COMPETITION BETWEEN FILLED AND HALF-FILLED STRIPES IN CUPRATES AND NICKELATES

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OUTLINE

- Types of stripes
- Experimental evidences
- Description of the cuprates
- Competition between stripes
- Modeling of the nickelates
- Competition between stripes
- Summary
**STRIPE PHASES**

- 1D domain walls of holes which separate AF domains of opposite phases.
- They might be:
  - **site-centered** centered on rows of metal atoms
  - **bond-centered** centered on rows of oxygen atoms bridging two metal sites
- Their shape and properties are material dependent
TYPICAL MATERIALS

- $\text{La}_{2-x-y}\text{Nd}_y\text{Sr}_x\text{CuO}_4$, $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$
- superconducting above $x \simeq 0.06$
- $Q_s = \pi (1 \pm 2\epsilon, 1)$, $Q_s = \pi (1, 1 \pm 2\epsilon)$ with $\epsilon \simeq x$ for $0.06 \leq x \leq 1/8$
- half–filled vertical/horizontal stripes (0.5 hole per Cu atom in a domain wall)
- $Q_s = \pi (1 \pm \sqrt{2}\epsilon, 1 \pm \sqrt{2}\epsilon)$ with $\epsilon \simeq x$ for $x \leq 0.06$
- filled diagonal stripes (one hole per Cu atom in a domain wall)
- $3d^9$: Cu$^{2+}$ ($S = 1/2$), Cu$^{3+}$ ($S = 0$) ⇒ orbital degeneracy is absent
- quantum fluctuations important
- proper treatment of strong electron correlations required

- $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$, $\text{La}_2\text{NiO}_4+\delta$
- insulator up to $x \simeq 1$
- $Q_s = \pi (1 \pm \epsilon, 1 \pm \epsilon)$ with $\epsilon \simeq x$ for $x \leq 1/3$
- filled diagonal stripes (one hole/Ni ion in a domain wall)
- $3d^8$: Ni$^{2+}$ ($S = 1$), Ni$^{3+}$ ($S = 1/2$) ⇒ orbital degeneracy
- more classical
- Hartree approach should capture the physics of the nickelates
Summary of experimental data illustrating the doping dependence of incommensurability $\epsilon$ in the cuprates. In LSCO, $\epsilon$ has been defined as a distance from the IC peak position to the AF wave vector (1/2, 1/2) either in the orthorhombic ($x < 0.06$) or tetragonal ($x > 0.06$) notation, whereas at $x = 0.06$, both definitions are used due to the coexistence of diagonal and parallel to the Cu-O bonds spin modulations.
Summary of the results for $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$ (filled circles), $\text{Nd}_{2-x}\text{Sr}_x\text{NiO}_4$ (diamonds), and $\text{La}_{2-x}\text{Sr}_x\text{NiO}_4+\delta$ (empty circles) for different net dopant induced hole concentration $n_h = x + 2\delta$ dependence of: (a) transition temperature for a checkerboard-type charge order ($T_{\text{CO}}^\text{C}$) as well as a stripe-type charge ($T_{\text{CO}}^\text{IC}$) and spin ($T_N$) order, and (b) incommensurability $\epsilon$, after Kajimoto et al., Phys. Rev. B 67, 014511 (2003).
Temperature dependence of:

(a) incommensurability $\epsilon$
Kajimoto et al., Phys. Rev. B 64, 144432 (2001);

(b) phonon thermal conductivity $\kappa$
Hess et al., Phys. Rev. B 59, R10397 (1999);

(c) specific heat $C'$
Ramirez et al., Phys. Rev. Lett. 76, 447 (1996);

(d) logarithmic resistivity $\log \rho$
Cheong et al., Phys. Rev. B 49, 7088 (1994);

inset: optical conductivity $\sigma(\omega)$
SLAVE-BOSON APPROACH

- single-band Hubbard model with the next-nearest-neighbor hopping $t'$

$$H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

- in terms of the SB operators

$$H_{SB} = \sum_{ij} \sum_{\sigma\sigma'\sigma_1} t_{ijz_{i\sigma_1\sigma}^\dagger f_{j\sigma'}^\dagger f_{j\sigma'} z_{j\sigma'}^\dagger + U \sum_i d_i^\dagger d_i$$

