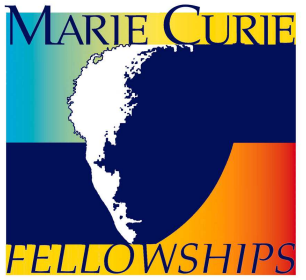

WŁAŚCIWOŚCI FAZ WSTĘGOWYCH W TLENKACH METALI PRZEJŚCIOWYCH

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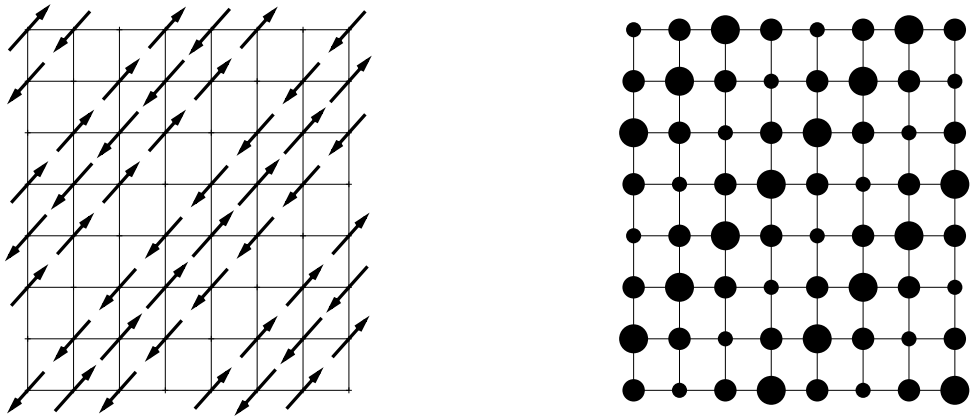
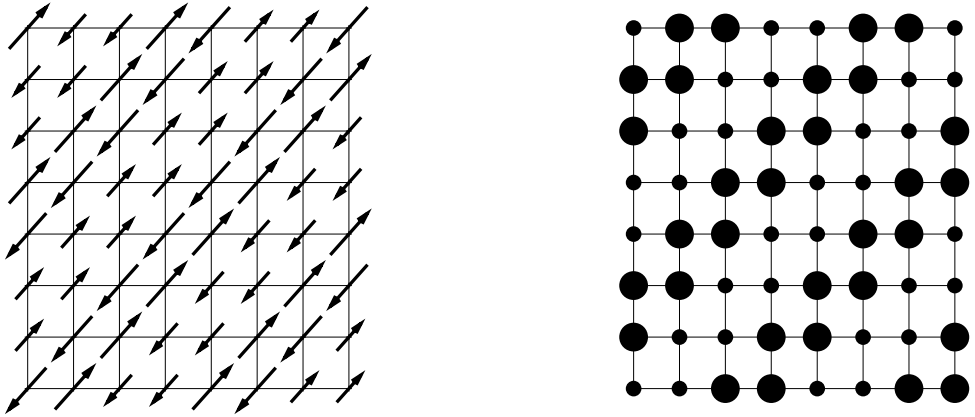
STRIPE PHASES

- 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



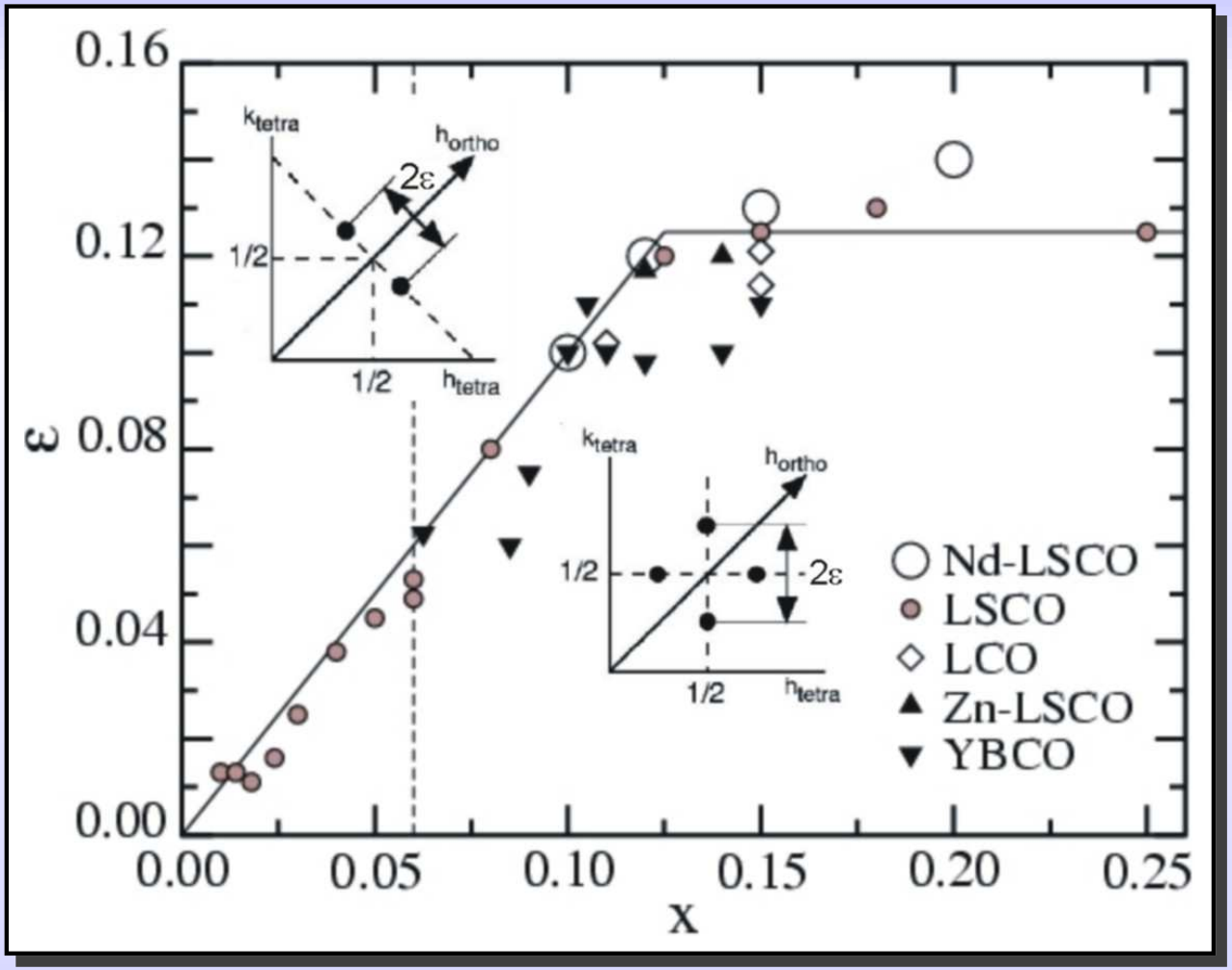
- their shape and properties are material dependent

