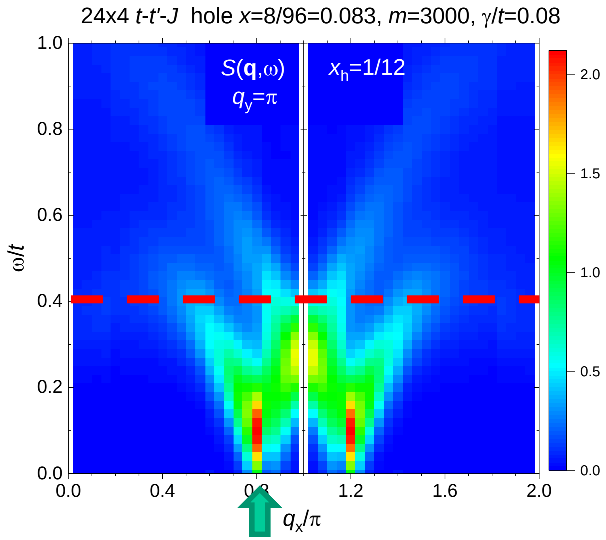


Minimum-energy position is close to $q_x = \pi(1-4x)$ as expected from stripe order.

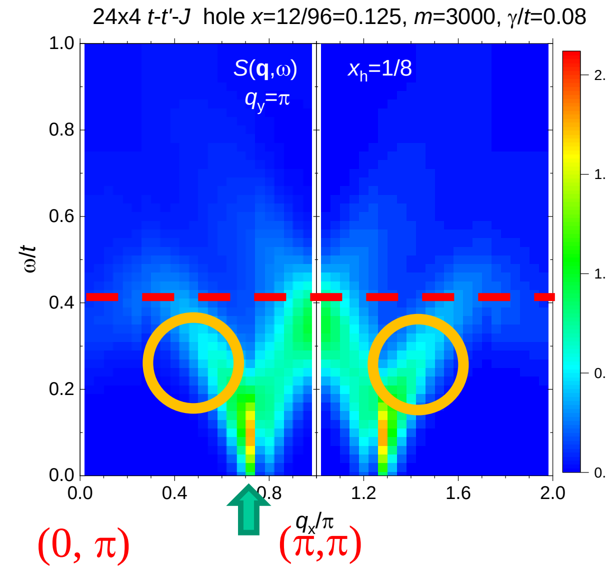
Dynamical spin structure factor in the 24x4 *t-t'-J* ladder

