Lattice distortions, stripes and superconductivity in high-Tc cuprates

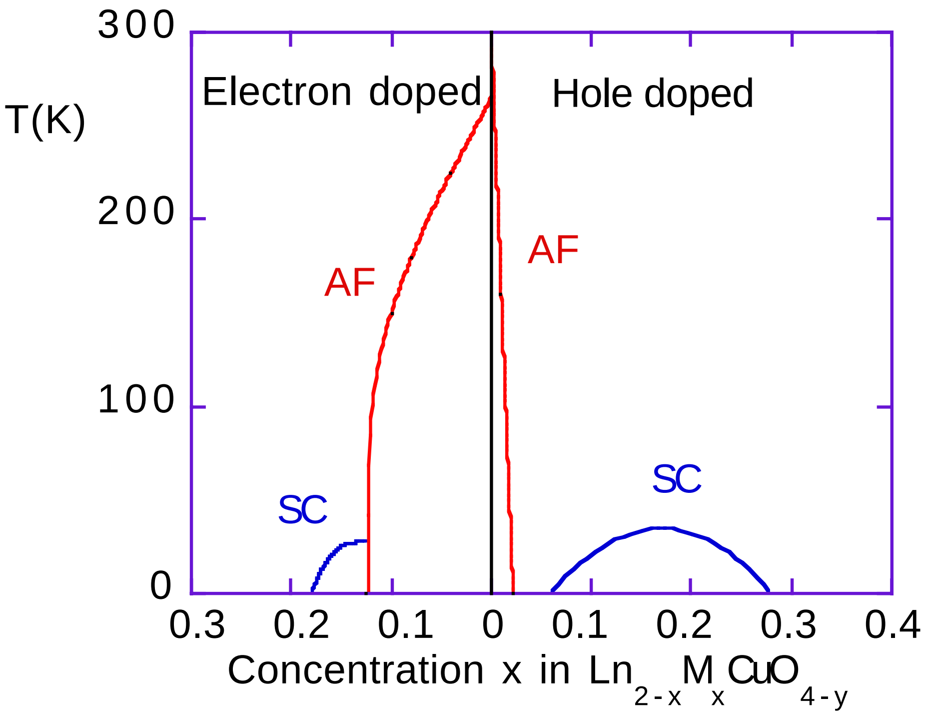
National Institute of Advanced Industrial Science and Technology (AIST)
Nanoelectronics Research Institute
T Yanagisawa
M Miyazaki
K Yamaji

Contents

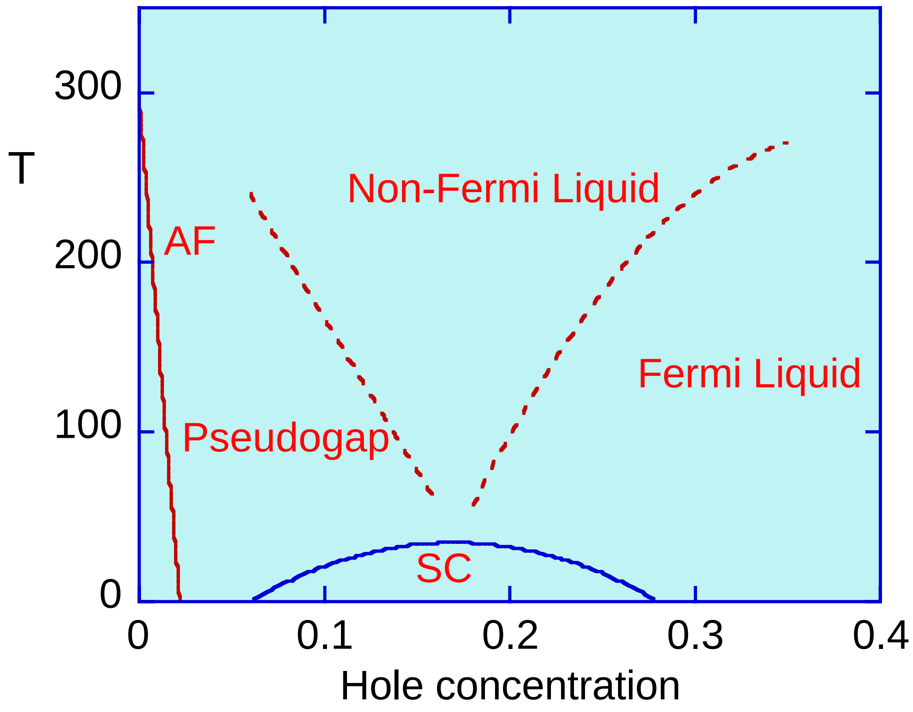
1. Introduction
    - Structural transition in cuprates
    - LTO,LTLO,LTT phases
    - Incommensurate spin correlation
2. Correlated d-wave State
    - Vertical Stripes
    - SC Condensation Energy
3. Stripes in the LTT and LTO phases
    - Diagonal stripes
4. Summary