TYPICAL MATERIALS

- $La_{2-x-y}Nd_ySr_xCuO_4$, $La_{2-x}Sr_xCuO_4$
- superconducting above $x \simeq 0.06$
- $\mathbf{Q}_s = \pi(1 \pm 2\epsilon, 1)$, $\mathbf{Q}_s = \pi(1, 1 \pm 2\epsilon)$ with $\epsilon \simeq x$ for $x \leq 1/8$
- half–filled vertical/horizontal stripes (0.5 hole per Cu atom in a domain wall)
- $3d^9$: Cu^{2+} ($S = 1/2$), Cu^{3+} ($S = 0$) $\Rightarrow$ orbital degeneracy is absent
- quantum fluctuations important
- proper treatment of strong electron correlations required

- $La_{2-x}Sr_xNiO_4$, $La_2NiO_{4+\delta}$
- insulator up to $x \simeq 1$
- $\mathbf{Q}_s = \pi(1 \pm \epsilon, 1 \pm \epsilon)$ 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+} ($S = 1/2$) $\Rightarrow$ orbital degeneracy
- more classical
- Hartree approach should capture the physics of the nickelates

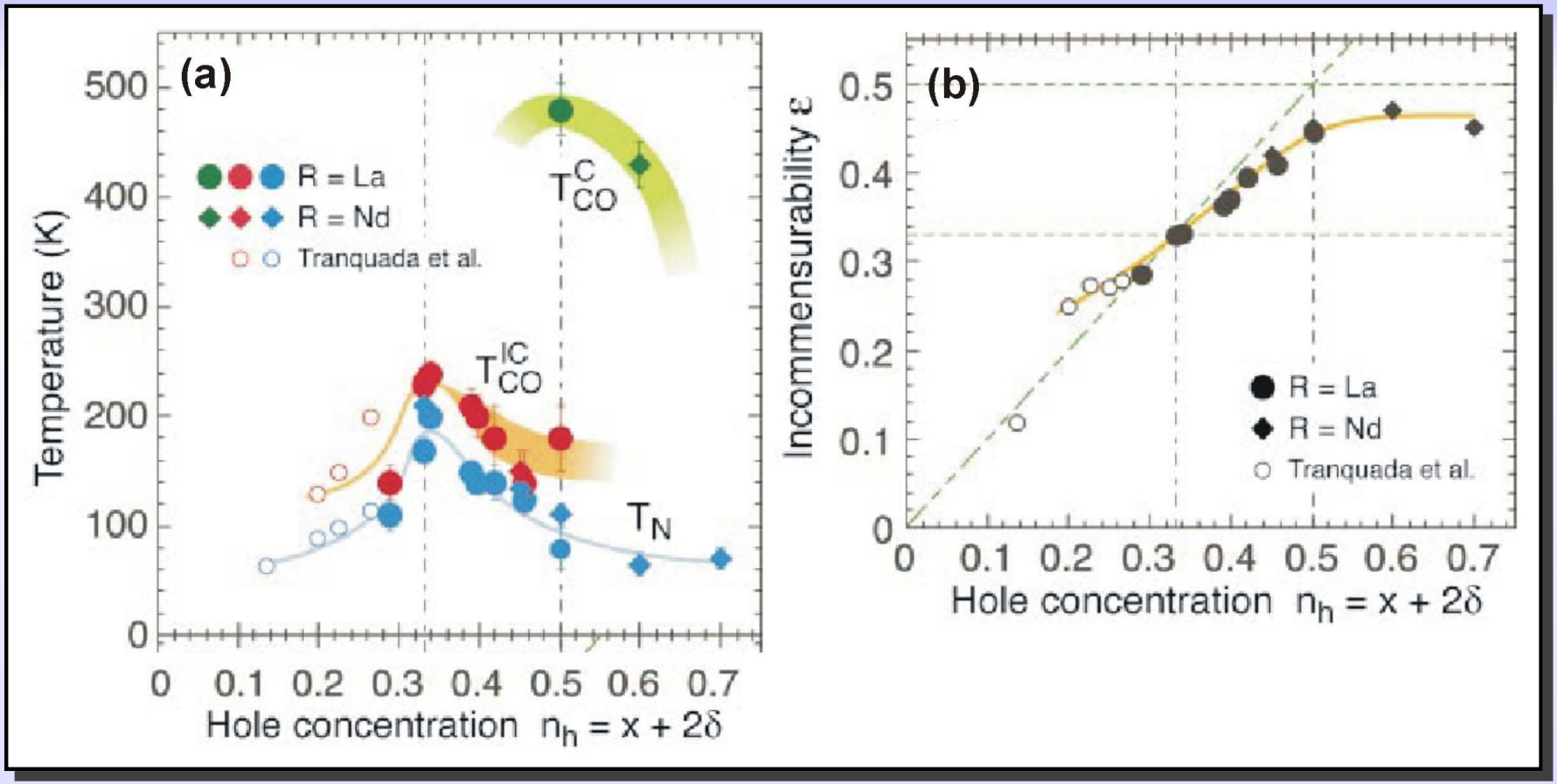
EXPERIMENTAL SIGNATURES OF STRIPES: CUPRATES



$La_{2-x-y}Nd_ySr_xCuO_4$ (Nd-LSCO)
$La_{2-x}Sr_xCuO_4$ (LSCO)
$La_2CuO_{4+\delta}$ (LCO)
$La_{2-x}Sr_xCu_{1-y}Zn_yO_4$ (Zn-LSCO)
$YBa_2Cu_3O_{6+\delta}$ (YBCO)

Summary of experimental data illustrating the doping dependence of incommensurability ϵ in the cuprates. In LSCO, ϵ 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.

EXPERIMENTAL SIGNATURES OF STRIPES: NICKELATES

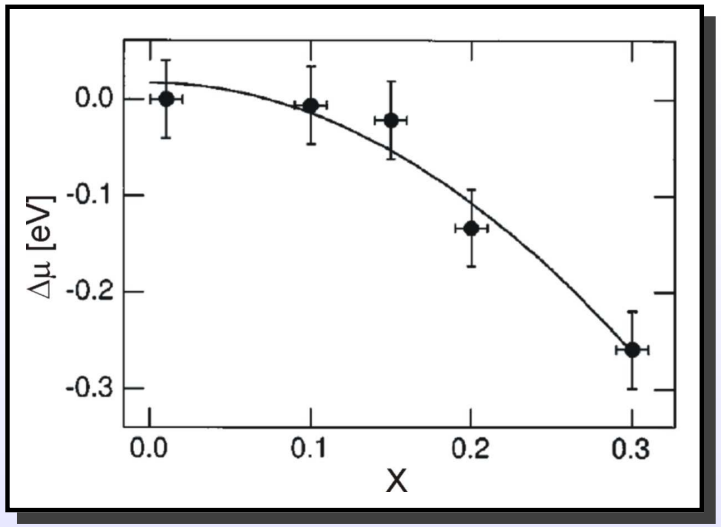


Summary of the results for $La_{2-x}Sr_xNiO_4$ (filled circles), $Nd_{2-x}Sr_xNiO_4$ (diamonds), and $La_{2-x}Sr_xNiO_{4+\delta}$ (empty circles) for different net dopant induced hole concentration $n_h = x + 2\delta$ dependence of: (a) transition temperature for a checkerboard-type charge order (T_{CO}^{C}) as well as a stripe-type charge (T_{CO}^{IC}) and spin (T_N) order, and (b) incommensurability ϵ, after Kajimoto *et al.*, Phys. Rev. B **67**, 014511 (2003).