hole doping

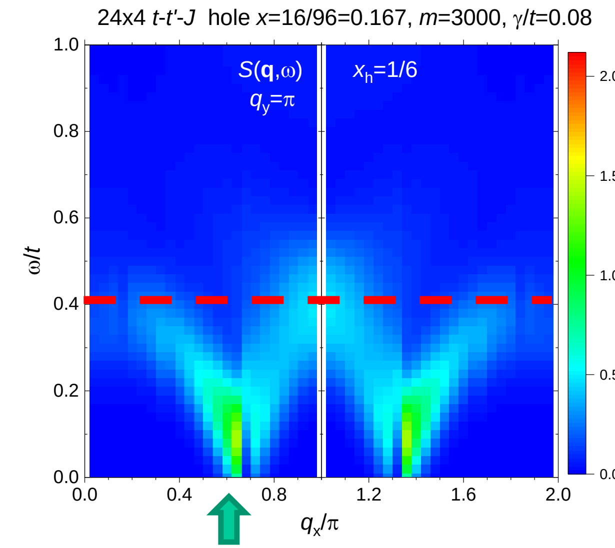
x=1/12

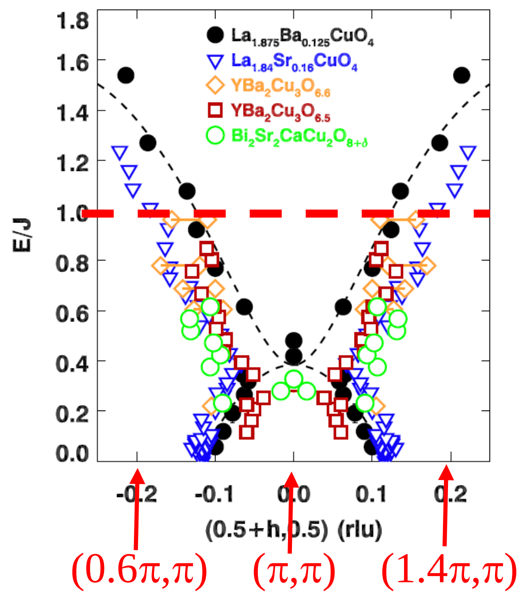


x=1/8



x=1/6



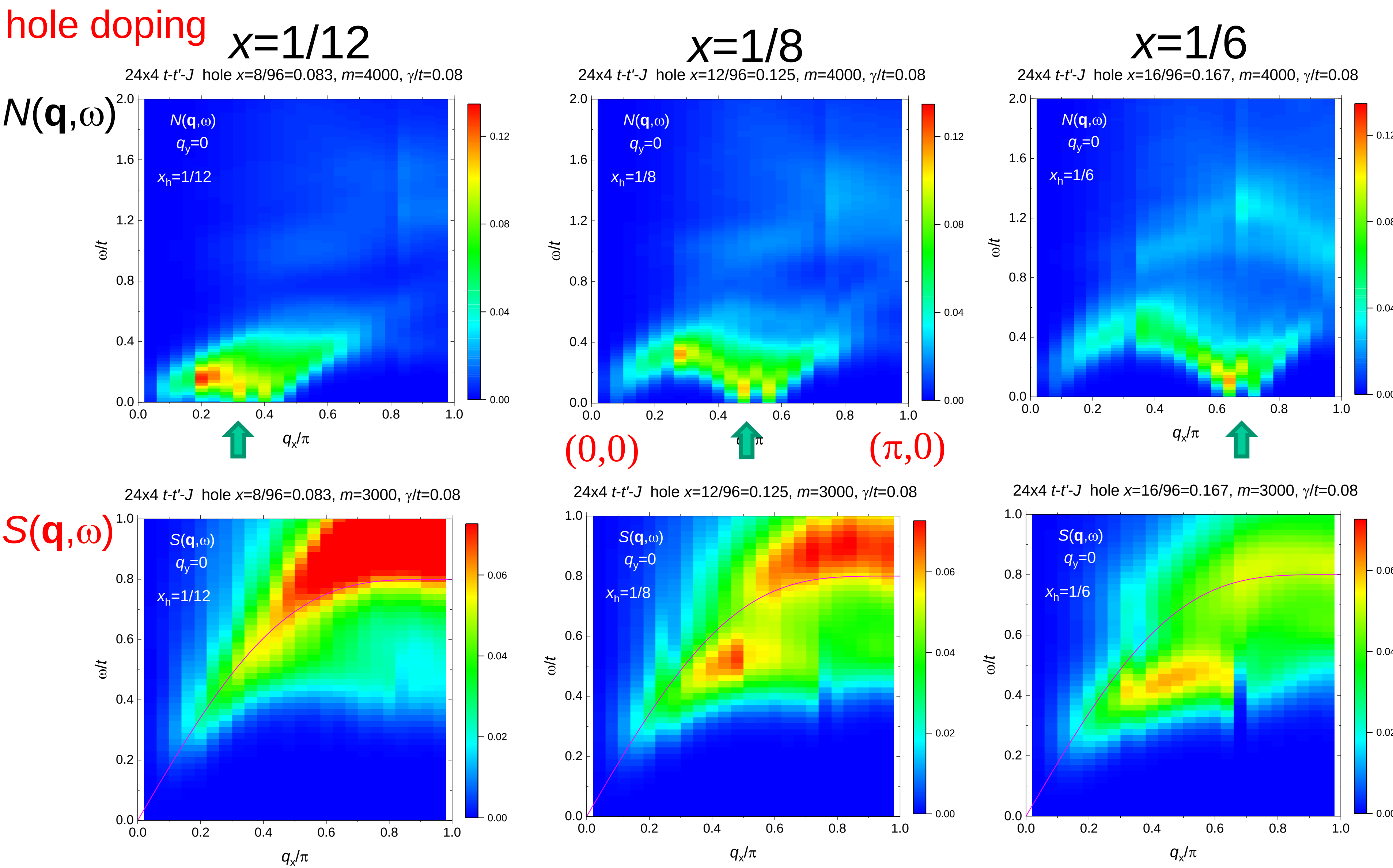


- Incommensurate q_x is $\pi(1-2x)$.

- Calculated $\mathbf{q}=(\pi,\pi)$ excitations are higher in energy than the experimental data.

- Strong "outward" weight, inconsistent with experiments

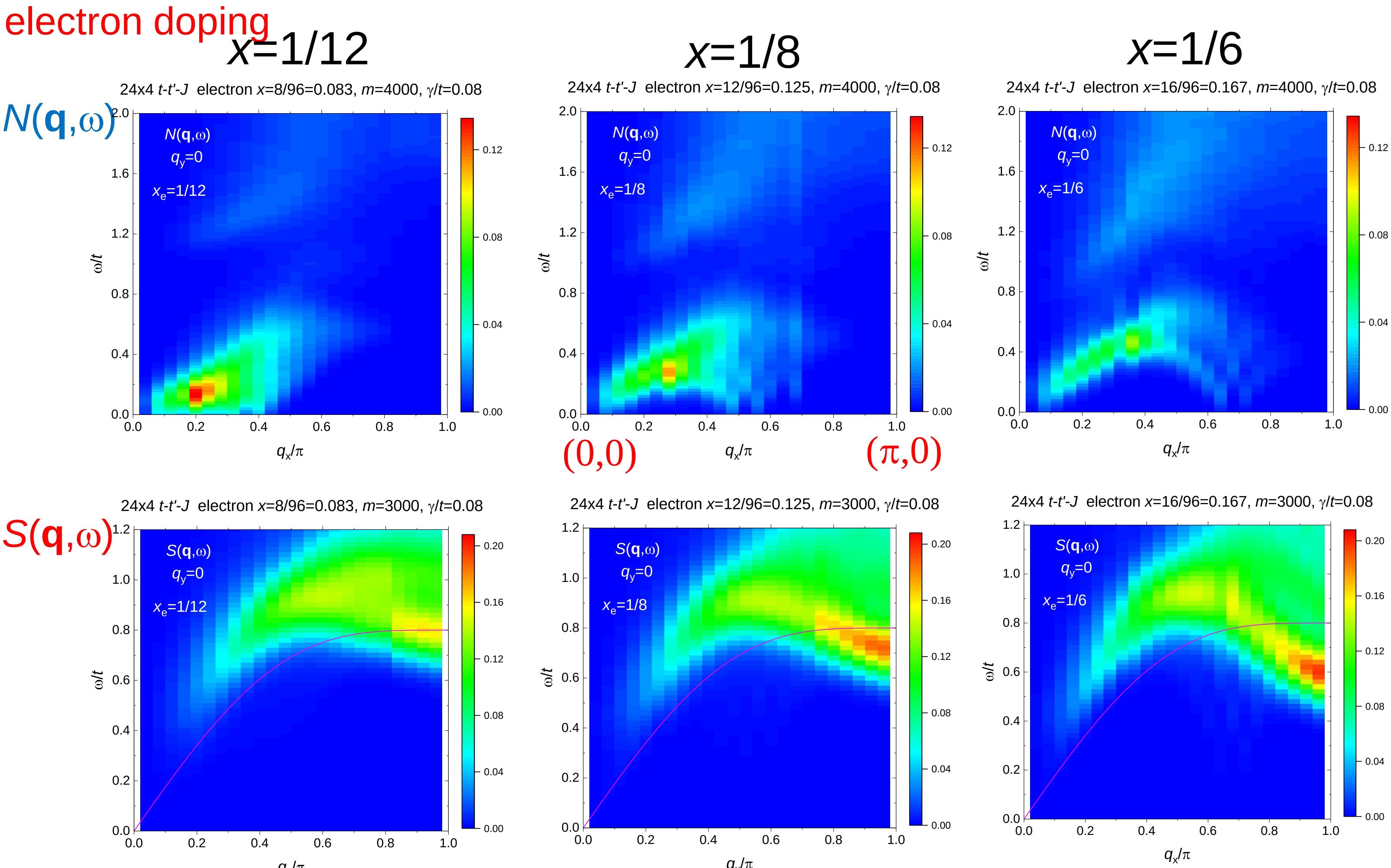
Dynamical charge and spin structure factor in the 24x4 *t-t'-J* ladder



- A step structure at the charge order vector q_x for x=1/8 and 1/6

→ strong coupling between charge and spin; ferromagnetic coupling across the stripes

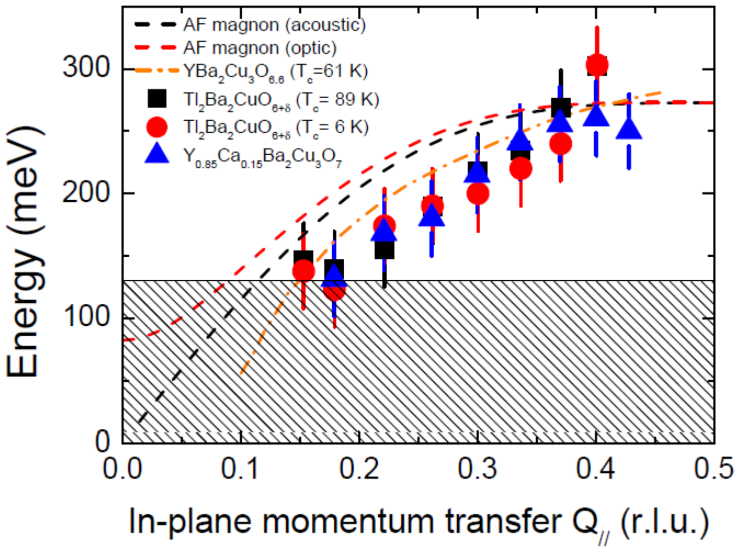
Dynamical charge and spin structure factor in the 24x4 *t-t′-J* ladder