High-Tc Superconductor: Phase diagram

Phase diagram



Theoretical suggestions

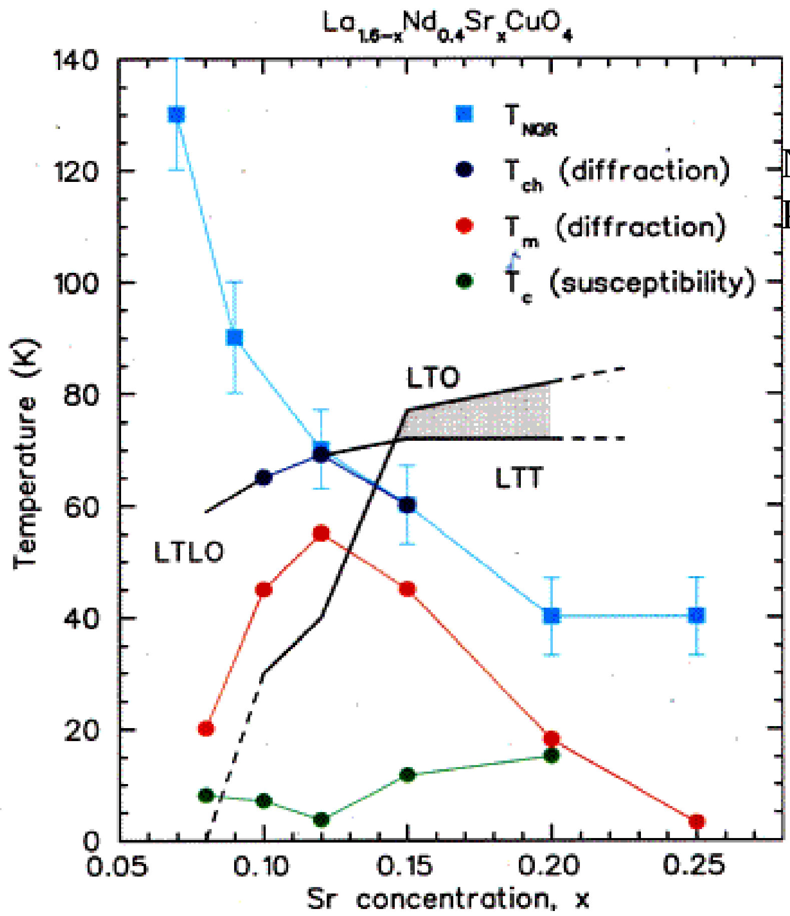


1. Introduction: Stripes and structural transition

Structural transitions: Lattice distortions

LTT,LTO,LTLO,HTT

Stripes: suggested by Incommensurability



N.Ichikawa et al. PRL85, 1738('00)

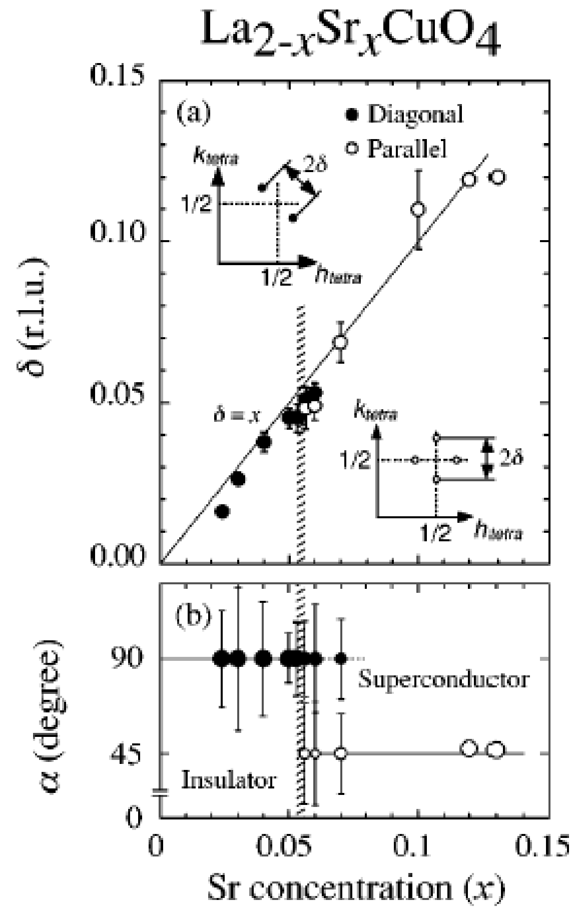


FIG. 7. Sr-concentration dependence of (a) the incommensurability δ and (b) the angle a defined in Fig. 3. Previous results for $x=0.024$ (Ref. 11), 0.04 (Ref. 10), 0.05 (Ref. 10), 0.12 (Ref. 5), 0.1 (Ref. 15), and 0.13 (Ref. 15) are included. In both figures, the solid and open symbols represent the results for the diagonal and parallel components, respectively.

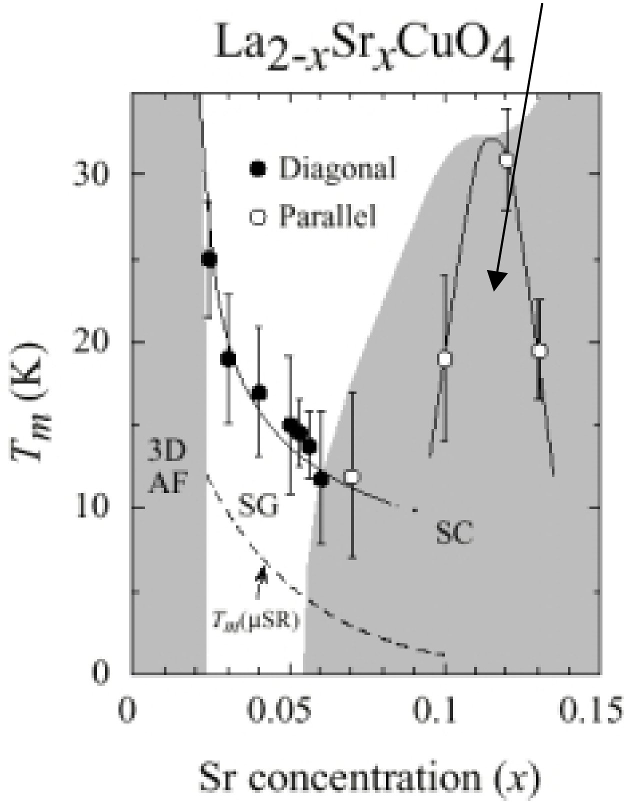
M.Fujita et al. Phys. Rev.B65,064505('02)

Lattice distortions and stripes

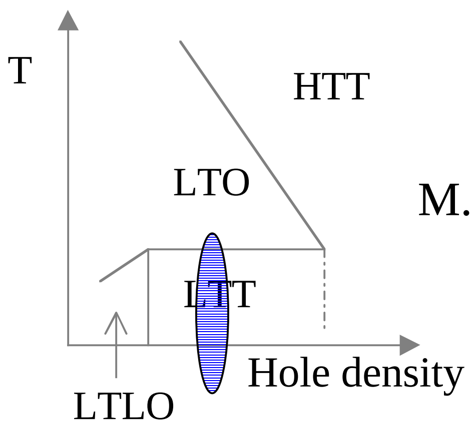
Quantum Variational Monte Carlo method

SC+stripes
Coexistence

1. Stable stripes in LTT phase
   - Vertical stripes
   - Coexistence of stripes and SC
   - SC Condensation energy
   - Stripes and tilt axis
2. Stripes and Spin-Orbit in LTO phase
   - Diagonal stripes for lightly doping
   - Flux phase