- SB operators have to fulfill a set of constraints at each site

$$e_i^\dagger e_i + d_i^\dagger d_i + \sum_{\mu} p_{i\mu}^\dagger p_{i\mu} = 1$$

$$2d_i^\dagger d_i + \sum_{\mu} p_{i\mu}^\dagger p_{i\mu} = \sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma}$$

$$p_{0i}^\dagger p_i + p_i^\dagger p_{0i} - i p_i^\dagger \times p_i = \sum_{\sigma\sigma'} \tau_{\sigma\sigma'} f_{i\sigma'}^\dagger f_{i\sigma}$$

- The corresponding action is handled on the saddle-point level.

$$F = \sum_i \left\{ -\beta_{0i}(p_{0i}^2 + p_i^2 + 2d_i^2) + U_i d_i^2 - 2\beta_i \cdot p_i p_{0i} \right\} - \beta^{-1} \sum_{q\sigma} \ln(1 + e^{-\beta q\sigma}) + \mu N_{el}$$
For large systems one need a proper unit cell

(a) Vertical stripe phase, its unit cell, and two periodicity vectors $g_1 = (4, 1)$ and $g_2 = (0, 2)$. (b) Diagonal SC stripe phase, its unit cell, and two periodicity vectors $g_1 = (1, 1)$ and $g_2 = (4, -4)$.

in the reciprocal space representation the large original fermionic matrix is decoupled into $(2N_c \times 2N_c)$ blocks.
The interaction energy is reduced when:

- The (local) density is reduced
- A local magnetic moment is formed

Characteristics of simple bond-centered and site-centered stripes

\((U/t = 12, t'/t = -0.15, \beta t = 100)\)
**Finite size effects** \( (U/t = 12, \beta t = 1000, x = 1/8) \)

(half-filled domain walls)  

<table>
<thead>
<tr>
<th>N</th>
<th>F/t</th>
</tr>
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<tbody>
<tr>
<td>128x128</td>
<td>-0.569</td>
</tr>
<tr>
<td>32x32</td>
<td>-0.568</td>
</tr>
<tr>
<td>24x24</td>
<td>-0.567</td>
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<tr>
<td>64x64</td>
<td>-0.566</td>
</tr>
<tr>
<td>8x8</td>
<td>-0.567</td>
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</table>

(vertical)

The behavior is stripe dependent
Influence of electron correlations on SC stripe profiles \((U/t = 6, x = 1/8)\)

(filled domain walls) (half-filled domain walls)
Influence of the next-neighbor hopping $t'$ (SBA: $U = 12t$, $x = 1/8$)

SB free energy of various phases at temperature $\beta t = 100$ on a $128 \times 128$ cluster

<table>
<thead>
<tr>
<th>$t/t'$</th>
<th>phase</th>
<th>$F/t$</th>
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<tr>
<td>0.0</td>
<td>PM</td>
<td>-0.5040</td>
</tr>
<tr>
<td></td>
<td>HDSC</td>
<td>-0.5339</td>
</tr>
<tr>
<td></td>
<td>AF</td>
<td>-0.5393</td>
</tr>
<tr>
<td></td>
<td>HVSC</td>
<td>-0.5689</td>
</tr>
<tr>
<td></td>
<td>VSC</td>
<td>-0.5751</td>
</tr>
<tr>
<td></td>
<td>DSC</td>
<td>-0.5821</td>
</tr>
<tr>
<td>-0.3</td>
<td>VSC</td>
<td>—</td>
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<tr>
<td></td>
<td>PM</td>
<td>-0.4822</td>
</tr>
<tr>
<td></td>
<td>AF</td>
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<tr>
<td></td>
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<td></td>
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<tr>
<td></td>
<td>HVSC</td>
<td>-0.5749</td>
</tr>
</tbody>
</table>

SB band structure of the HVSC stripe phase

$t'/t=0.0$

$t'/t=-0.3$
Doping dependence of the vertical stripe ground state (SBA: $U = 12t$)

(site-centered domain walls)