FINGERPRINT OF STRIPES ?

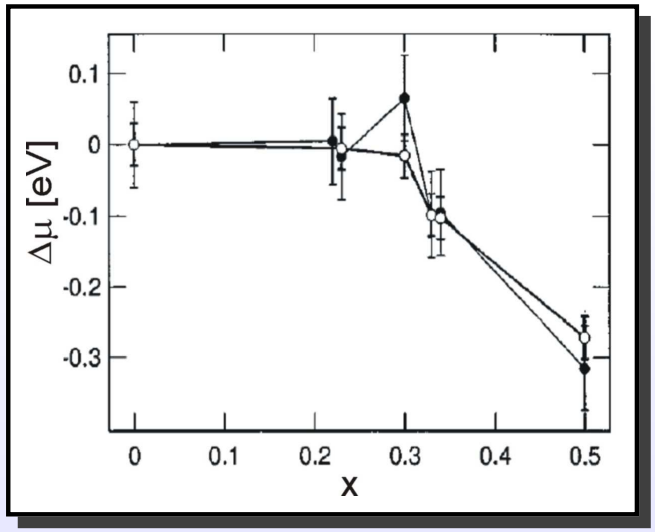
(a) chemical potential shift $\Delta\mu$:

$La_{2-x}Sr_xCuO_4$



Ino *et al.*, Phys. Rev. Lett. **79**, 2101 (1997).

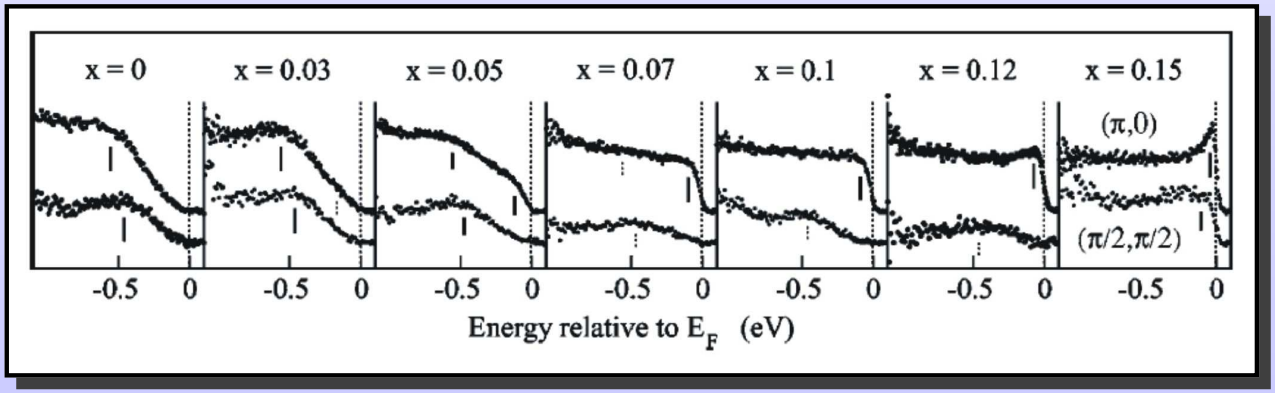
$La_{2-x}Sr_xNiO_4$



Satake *et al.*, Phys. Rev. B **61**, 15515 (2000).

(b) ARPES spectra: $La_{2-x}Sr_xCuO_4$

A. Ino, *et al.*, Phys. Rev. B **62**, 4137 (2000).



SLAVE-BOSON APPROACH

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

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

- in terms of the SB operators

$$H_{SB} = \sum_{ij} \sum_{\sigma\sigma'\sigma_1} t_{ij} z^{\dagger}_{i\sigma_1\sigma} f^{\dagger}_{i\sigma} f_{j\sigma'} z_{j\sigma'\sigma_1} + U \sum_{i} d^{\dagger}_{i} d_{i}$$

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

$$e^{\dagger}_{i} e_{i} + d^{\dagger}_{i} d_{i} + \sum_{\mu} p^{\dagger}_{i\mu} p_{i\mu} = 1$$

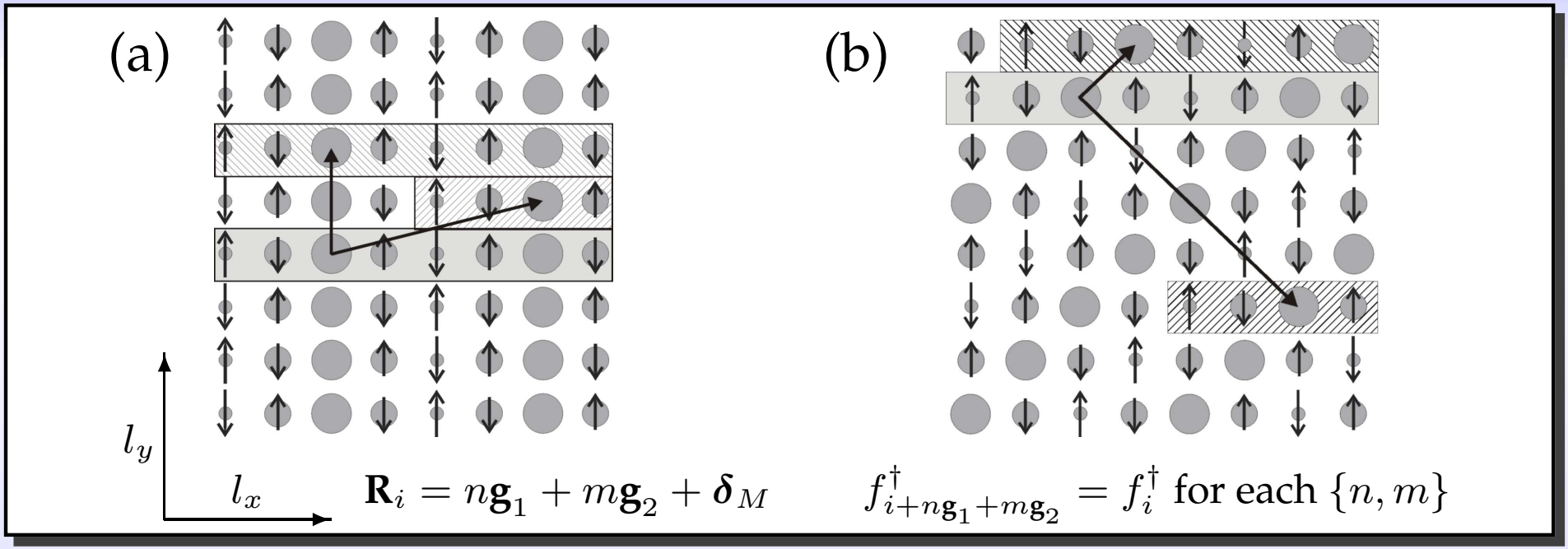
$$2 d^{\dagger}_{i} d_{i} + \sum_{\mu} p^{\dagger}_{i\mu} p_{i\mu} = \sum_{\sigma} f^{\dagger}_{i\sigma} f_{i\sigma}$$