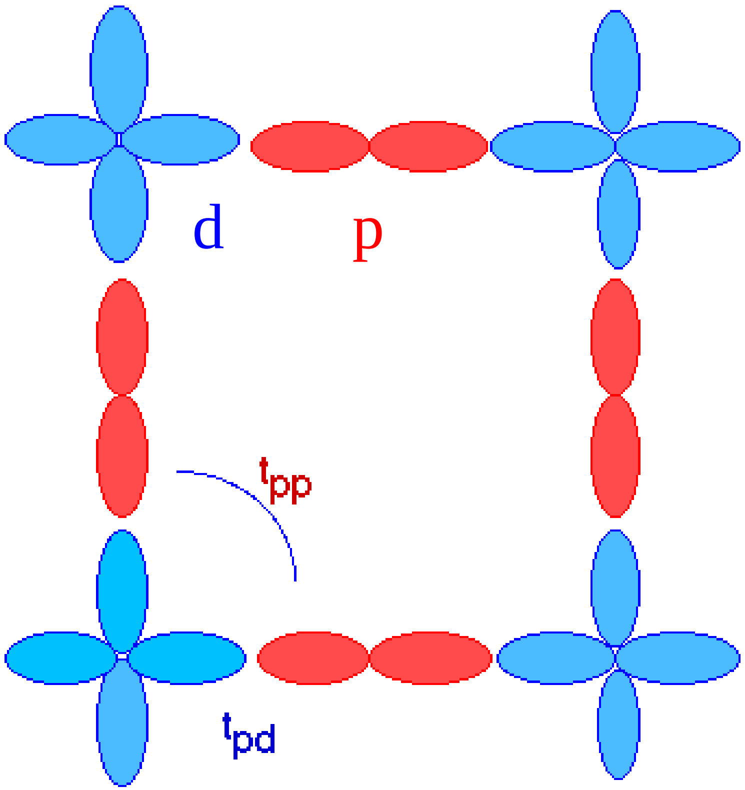
S.Wakimoto et al. PRB



M. K. Crawford et. al.

2. Correlated wave functions

3-band Hubbard model
(d-p model)



Gutzwiller function

$$H_{dp}^0 = \sum_{ij\sigma} \left(d_{i\sigma}^+ p_{i+x/2\sigma}^+ p_{i+y/2\sigma}^+ \right) \left(H_{ij\sigma}^0 \right) \begin{pmatrix} d_{j\sigma} \\ p_{j+x/2\sigma} \\ p_{j+y/2\sigma} \end{pmatrix}$$

$$V_{potential} = \sum_{i\sigma} [\rho_{di} - \sigma(-1)^{x_i + y_i} m_i] d_{i\sigma}^+ d_{i\sigma}$$

$$(H^0 + V)_{ij} u_j^\lambda = E^\lambda u_i^\lambda$$

weight

$$w = \det(\phi^+ P_G P_G \phi) \qquad \phi_{j\lambda} = u_j^\lambda$$

Hubbard-Stratonovich variables

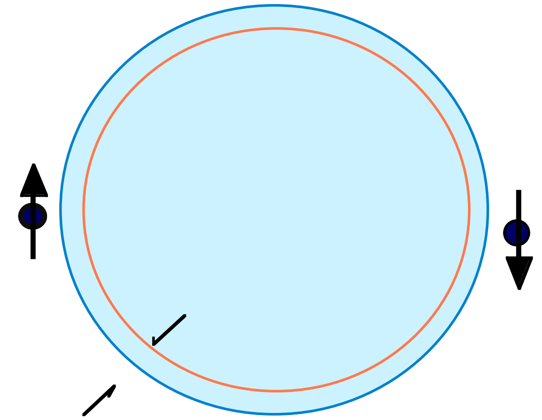
To include SC order parameter, we
Solve the Bogoliubov-de Gennes eq.

P_G = Gutzwiller operator

Superconducting state: Gossamer state

SC state in the strongly correlated electron system

$$\psi_{CdS} = P_G \prod_k (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow})|0\rangle$$



Gutzwiller Projection P_G

To control the on-site strong correlation

Weight g
Coulomb +U

Weight 1
Parameter 0<g<1

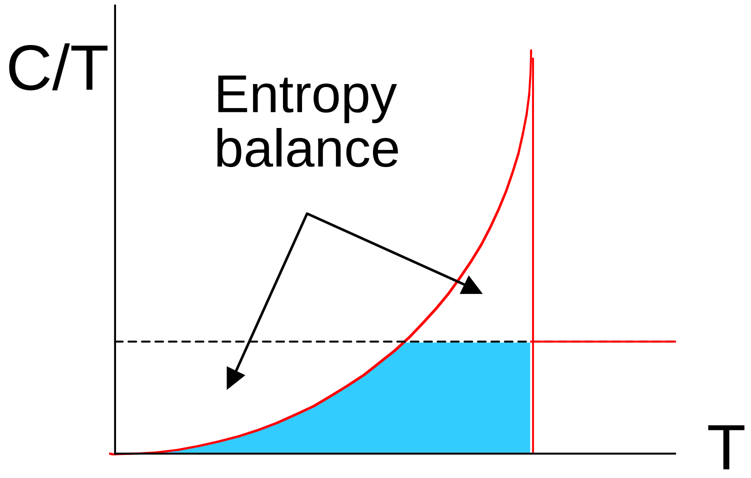
Essentially equivalent to
RVB state (Anderson)
Gossamer SC (Laughlin)
t-J, t-U-J model

Superconducting Condensation Energy

SC Condensation energy

$$\Delta E_{SC} = \Omega_n - \Omega_s = \int_0^{T_c} (S_n - S_s) dT$$

$$= \int_0^{T_c} (C_s - C_n) dT$$



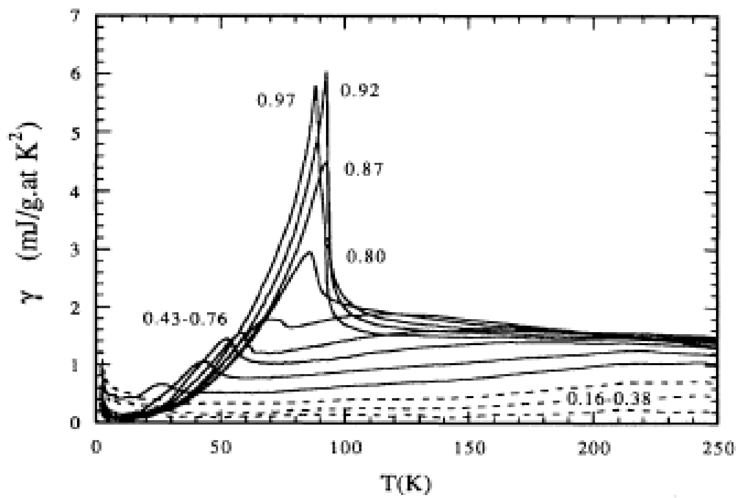


FIG. 4. Electronic specific heat coefficient $\gamma(x,T)$ vs T for $YBa_2Cu_3O_{6+x}$ relative to $YBa_2Cu_3O_6$. Values of x are 0.16, 0.29, 0.38, 0.43, 0.48, 0.57, 0.67, 0.76, 0.80, 0.87, 0.92, and 0.97.