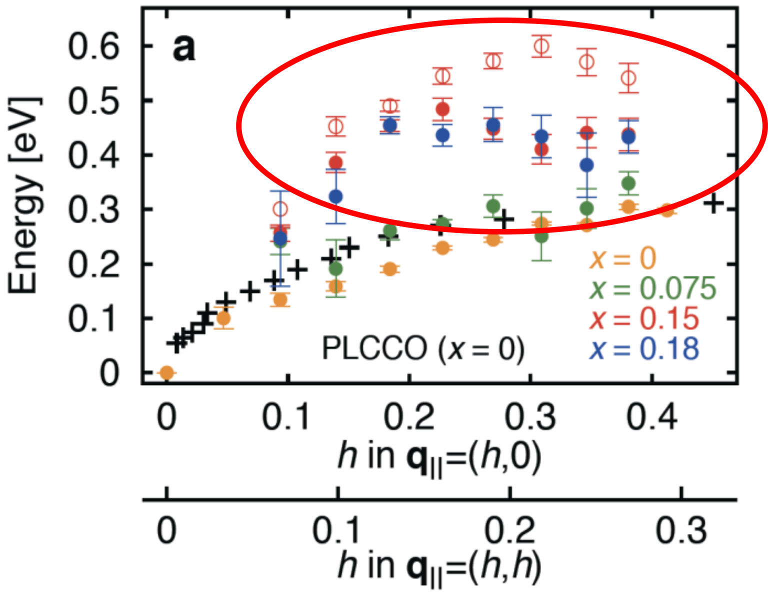
- No step-like structure in contrast to hole doping because of weak stripe order
- A downward spectral weight toward (π,0) → intrinsic for electron doping?

Doping dependence of magnetic excitation by RIXS

Hole doping



Electron doping



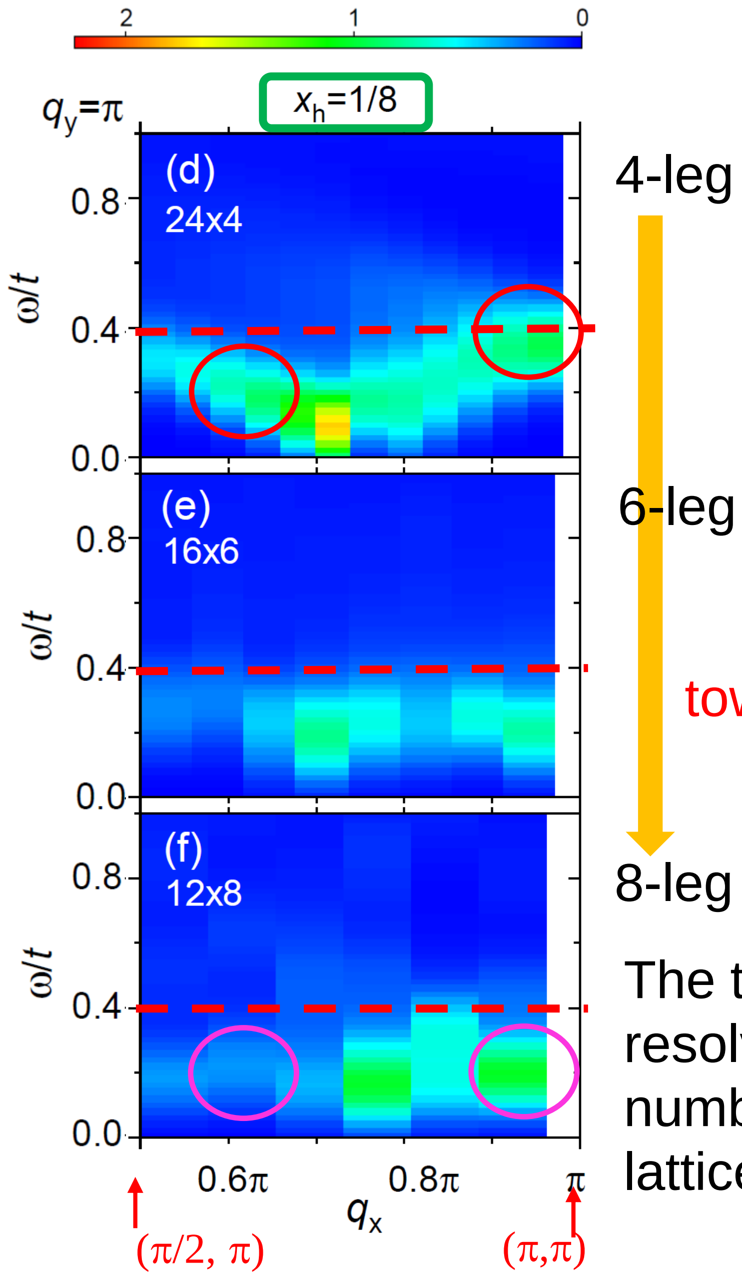
M. Le. Tacon *et al*., Nat. Phys. **7**, 725 (2011); PRB **88**, 020501(R) (2013)
M. P. M. Dean, JMMM **376**, 3 (2015)