(bond-centered domain walls)
Doping dependence of the vertical stripe ground state (SBA: $U = 12t$)

SB ground state free energy of the VSC and VBC stripes ($t' = -0.15t$)

<table>
<thead>
<tr>
<th>$x$</th>
<th>$d$</th>
<th>$F/t$</th>
<th>$d$</th>
<th>$F/t$</th>
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<tr>
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</tr>
<tr>
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</tr>
<tr>
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<td>2</td>
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<td>3</td>
<td>-0.8605</td>
</tr>
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A road to low energy modes?
Systems with orbital degeneracy

- Hamiltonian for $e_g$ electrons: $|x\rangle \sim |x^2 - y^2\rangle$ and $|z\rangle \sim |3z^2 - r^2\rangle$

$$\mathcal{H} = H_{\text{kin}} + H_{\text{int}} + H_{\text{cf}}$$

- kinetic energy

$$H_{\text{kin}} = \sum_{\langle ij \rangle} \sum_{\alpha\beta\sigma} t_{ij}^{\alpha\beta} c_i^{\alpha\sigma} c_j^{\beta\sigma}, \quad t_{ij}^{\alpha\beta} = -\frac{t}{4} \left( \frac{3}{\pm \sqrt{3}} \pm \frac{\sqrt{3}}{1} \right), \quad t_{ij}^{\alpha\beta} = -(t/2)\delta_{\alpha\beta}$$

- electron-electron interactions

$$H_{\text{int}} = U \sum_i (n_{ix\uparrow} n_{ix\downarrow} + n_{iz\uparrow} n_{iz\downarrow}) + (U - \frac{5}{2} J_H) \sum_i n_{ix} n_{iz}$$

$$-2J_H \sum_i S_{ix} \cdot S_{iz} + J_H \sum_i (c_{ix\uparrow}^\dagger c_{ix\downarrow}^\dagger c_{iz\downarrow} c_{iz\uparrow} + c_{iz\uparrow}^\dagger c_{iz\downarrow}^\dagger c_{ix\downarrow} c_{ix\uparrow})$$

- crystal-field splitting between $|x\rangle$ and $|z\rangle$ orbitals along the $c$ axis

$$H_{\text{cf}} = \frac{1}{2} E_0 \sum_{i\sigma} (n_{ix\sigma} - n_{iz\sigma})$$
Mean-field phase diagram for $e_g$ electrons

Intricate interplay between ferromagnetic and antiferromagnetic phases
Doping dependence of the BC stripe ground state (HA: $U = 8t$, $J_H = 1.5t$)  

($e_g$ model)  

(equivalent band model)
Diagonal bond-centered stripes \((U = 8t, J_H = 1.5t, E_z = 0, x = 1/8)\)

- intraorbital double occupancy

\[
D(l_x) = \sum_\alpha n_{\alpha\uparrow}(l_x)n_{\alpha\downarrow}(l_x)
\]

- interorbital double occupancies

\[
D^{\sigma\bar{\sigma}}_{xz}(l_x) = \sum_\sigma n_{x\sigma}(l_x)n_{z\bar{\sigma}}(l_x)
\]

\[
D^{\sigma\sigma}_{xz}(l_x) = \sum_\sigma n_{x\sigma}(l_x)n_{z\sigma}(l_x)
\]
Filled diagonal BC stripes \((U = 8t, J_H = 1.5t, E_z = 0, x = 1/8)\)

Density of states

- Two 1-d bands
- The lowest one hybridizes with the 2-d background
- Metallic state
- Needs to go beyond mean-field
SUMMARY

- we have developed a simple but powerful approach which allows one to investigate stripe phases with a large unit cell and carry out the calculation on large ($\sim 100 \times 100$) clusters, eliminating the role of finite size effects
- the stripe phases allow for a description of the Hubbard model that involves lower and upper Hubbard bands, and a quasiparticle band on mean-field level
- the description of half-filled vertical stripes in the cuprates involves a proper treatment of strong electron correlations in the $t-t'-U$ model
- filled diagonal stripe phases observed in the nickelates are a generic feature of the model with two $e_g$ electrons
- there is a need to go beyond mean-field to describe the nickelates

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