Loram et al. PRL 71, 1740 ('93)

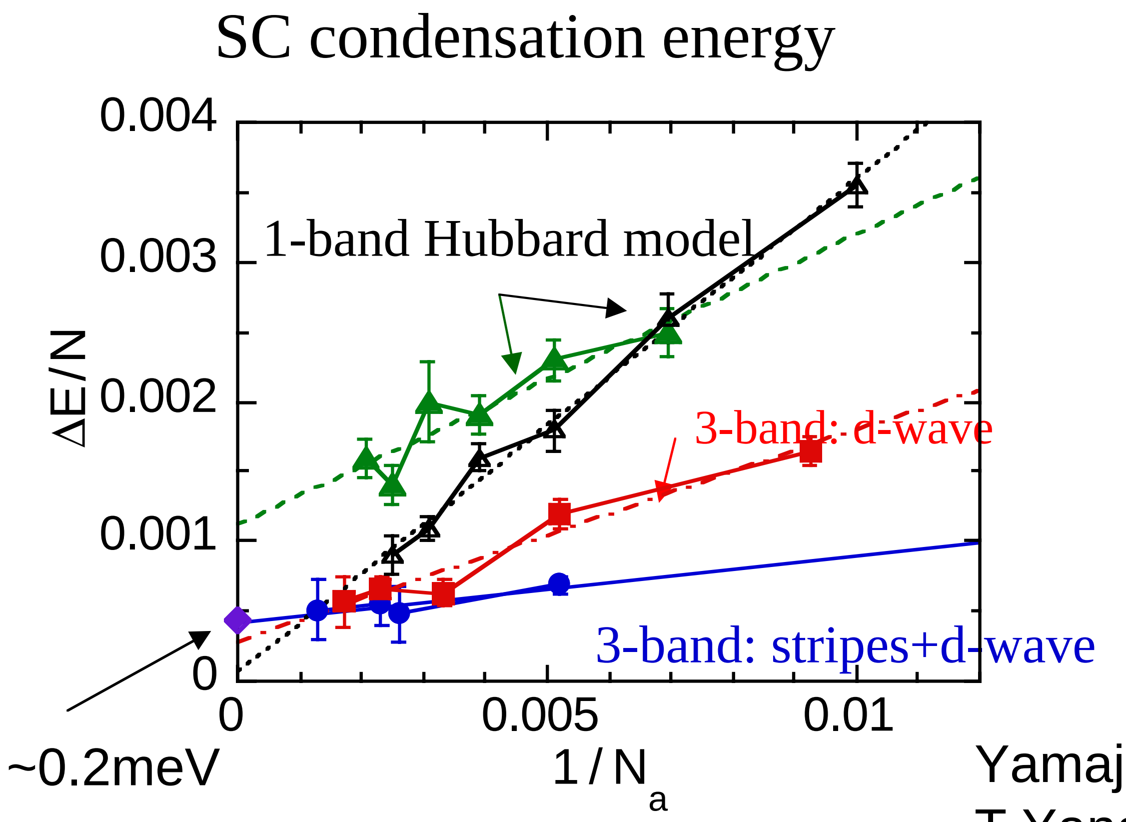
optimally doped YBCO

SC Condensation energy
~ 0.2 meV

SC Condensation Energy in VMC

SC Condensation energy in the bulk limit

Variational Monte Carlo evaluations



ΔE_{sc} = 0.00117t
= 0.59 meV/site
(ρ=0.86, t'=-0.2, U=8)

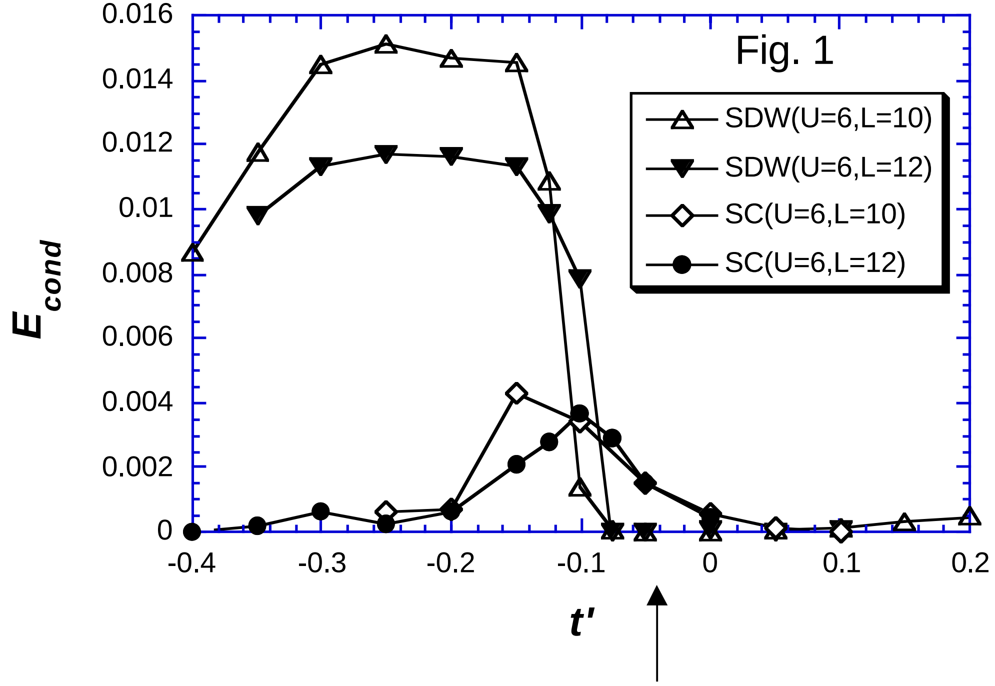
Experiments
0.26 meV/site
(critical field H_c)
0.17~0.26 (C/T)

Agreement is good!

