Spin and Charge Excitations in Stripe-Ordered Cuprates

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- 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


- 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 $\text{La}_{1.875}\text{La}_{0.125}\text{CuO}_4$.

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

Inelastic neutron scattering
“hourglass” around \((\pi, \pi)\)

Resonant inelastic x-ray scattering
“plateau” around \((0.5\pi, 0)\)

stripe-ordered \(\text{La}_{1.875}\text{Ba}_{0.125}\text{CuO}_4\)


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)
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

$$S (q, \omega) = -\frac{1}{\pi} \text{Im} \langle 0 | S^z_{-q} \frac{1}{\omega - H_{tJ} + E_0 + i\gamma} S^z_q | 0 \rangle$$

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

24x4 $t$-$t'$-$J$ ladder
x (leg) direction $\rightarrow$ open boundary
y (rung) direction $\rightarrow$ periodic boundary

Dynamical density-matrix renormalization group (DDMRG)

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

**hole doping** $x=1/12$

24x4 $t-t'-J$ hole $x=8/96=0.083$, $m=4000$, $\gamma/t=0.08$

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

**hole doping** $x=1/8$

24x4 $t-t'-J$ hole $x=12/96=0.125$, $m=4000$, $\gamma/t=0.08$

**hole doping** $x=1/6$

24x4 $t-t'-J$ hole $x=16/96=0.167$, $m=4000$, $\gamma/t=0.08$
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 $q=(\pi,\pi)$ 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

**hole doping** \( x = 1/12 \)

24x4 \( t-t'-J \) hole \( x = 8/96 = 0.083, m = 4000, \gamma/t = 0.08 \)

- 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

Electron doping $x=1/12$

- No step-like structure in contrast to hole doping because of weak stripe order
- A downward spectral weight toward $(\pi,0) \rightarrow$ 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)

W. S. Lee et al., Nat. Phys. 10, 883 (2014)
Dynamical spin structure factor in the $t$-$t'$-$J$ model

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

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

absorption process
(=XAS)

intermediate state

emission process
(=XES)

ground state

3d

2p

\[ I(q, \Delta \omega) \sim \sum_f \left| \left\langle f \right| D_{k_0, \varepsilon_0}^{\dagger} \frac{1}{\omega_i - H + E_0 + i\Gamma} D_{k_i, \varepsilon_i} |0\rangle \right|^2 \delta(\Delta \omega - E_f + E_0) \]

\[ \Delta \omega = \omega_i - \omega_o \]

\[ q = k_i - k_o \]

\[ |0\rangle : \text{ground state (no Cu2p hole)} \]

\[ |f\rangle : \text{‘final’ state with momentum } q \]

\[ D_{k_i, \varepsilon_i} = \sum_{\mu, \sigma, j_z} \langle 3d; \mu \sigma | \varepsilon_{i(o)} \cdot r | 2p; jj_z \rangle \sum_k d_{k, \mu, \sigma}^+ P_{k-k_{i(o)}, j, j_z} \] : dipole transition operator
RIXS for cuprates

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

$$ \langle f \mid D_{k_0,\epsilon_0}^\dagger \frac{1}{\omega_i - H + E_0 + i\Gamma} D_{k_i,\epsilon_i} \mid 0 \rangle \Rightarrow \langle f \mid \alpha_N^j N_q^j + \alpha_S^j S_q^j \mid 0 \rangle $$

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

$N_q^j = B_q^{j \uparrow \uparrow} + B_q^{j \downarrow \downarrow}$

Non spin-flip process

$S_q^j = (B_q^{j \uparrow \uparrow} - B_q^{j \downarrow \downarrow})/2$

Spin-flip process

$$ B_q^{j \sigma' \sigma} = \sum_l e^{-i\mathbf{q} \cdot \mathbf{R}_l} d_{l\sigma'}^\dagger \frac{1}{\omega_i - H_l^j + E_0 + i\Gamma} d_{l\sigma} $$

$$ H_l^j = H_{3d} + U_c \sum_\sigma n_{l\sigma} + \epsilon_j $$

$$ 2\alpha_N^{j=1/2} = \alpha_N^{j=3/2} = \frac{2}{15} (\epsilon_o \cdot \epsilon_i - \epsilon_{o\sigma} \epsilon_{i\sigma}) $$

$$ \alpha_S^{j=1/2} = -\alpha_S^{j=3/2} = -\frac{2}{15} i(\epsilon_o \times \epsilon_i)_z $$

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 $\omega_i$ dependence of RIXS intensity

hole doping (11%)

18 sites $t'=-0.25t$
$U=10t$ $U_{\text{core}}=12t$ $\Gamma=t$

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

A change from "two-magnon" to "charge" $\rightarrow$ fluorescence-like behavior

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

M. Minola et al., PRL 114, 217003 (2015)
One-dimensional extended Hubbard model

\[
H = -t \sum_{i\sigma} (c_{i\sigma}^\dagger c_{i+1\sigma} + \text{h.c.}) - U \sum_i n_{i\uparrow} n_{i\downarrow} - V \sum_i (n_{i\uparrow} + n_{i\downarrow})(n_{i+1\uparrow} + n_{i+1\downarrow})
\]

Half-filling

Singlet super


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

- $S(q, \omega)$
  - $U=-4, V=+0.25$
  - $U=-4, V=-0.25$

- CDW
  - $U_c=4, \omega_i$: edge

- Singlet super. (SS)
  - $\Delta K=\pi$

- No difference between CDW and SS

- Excitations at high-energy

Hubbard model at half-filling

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

In the Hubbard model at half-filling, the behavior of $S(q, \omega)$ and $N(q, \omega)$ changes depending on the sign of $U$. For $U<0$, the number of states $N(q, \omega)$ is dominant, while for $U>0$, the structure factor $S(q, \omega)$ becomes significant.
RIXS for non-spin-flip process and $N(q,\omega)$

- **CDW**
  - RIXS and $N(q,\omega)$ similar
  - Clear difference between CDW and SS

- **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
- Absorption at empty sites

**spin-flip**

- Large intensity at low-energy XAS
- Large intensity at high-energy XAS
☐ RIXS, $S(q,\omega)$, and $N(q,\omega)$ with charge-stripe order


- “hourglass” in $S(q,\omega)$
- A step-like behavior with $S(q,\omega)$ along $(0,0)$-$(\pi,0)$

hole doping: stripe order in the ground state

electron doping: weak stripe order in the ground state

- A downward behavior in $S(q,\omega)$ along $(0,0)$-$(\pi,0)$.

← itinerant nature in strong antiferromagnetic correlation

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

- Weakening of charge stripe $\rightarrow$ 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