$$p^{\dagger}_{0i} \mathbf{p}_{i} + \mathbf{p}^{\dagger}_{i} p_{0i} - i \mathbf{p}^{\dagger}_{i} \times \mathbf{p}_{i} = \sum_{\sigma\sigma'} \boldsymbol{\tau}_{\sigma\sigma'} f^{\dagger}_{i\sigma'} f_{i\sigma}$$

- one replaces the Bose fields by their time-independent averages, determined from the saddle-point equations $\nabla F = 0$ with

$$F = \sum_{i} \Big\{ -\beta_{0i} (p^{2}_{0i} + p^{2}_{i} + 2 d^{2}_{i}) + U_{i} d^{2}_{i} - 2 \boldsymbol{\beta}_{i} \cdot \mathbf{p}_{i} p_{0i} \Big\} - \beta^{-1} \sum_{\mathbf{q}\sigma} \ln\big(1 + e^{-\beta \varepsilon_{\mathbf{q}\sigma}}\big) + \mu N_{el}$$

- remedy: choose a proper unit cell

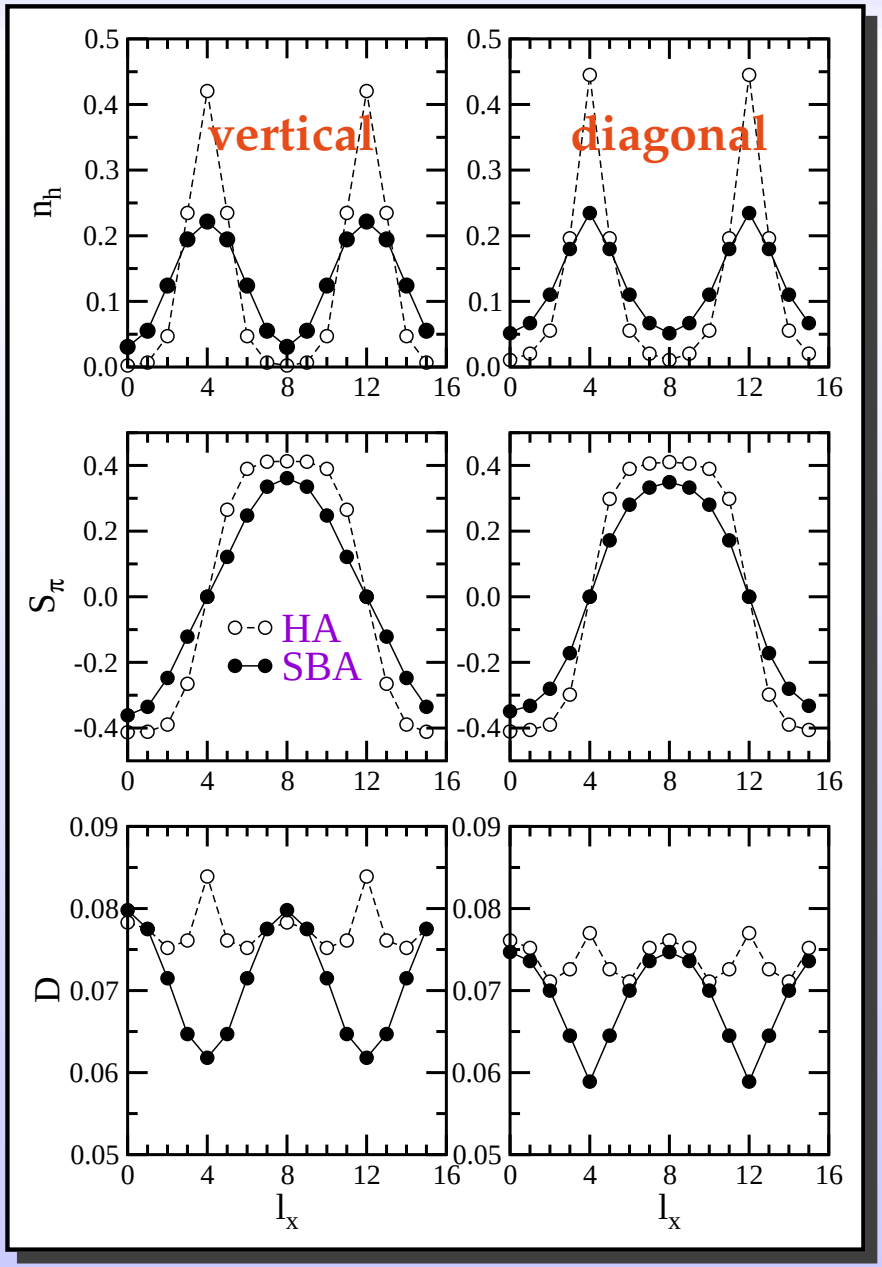


(a) Vertical stripe phase, its unit cell, and two periodicity vectors $\mathbf{g}_1 = (4, 1)$ and $\mathbf{g}_2 = (0, 2)$. (b) Diagonal SC stripe phase, its unit cell, and two periodicity vectors $\mathbf{g}_1 = (1, 1)$ and $\mathbf{g}_2 = (4, -4)$.