Yamaji et al., Physica C304, 225('98)
T.Yanagisawa, Phys. Rev.B67,132408

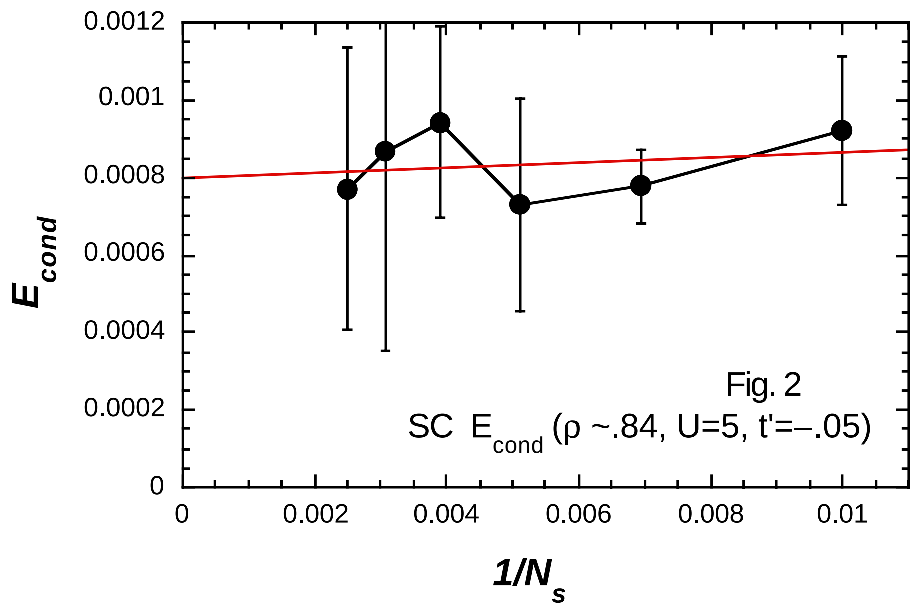
Superconductivity and Antiferromagnetism: Competition

SC and AF



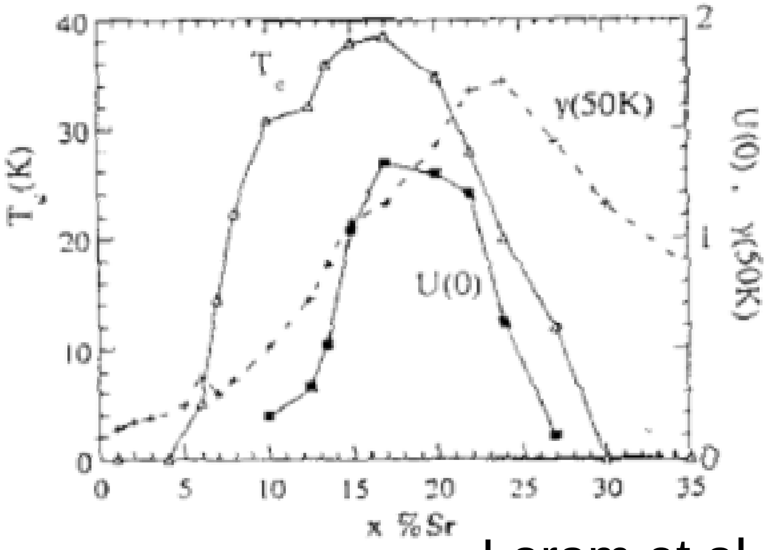
Pure d-wave SC

Size dependence of
SC condensation energy



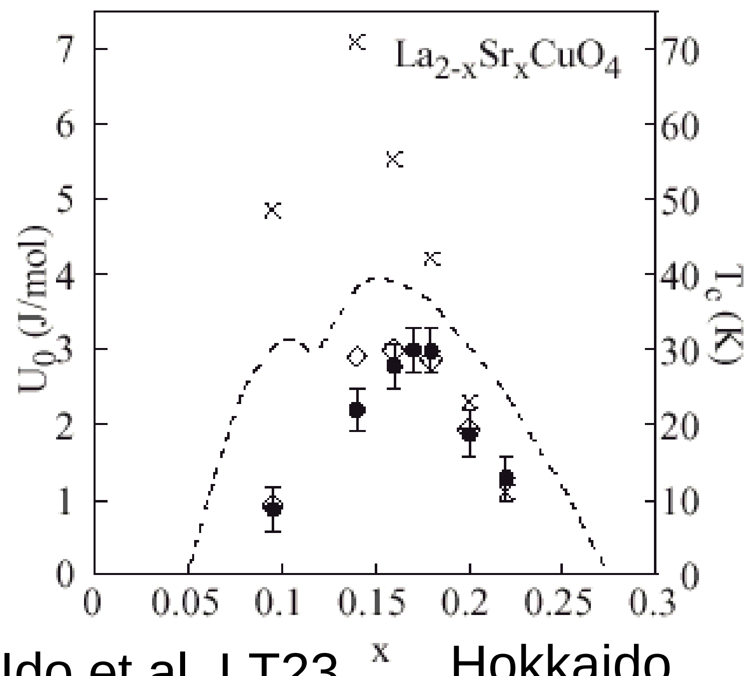
Carrier density dependence of condensation energy

Decrease of ΔE_{sc} due to Stripe order



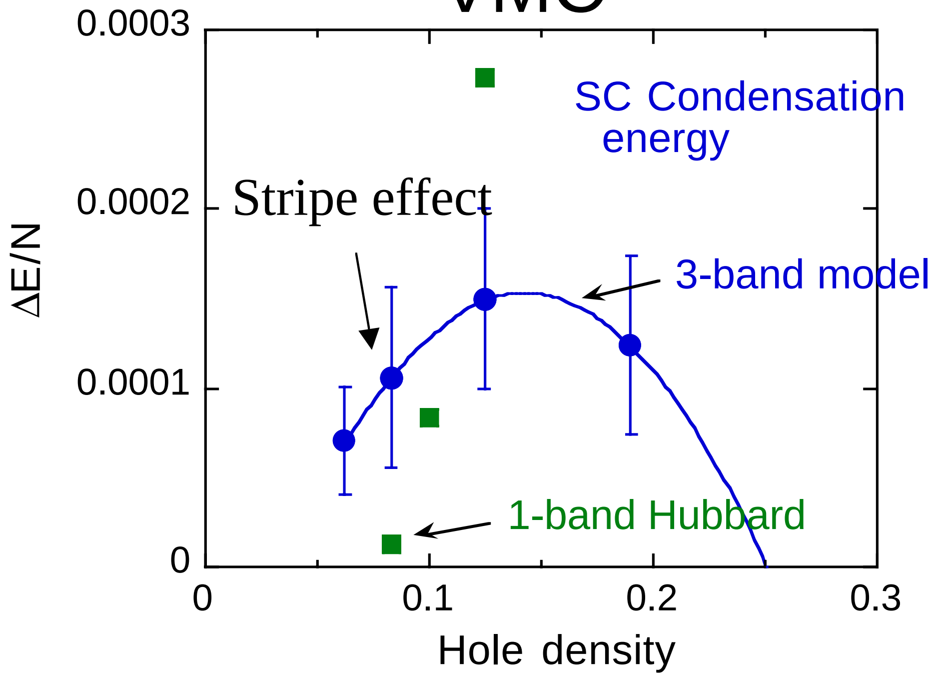
Loram et al.