K. Ishii, M. Fujita, T.T. *et al*., Nat. Commun. **5**, 3714 (2014)
W. S. Lee *et al*., Nat. Phys. **10**, 883 (2014)

Dynamical spin structure factor in the *t-t'-J* model

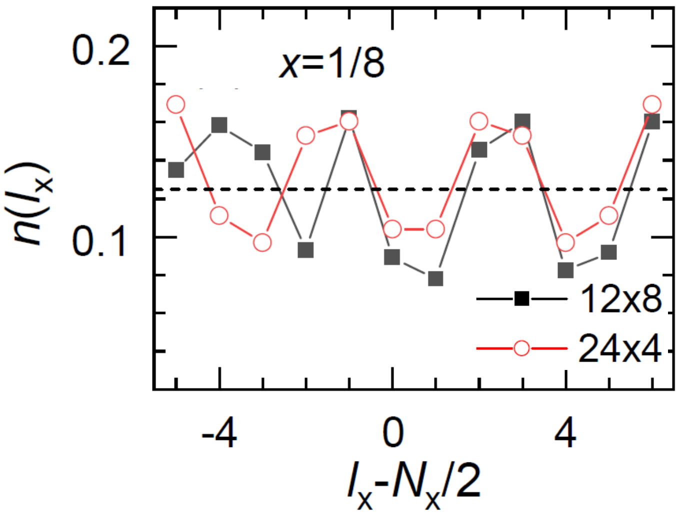
$S(\mathbf{q},\omega)$

J/t=0.4
t'/t=-0.25

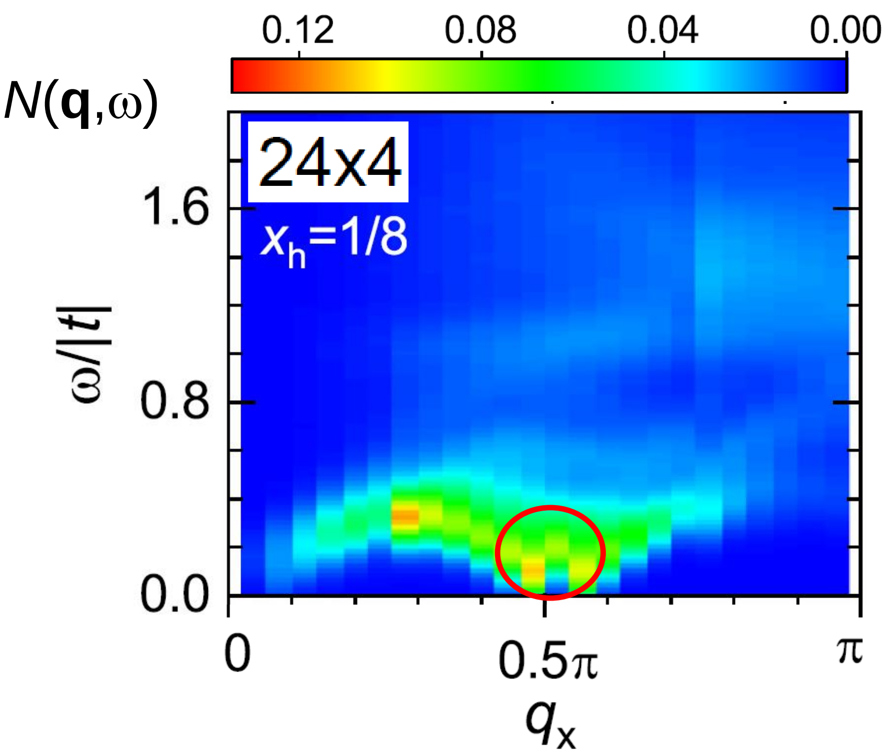


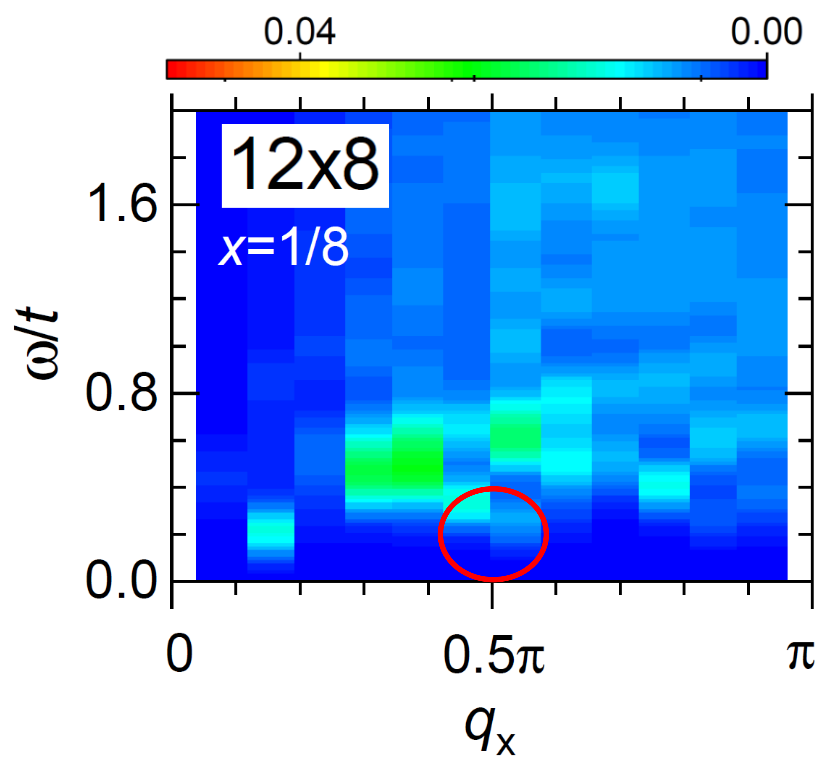
The two discrepancies are resolved with increasing leg number, i.e., toward square lattice.

Charge stripes from 4-leg to 8-leg ladders

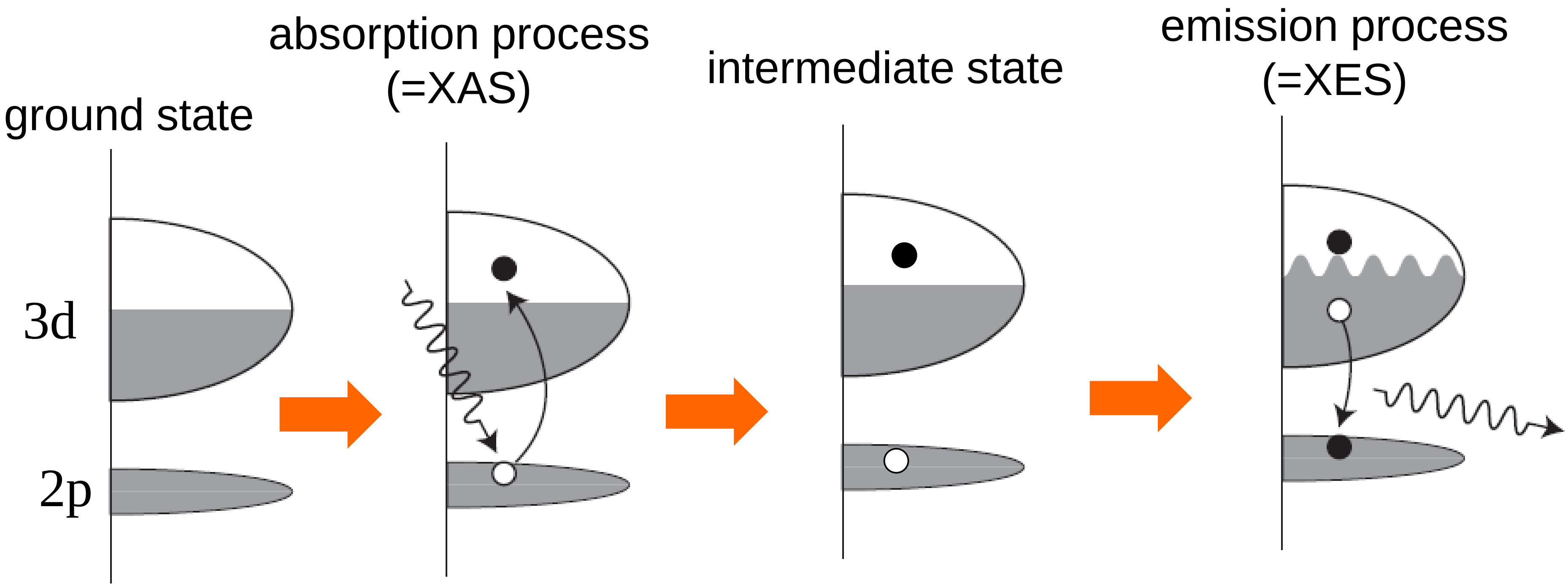


Weakening of stripes from 4-leg to 8-leg systems toward square lattice





RIXS for L-edge



$$I\left(\mathbf{q},\Delta\omega\right)\sim\sum_{f}\left|\left\langle f\right|D^{\dagger}_{\mathbf{k}_{\mathrm{o}},\varepsilon_{\mathrm{o}}}\frac{1}{\omega_{\mathrm{i}}-H+E_0+i\Gamma}D_{\mathbf{k}_{\mathrm{i}},\varepsilon_{\mathrm{i}}}\left|0\right\rangle\right|^2\delta\left(\Delta\omega-E_f+E_0\right)$$

$$\Delta\omega=\omega_{\mathrm{i}}-\omega_{\mathrm{o}}$$

$$\mathbf{q}=\mathbf{k}_{\mathrm{i}}-\mathbf{k}_{\mathrm{o}}$$

$\left|0\right\rangle$: ground state (no Cu2p hole)

$\left|f\right\rangle$: ‘final’ state with momentum q

$$D_{K_{\mathrm{i(o)}},\boldsymbol{\varepsilon}_{\mathrm{i(o)}}}=\sum_{\mu,\sigma,j_z}\left\langle 3d;\mu\sigma\right|\boldsymbol{\varepsilon}_{\mathrm{i(o)}}\cdot\mathbf{r}\left|2p;jj_z\right\rangle\sum_{\mathbf{k}}d^{+}_{\mathbf{k},\mu,\sigma}P_{\mathbf{k}-\mathbf{k}_{\mathrm{i(o)}},j,j_z}$$: dipole transition operator