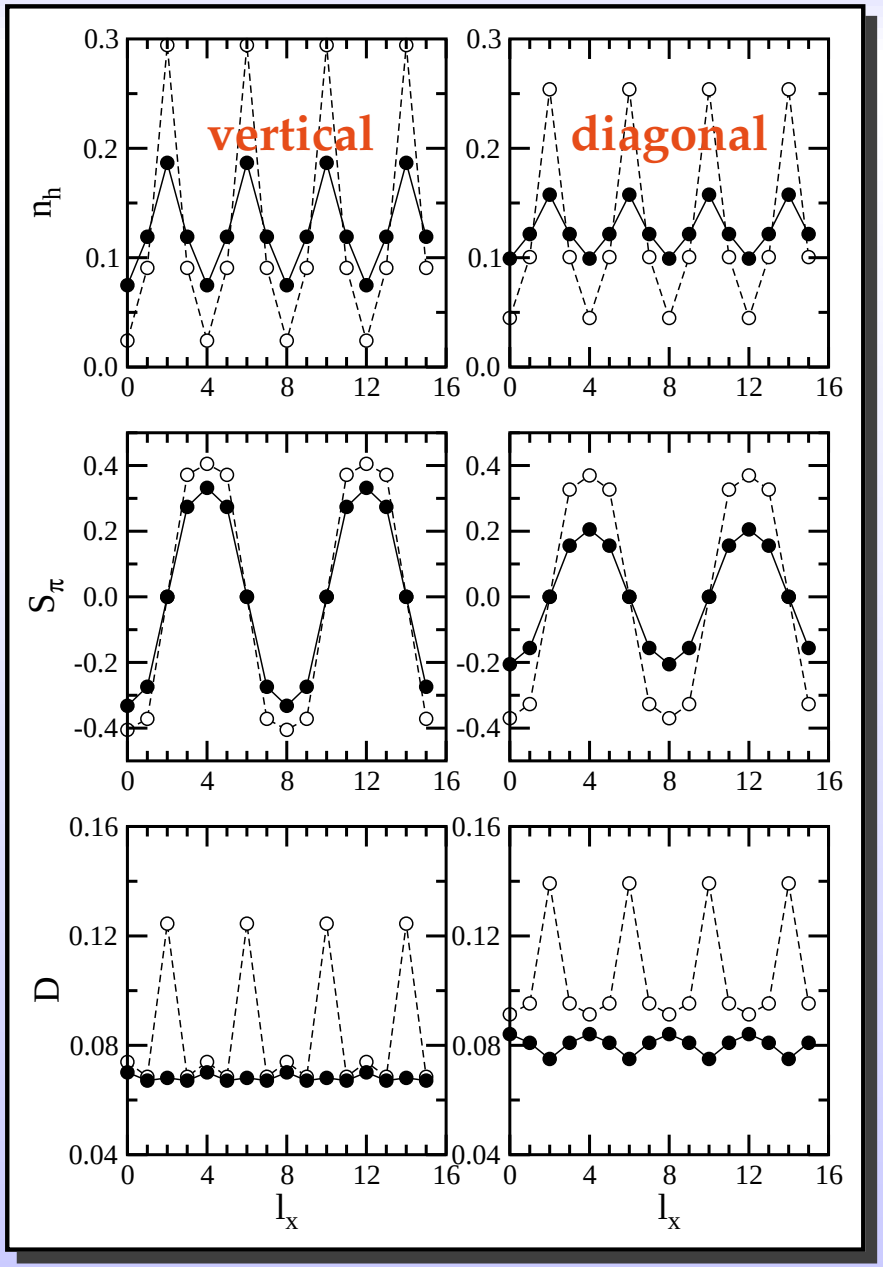
- in the reciprocal space representation one can reduce a large original fermionic matrix into decoupled submatrices, which gives a considerable time gain during numerical diagonalization

Influence of electron correlations on SC stripe profiles ($U/t = 6$, $x = 1/8$)

(filled domain walls)



(half-filled domain walls)

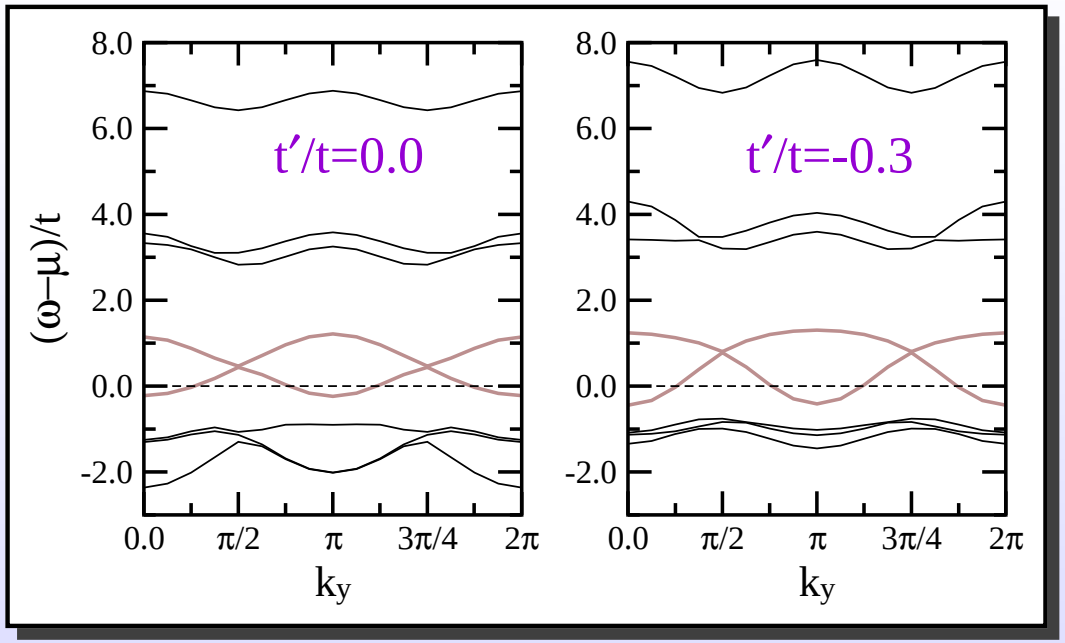


Influence of the next-neighbor hopping t' (SBA: $U = 12t$, $x = 1/8$)

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

t/t'	phase	F/t
0.0	PM	-0.5040
	HDSC	-0.5339
	AF	-0.5393
	HVSC	-0.5689
	VSC	-0.5751
	DSC	-0.5821
-0.3	VSC	—
	PM	-0.4822
	AF	-0.5341
	HDSC	-0.5534
	DSC	-0.5655
	HVSC	-0.5749