Figure 18 T_c, $U(0)$ (J/g-at) and $\gamma(50K)$ (mJ/g-at.K²) for $La_{2-x}Sr_xCuO_4$



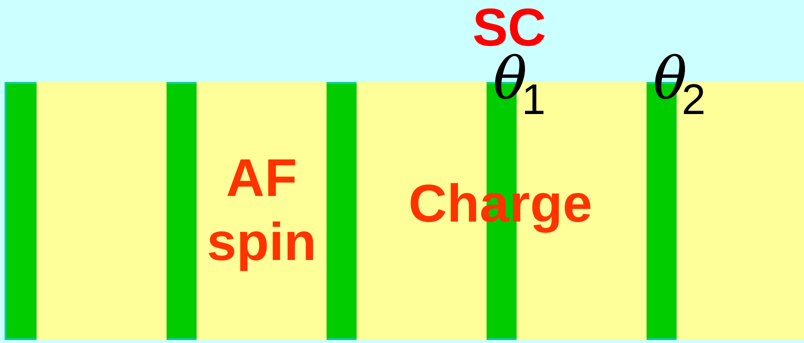
M.Ido et al. LT23 Hokkaido

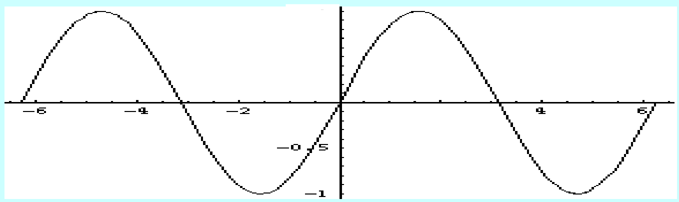
VMC



Coexistence of d-wave SC and stripes

Inhomogeneous SC state





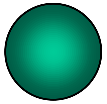
SC order parameter

Vanishing SC order parameter in AF (hole poor) domain

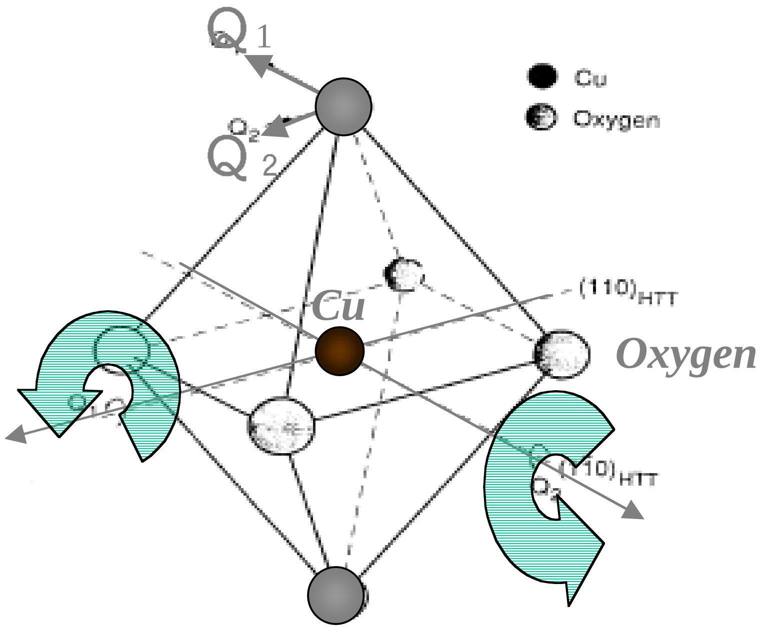
Relative π-phase shift across the AF domain

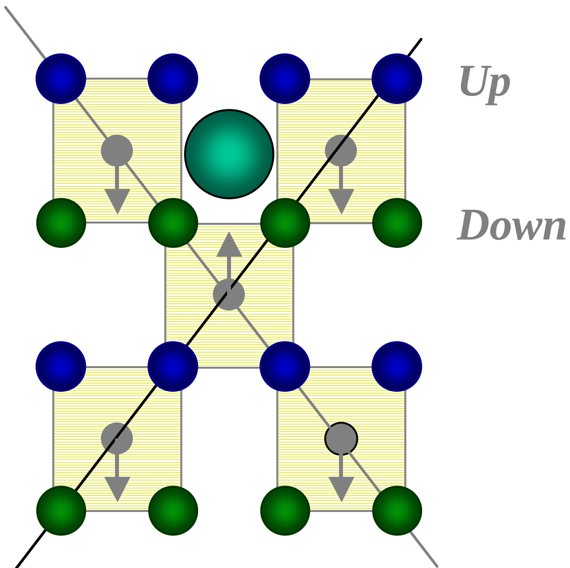
$$\theta_1 - \theta_2 = \pi$$

3. Lattice distortions

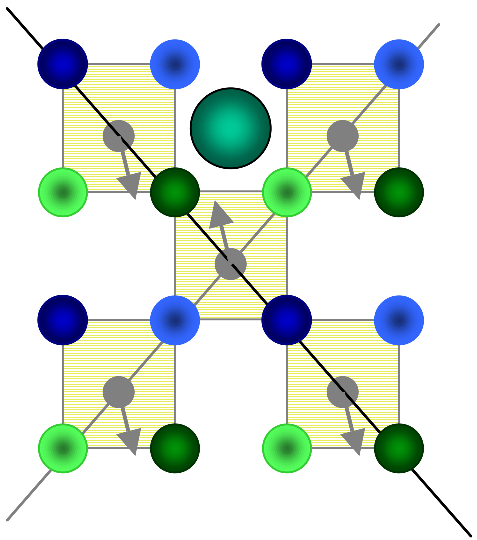


Lanthanide (La, Nd, Eu)
Sr, Ba

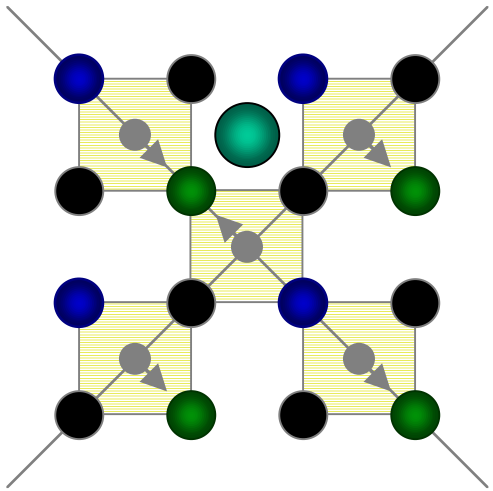




LTO (Q1=0,Q2≠0)