RIXS for cuprates

Cu^{2+}: $3d^9$ 1 hole on x^2-y^2 orbital with in-plane spin orientation

$$\langle f | D^{\dagger}_{\mathbf{k}_o,\varepsilon_o} \frac{1}{\omega_i - H + E_0 + i\Gamma} D_{\mathbf{k}_i,\varepsilon_i} |0\rangle \quad \Rightarrow \quad \langle f | \alpha^j_N N^j_{\mathbf{q}} + \alpha^j_S S^j_{\mathbf{q}} |0\rangle$$

$$j = \frac{1}{2}, \frac{3}{2}$$

$$\boxed{N^j_{\mathbf{q}} = B^j_{\mathbf{q}\uparrow\uparrow} + B^j_{\mathbf{q}\downarrow\downarrow}}$$

Non spin-flip process

$$\boxed{S^j_{\mathbf{q}} = (B^j_{\mathbf{q}\uparrow\uparrow} - B^j_{\mathbf{q}\downarrow\downarrow})/2}$$

Spin-flip process

$$\boxed{B^j_{\mathbf{q}\sigma'\sigma} = \sum_l e^{-i\mathbf{q}\cdot\mathbf{R}_l} d^{\dagger}_{l\sigma'} \frac{1}{\omega_i - H^j_l + E_0 + i\Gamma} d_{l\sigma}}$$

$$H^j_l = H_{3d} + U_c \sum_\sigma n_{l\sigma} + \varepsilon_j$$

$$2\alpha_N^{j=1/2} = \alpha_N^{j=3/2} = \frac{2}{15}\left(\boldsymbol{\varepsilon}_o \cdot \boldsymbol{\varepsilon}_i - \boldsymbol{\varepsilon}_{oz}\boldsymbol{\varepsilon}_{iz}\right) \qquad \alpha_S^{j=1/2} = -\alpha_S^{j=3/2} = -\frac{2}{15} i\left[\boldsymbol{\varepsilon}_o \times \boldsymbol{\varepsilon}_i\right]_z$$

M. W. Haverkort, PRL **105**, 167404 (2010)
J. Igarashi and T. Nagao, PRB **85**, 064421 (2012)
S. Kourtis, J. van den Brink, and M. Daghofer, PRB **85**, 064423 (2012)

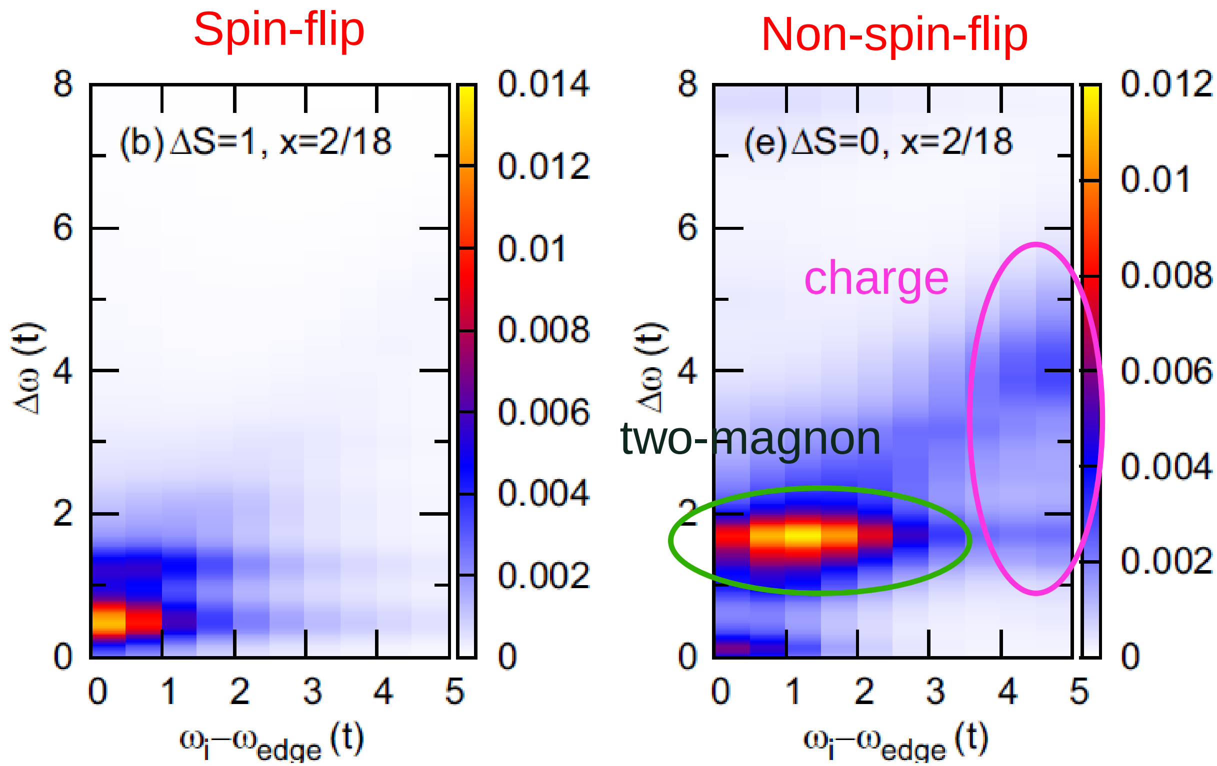
Incident-photon energy ω_i dependence of RIXS intensity

hole doping (11%)