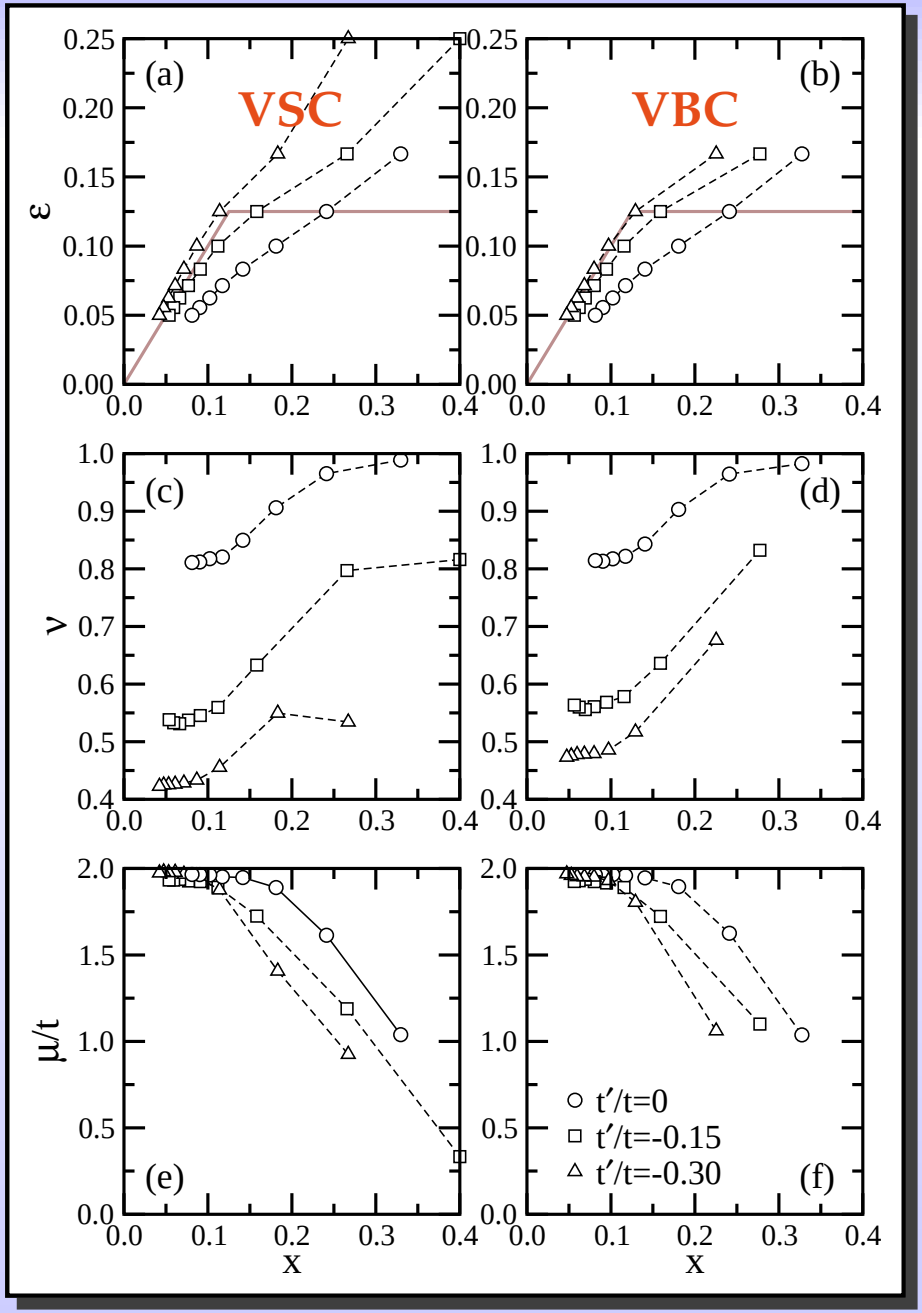
SB band structure of the HVSC stripe phase



Doping dependence of the vertical stripe ground state (SBA: $U = 12t$)

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

	VSC		VBC	
x	d	F/t	d	F/t
0.050	11	−0.4263	11	−0.4263
0.055	10	−0.4360	10	−0.4359
0.060	9	−0.4456	9	−0.4455
0.070	8	−0.4649	8	−0.4648
0.080	7	−0.4841	7	−0.4840
0.090	6	−0.5034	6	−0.5032
0.100	5	−0.5225	6	−0.5224
0.120	5	−0.5607	5	−0.5607
0.140	4	−0.5985	4	−0.5983
0.160	4	−0.6342	4	−0.6342
0.180	4	−0.6671	4	−0.6670
0.200	3	−0.6978	3	−0.6983
0.250	3	−0.7682	3	−0.7689
0.300	3	−0.8242	3	−0.8245
0.350	2	−0.8627	3	−0.8605



Systems with orbital degeneracy

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

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

- kinetic energy

$$H_{kin} = \sum_{\langle ij \rangle} \sum_{\alpha\beta\sigma} t_{ij}^{\alpha\beta} c_{i\alpha\sigma}^{\dagger} c_{j\beta\sigma}, \qquad t_{ij}^{\alpha\beta} = -\frac{t}{4} \begin{pmatrix} 3 & \pm\sqrt{3} \\ \pm\sqrt{3} & 1 \end{pmatrix}, \qquad t_{ij}^{\alpha\beta} = -(t/2)\delta_{\alpha\beta}$$

- electron-electron interactions

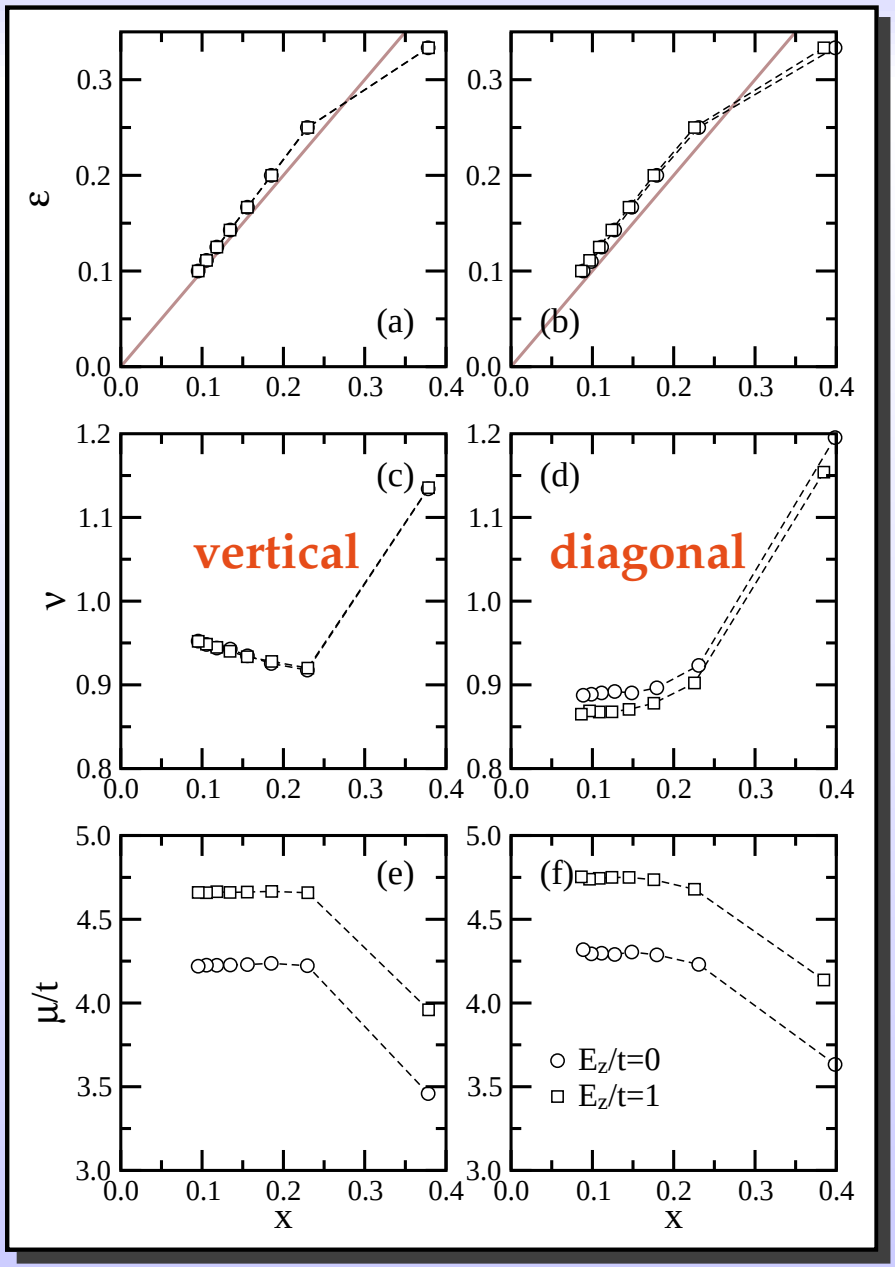
$$H_{int} = U \sum_i \left(n_{ix\uparrow} n_{ix\downarrow} + n_{iz\uparrow} n_{iz\downarrow} \right) + \left(U - \tfrac{5}{2} J_H \right) \sum_i n_{ix} n_{iz}$$
$$- 2J_H \sum_i \mathbf{S}_{ix} \cdot \mathbf{S}_{iz} + J_H \sum_i \left(c_{ix\uparrow}^{\dagger} c_{ix\downarrow}^{\dagger} c_{iz\downarrow} c_{iz\uparrow} + c_{iz\uparrow}^{\dagger} c_{iz\downarrow}^{\dagger} c_{ix\downarrow} c_{ix\uparrow} \right)$$