LTLO (Q1≠Q2≠0)

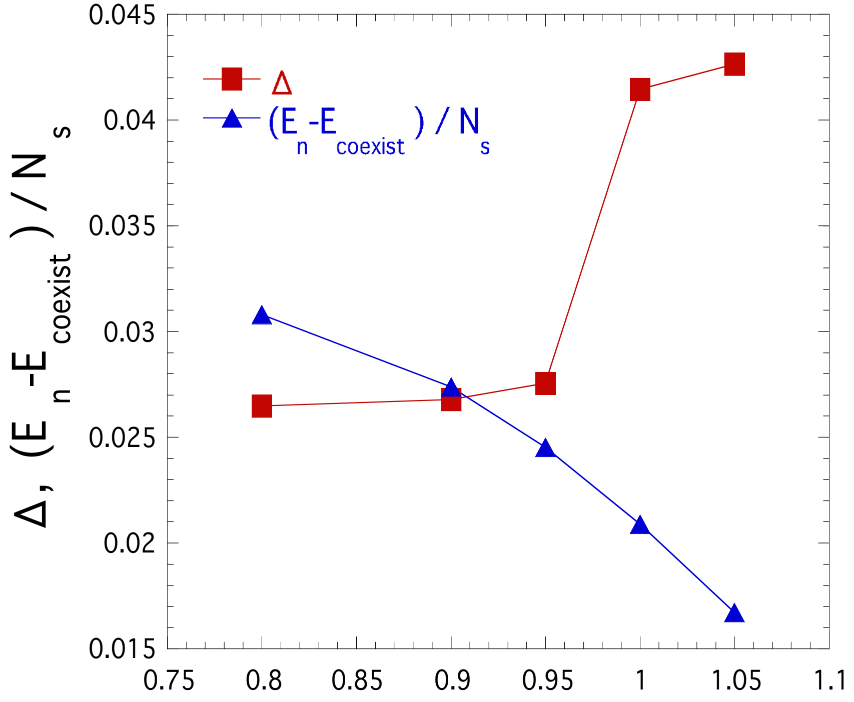


LTT (Q1= Q2 ≠0)

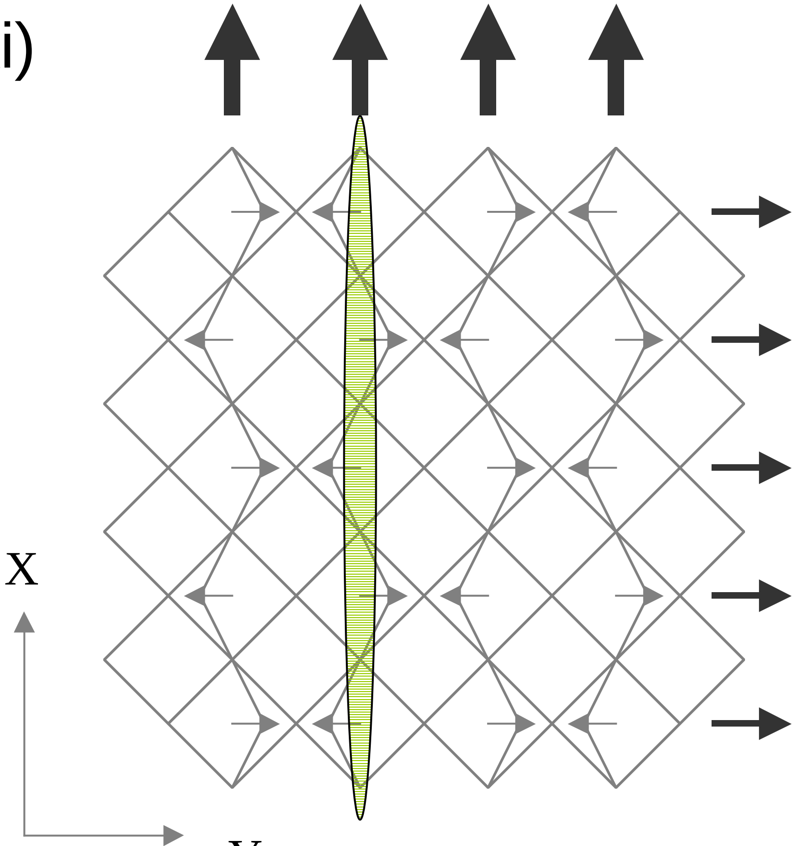
Anisotropy of the transfer integrals in LTT phase

Cf. A. P. Kampf et. al. PRB 64 (2001) 052509

One-band Hubbard model (Miyazaki)