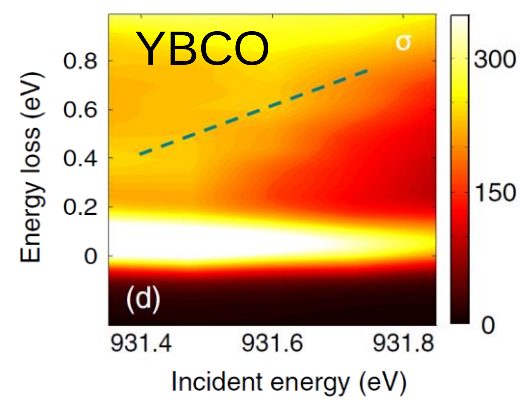
18 sites $t'=-0.25t$

$U=10t$ $U_{core}=12t$ $\Gamma=t$

K. Tsutsui, T.T., PRB **94**, 085144 (2016)



A change from “two-magnon” to “charge”
→ fluorescence-like behavior

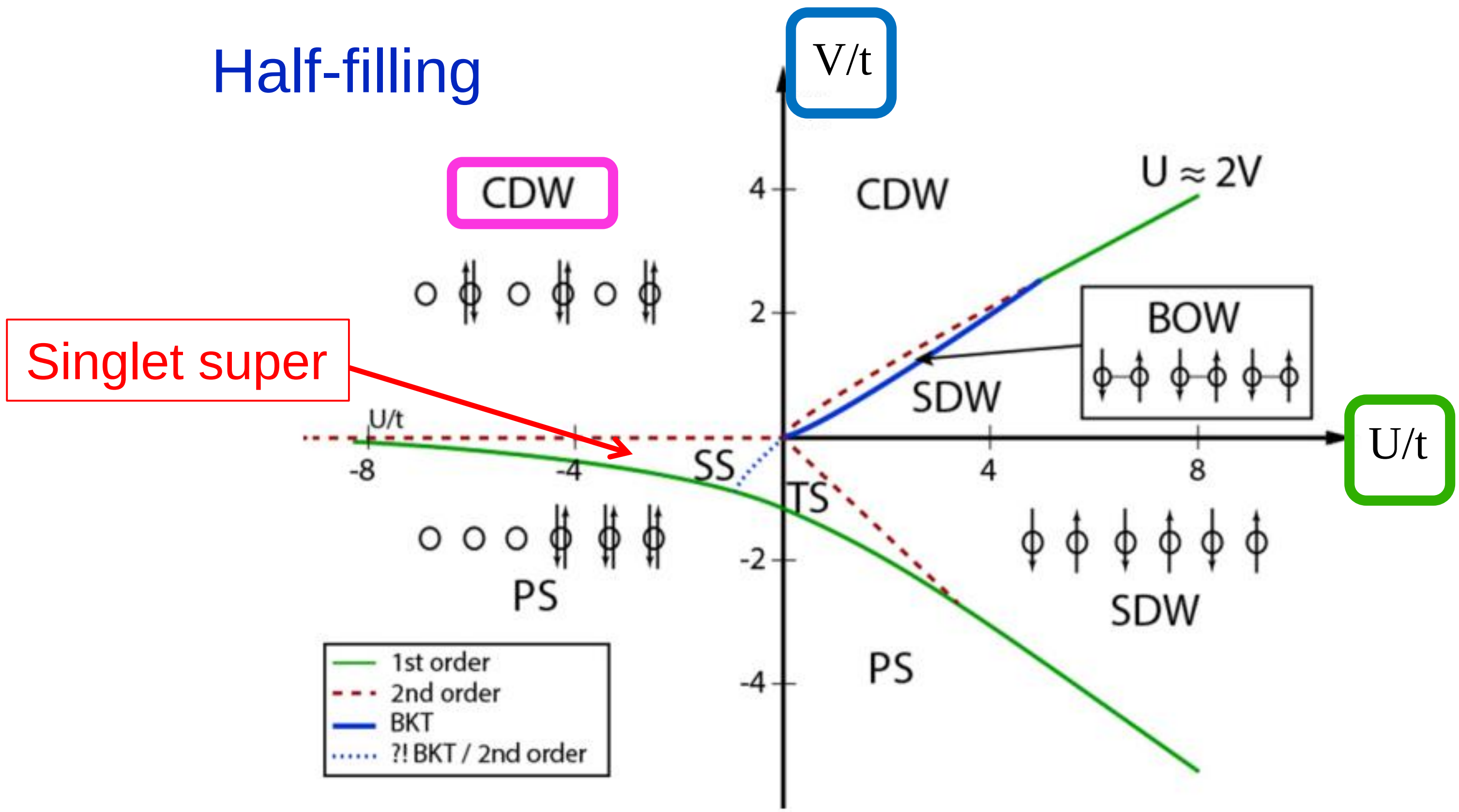


M. Minola *et al.*, PRL **114**, 217003 (2015)

How do RIXS spectra behave when attractive interactions are explicitly taken into account?

One-dimensional extended Hubbard model

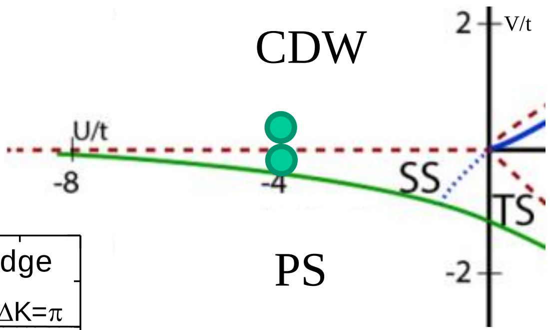
$$H=-t\sum_{i\sigma}\left(c_{i\sigma}^{\dagger}c_{i+1\sigma}+\text{h.c.}\right)+\boxed{U}\sum_{i}n_{i\uparrow}n_{i\downarrow}+\boxed{V}\sum_{i}\left(n_{i\uparrow}+n_{i\downarrow}\right)\left(n_{i+1\uparrow}+n_{i+1\downarrow}\right)$$



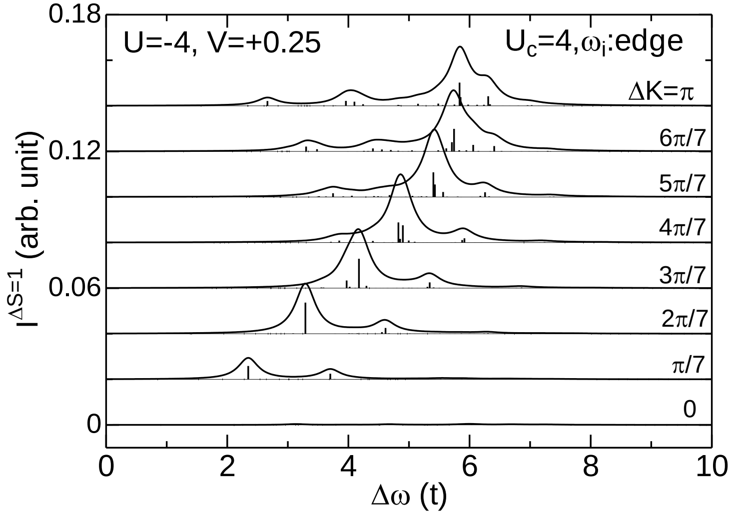
F. Iemini, T. O. Maciel, and R. O. Vianna, Phys. Rev. B **92**, 075423 (2015).

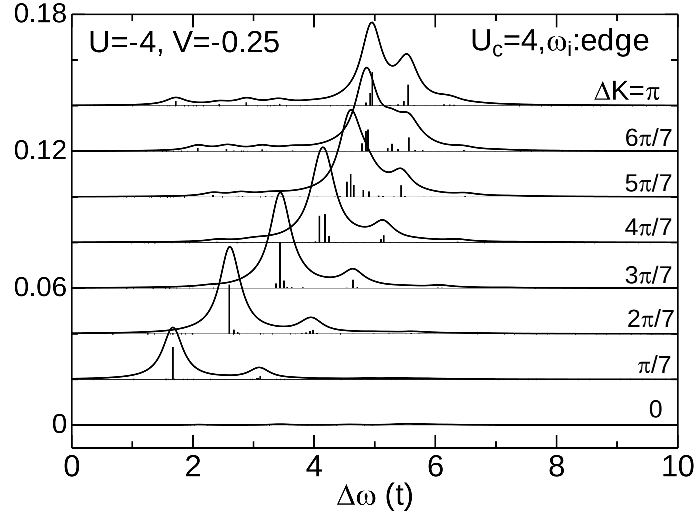
H. Q. Lin and J. E. Hirsch, Phys. Rev. B **33**, 8155 (1983).