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

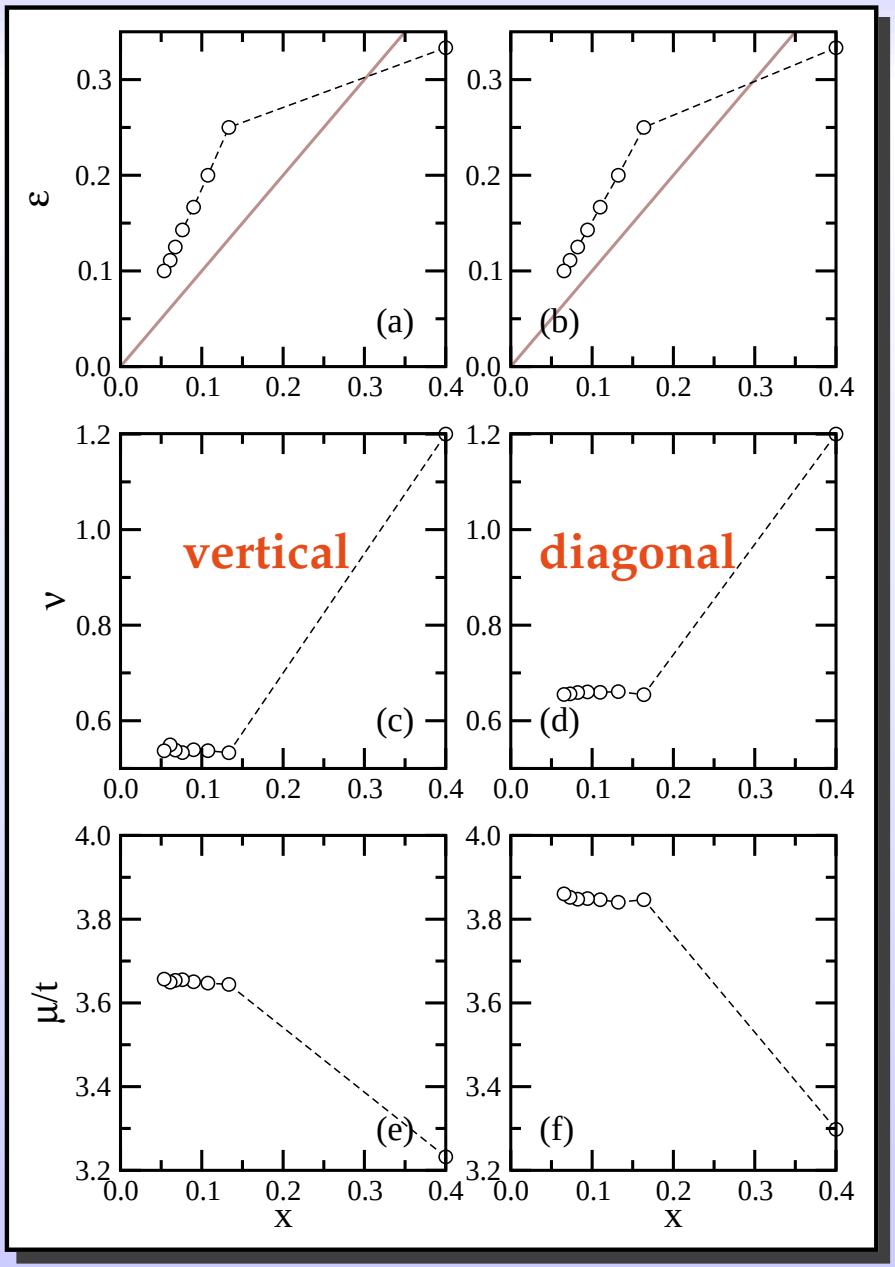
$$H_{cf} = \tfrac{1}{2} E_0 \sum_{i\sigma} (n_{ix\sigma} - n_{iz\sigma})$$

Doping dependence of the BC stripe ground state (HA: $U = 8t$, $J_H = 1.5t$)

(e_g model)