RIXS for spin-flip process and $S(q,\omega)$



RIXS





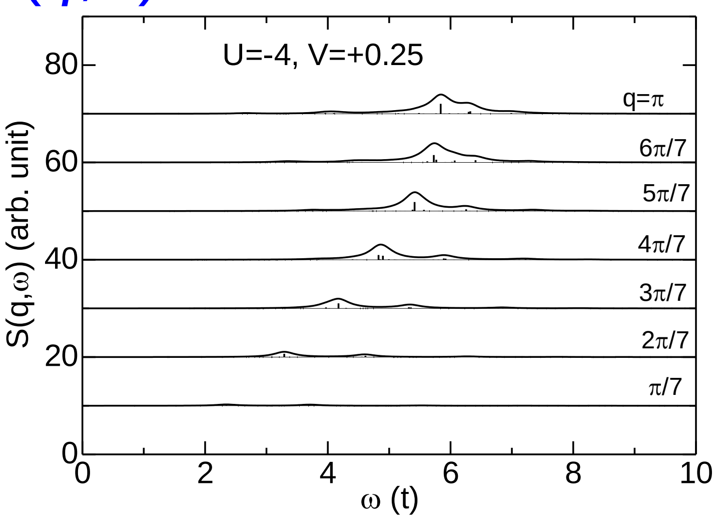
CDW

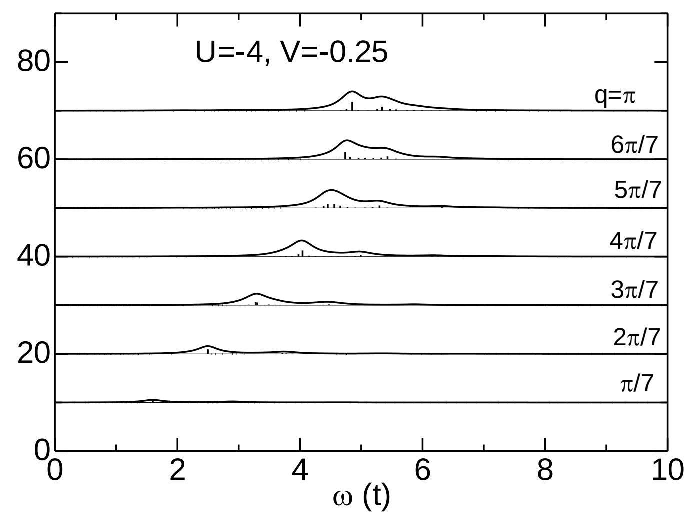
singlet super. (SS)

☑ No difference between CDW and SS

☑ Excitations at high-energy

$S(q,\omega)$

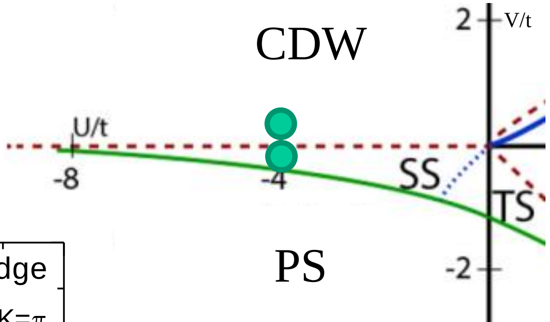




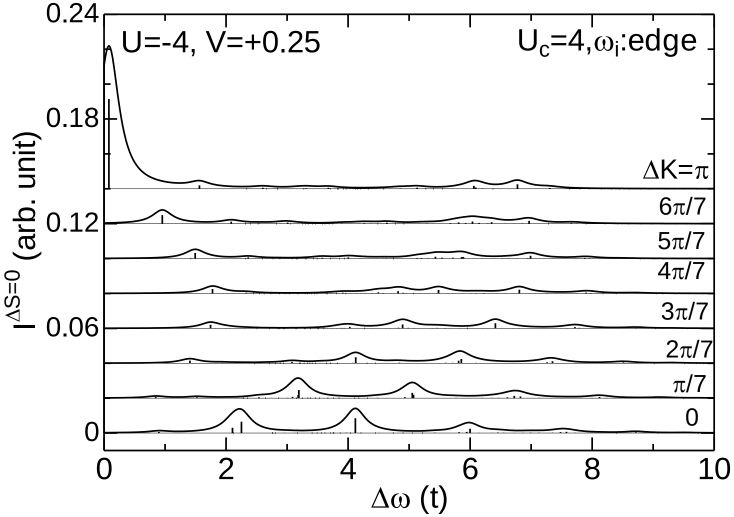
Hubbard model at half-filling

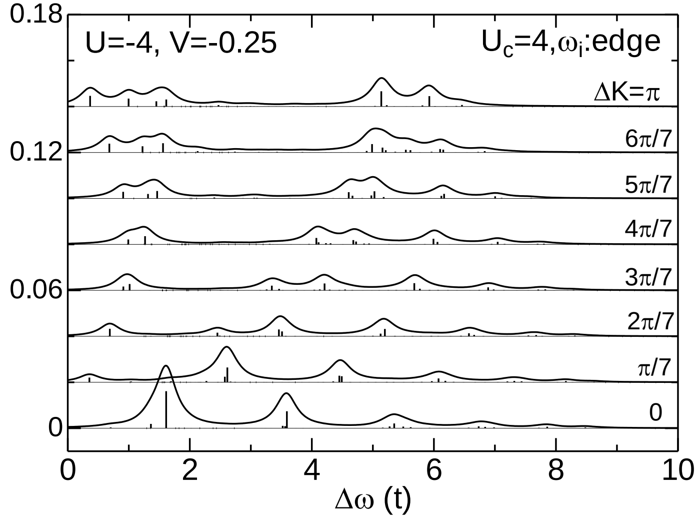
$U<0$	$U>0$
$N(q,\omega)$	$S(q,\omega)$
$S(q,\omega)$	$N(q,\omega)$

RIXS for non-spin-flip process and $N(q,\omega)$



RIXS

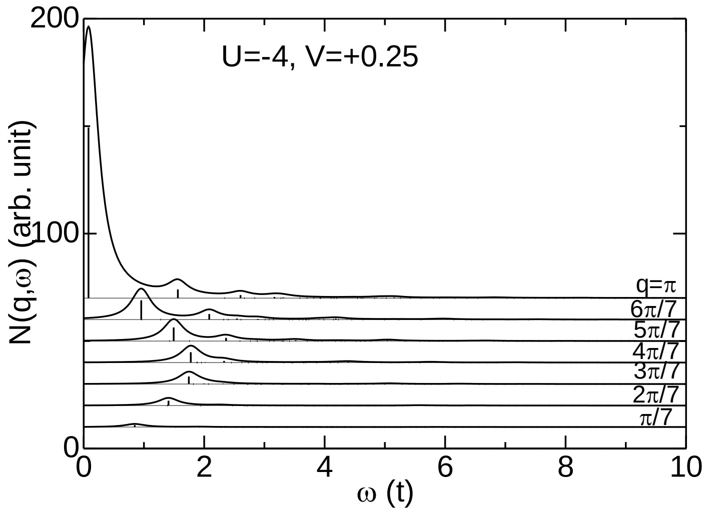


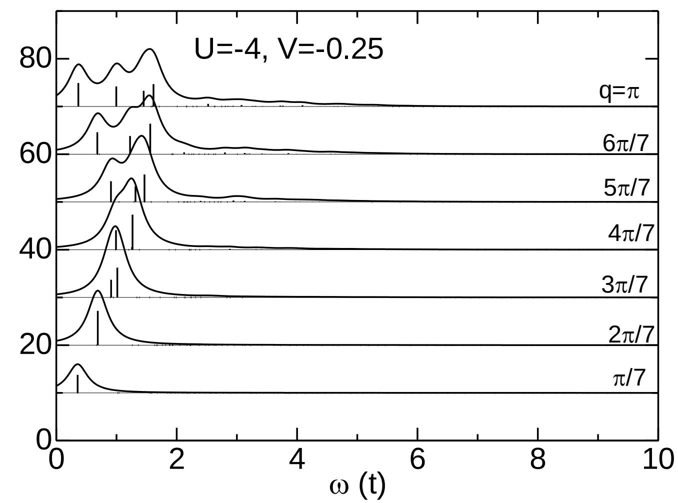


CDW

singlet super. (SS)