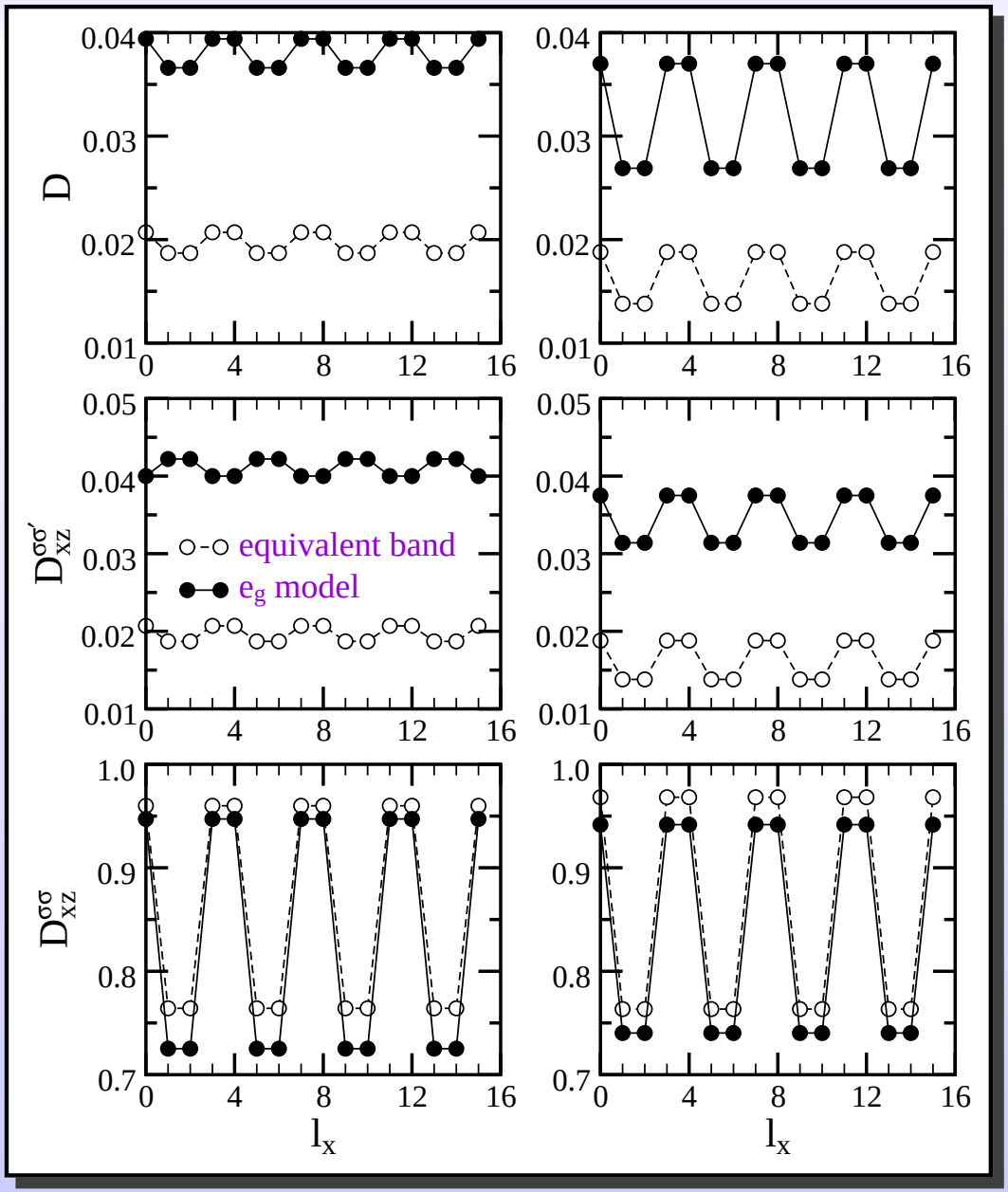


(equivalent band model)



Half-filled BC stripes ($U = 8t$, $J_H = 1.5t$, $E_z = 0$, $x = 1/8$)

vertical **diagonal**



- intraorbital double occupancy

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

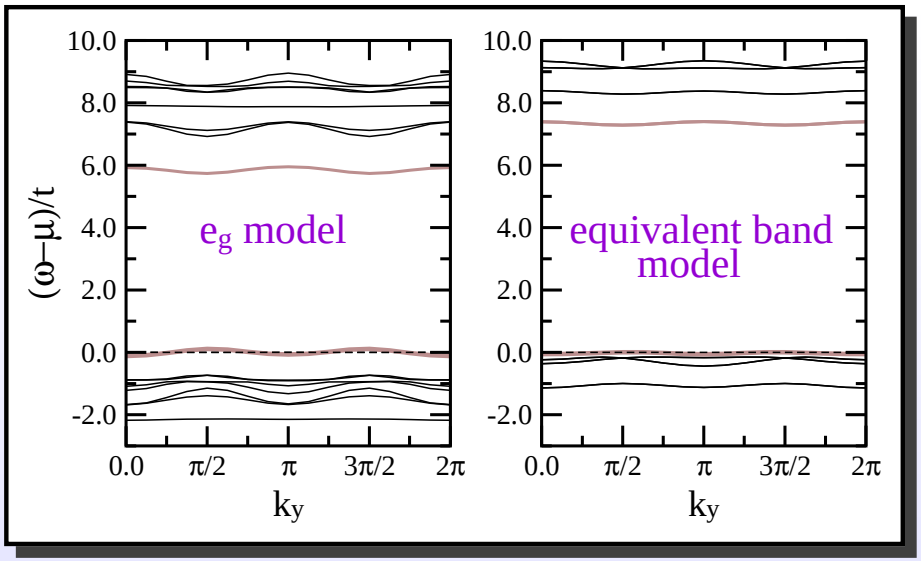
- interorbital double occupancies

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

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

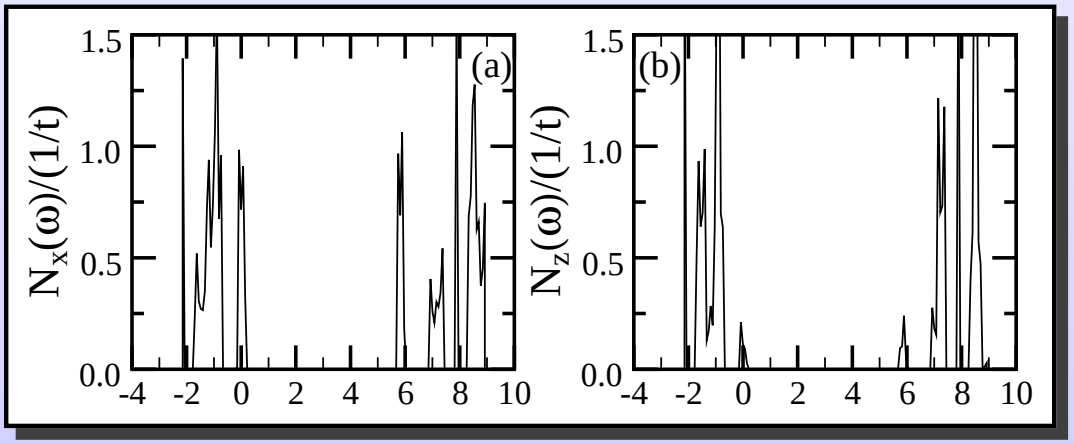
Half-filled vertical BC stripes ($U = 8t$, $J_H = 1.5t$, $E_z = 0$, $x = 1/8$)

Hartree band structure



Partial density of states

$$N_\alpha(\omega) = \frac{1}{N} \sum_{\mathbf{k}} \sum_{i\sigma} |\Psi_{i\alpha\sigma}(\mathbf{k})|^2 \delta(\omega - \varepsilon_{\mathbf{k}\sigma})$$



SUMMARY

- our goal was first and foremost to understand the properties of stripe phases and to determine the reasons of differences between the doped layered cuprates and nickelates
- 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 ($\sim 100\times100$) clusters
- it allows to obtain unbiased results at low temperature $\beta t = 100$ and to eliminate the role of finite size effects
- stripe phases found in the present approach are stabilized not due to particular boundary conditions but they represent a generic tendency of doped strongly correlated electron systems
- adequate 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