$N(q,\omega)$

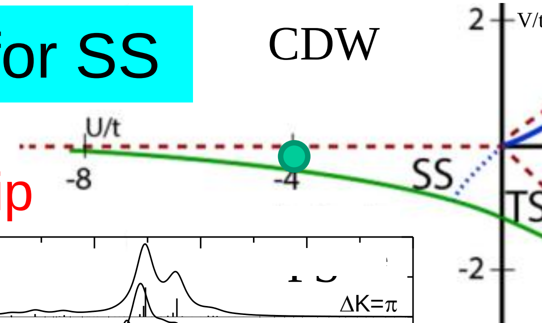




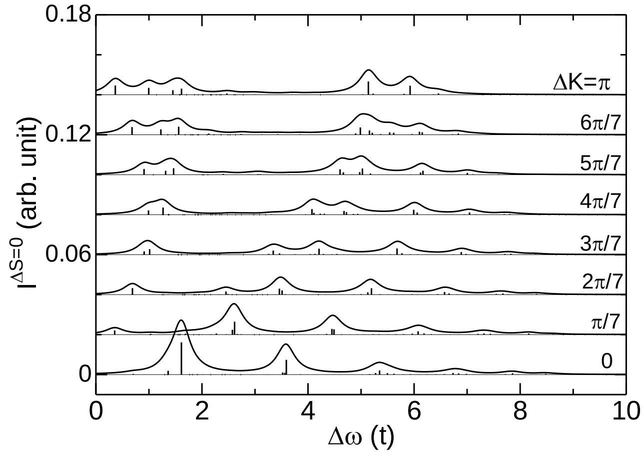
- ☑ Clear difference between CDW and SS
- ☑ CDW
  RIXS and $N(q,\omega)$ similar
- ☑ SS
  RIXS detects high-energy excitations that are the same as spin-flip case.

→ More incoherent nature in SS than CDW

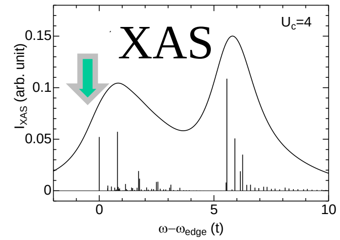
Incident-photon-energy dependence of RIXS for SS



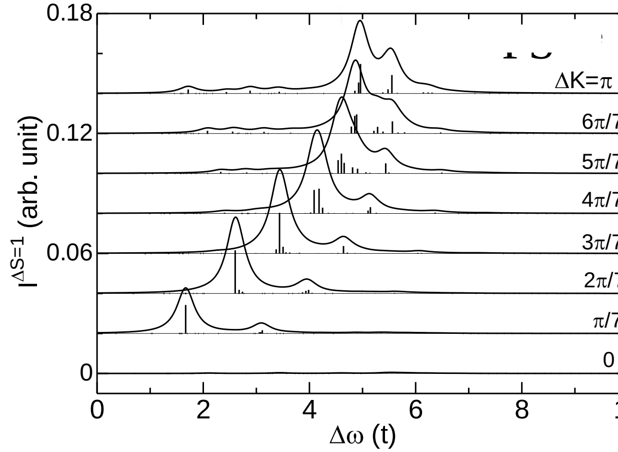
non-spin-flip



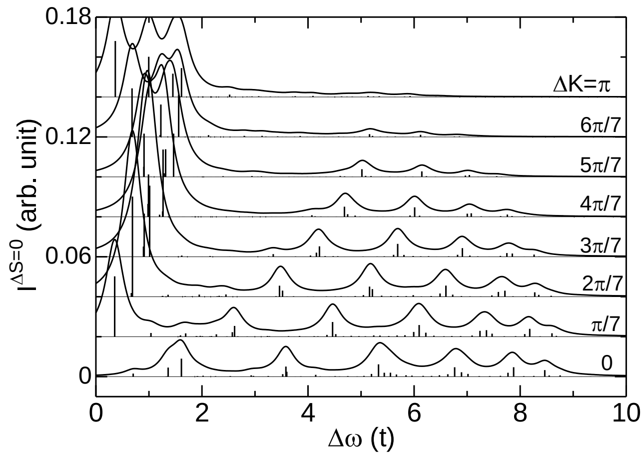
absorption at singly occupied sites



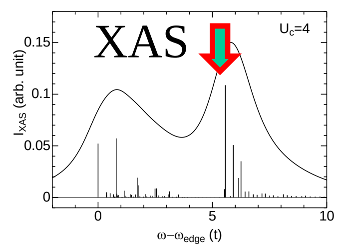
spin-flip



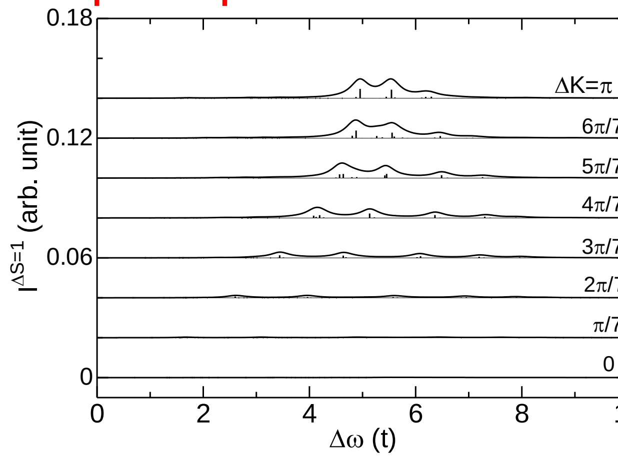
non-spin-flip



absorption at empty sites



spin-flip



spin-flip: large intensity at low-energy XAS

non-spin-flip: large intensity at high-energy XAS

Summary

☑ RIXS, $S(\mathbf{q},\omega)$, and $N(\mathbf{q},\omega)$ with charge-stripe order

T.T., M. Mori, and S. Sota, Phys. Rev. B **97**, 235137 (2018)

hole doping: stripe order in the ground state

- "hourglass" in $S(\mathbf{q},\omega)$
- A step-like behavior with $S(\mathbf{q},\omega)$ along (0,0)-(π,0)

electron doping: weak stripe order in the ground state

- A downward behavior in $S(\mathbf{q},\omega)$ along (0,0)-(π,0).
  ← itinerant nature in strong antiferromagnetic correlation

☑ Dimensionality effect on $S(\mathbf{q},\omega)$

- Weakening of charge stripe → change of "hourglass" behavior

T. T., S. Sota, S. Yunoki, in preparation

☑ RIXS in 1D extended Hubbard model

- Comparison between CDW and singlet superconducting phases

K. Tsutsui, T. T., in preparation