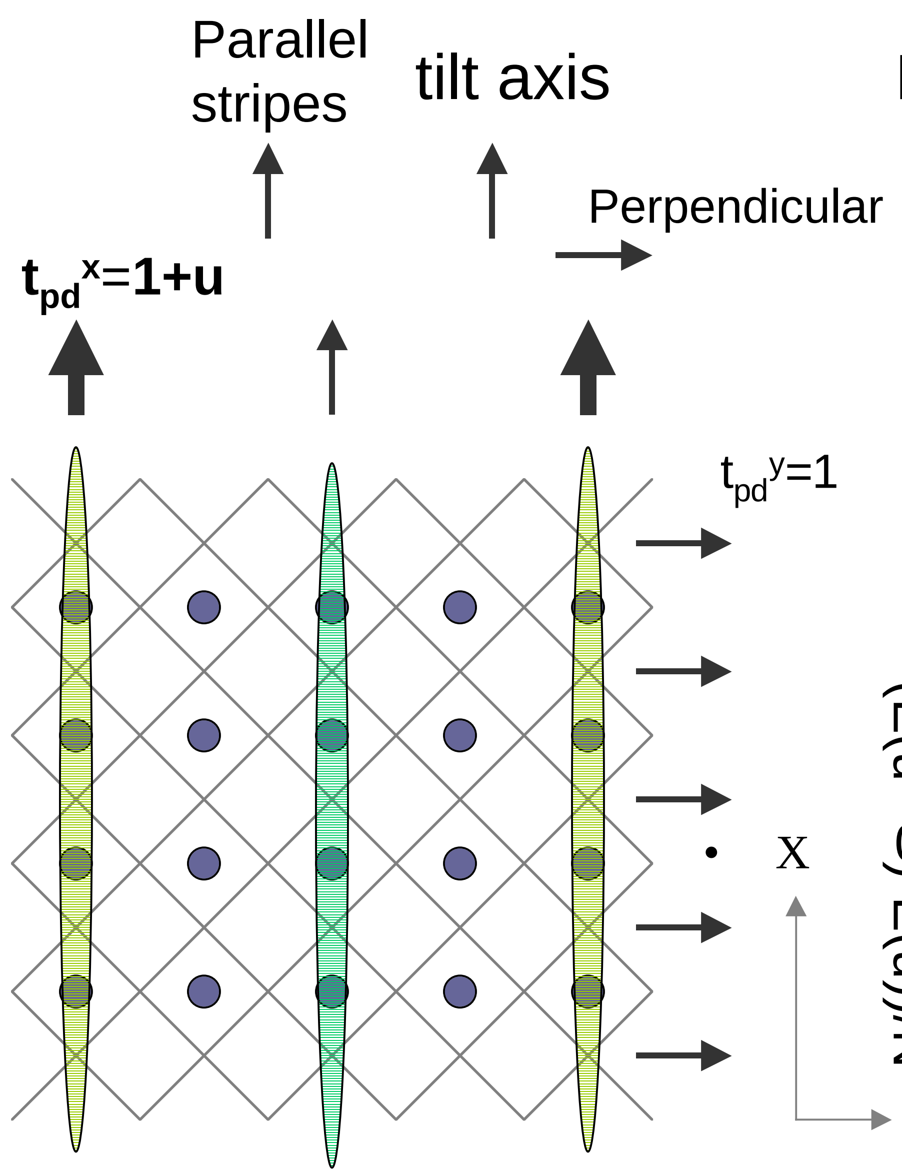
- $\beta = t_y / t_x$

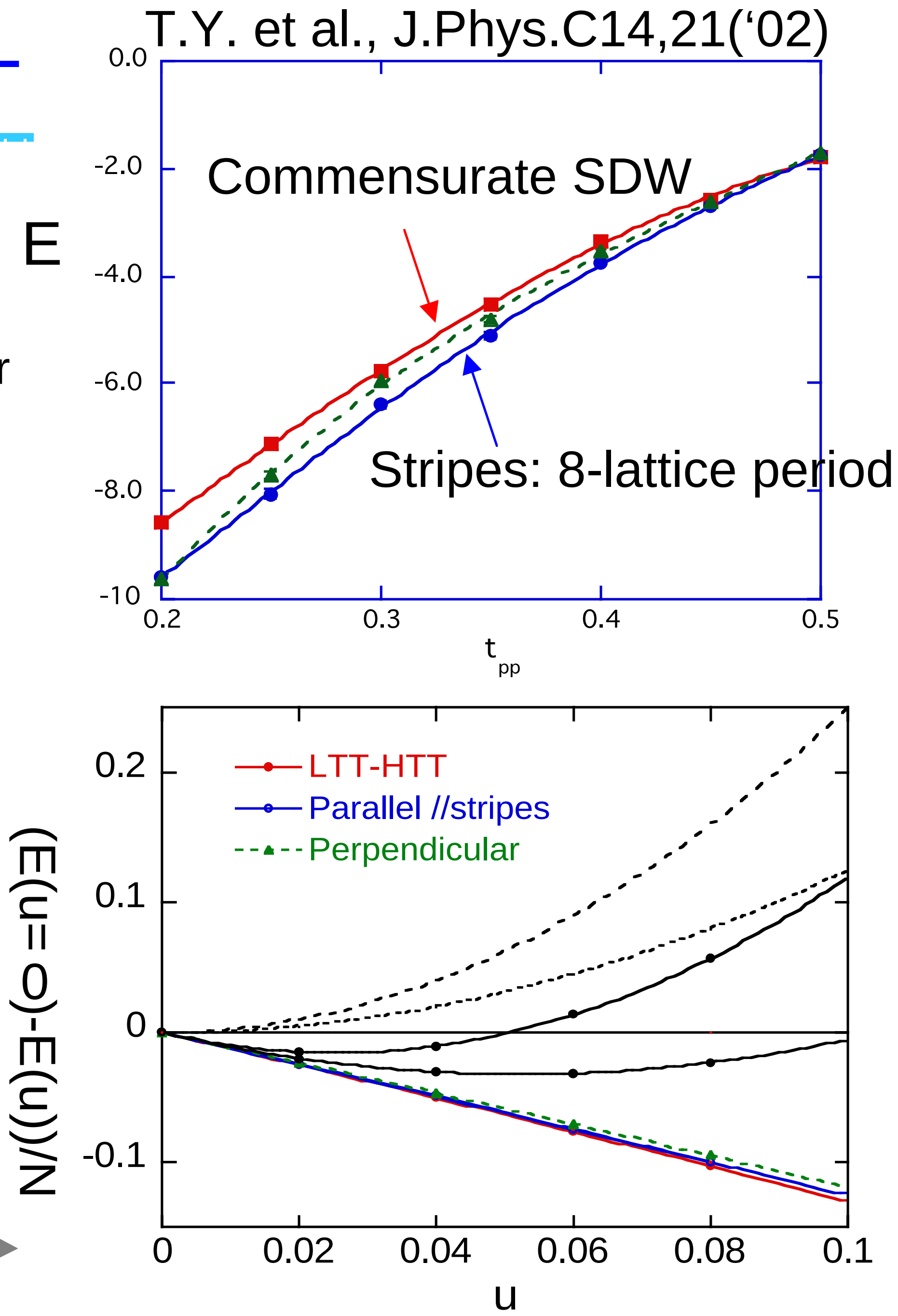


- X
- Y

LTT structural transitions stabilize stripes.

Vertical Stripes in LTT





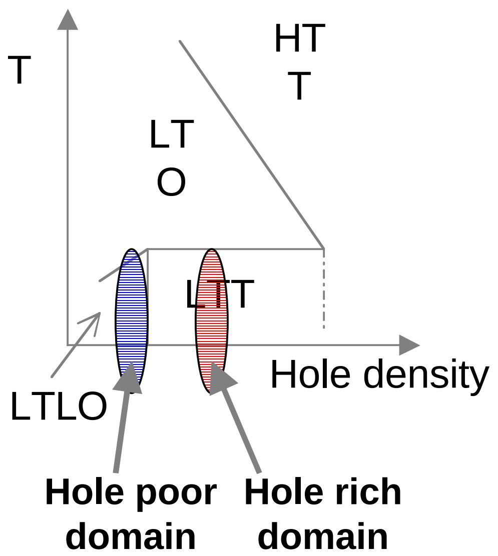
Possible Stripe Structures 1

E. S. Bozin et. al. PRB 59 (1999) 4445
Lanzara et. al. J. Phys. Cond. Mat 11 (1999) 541

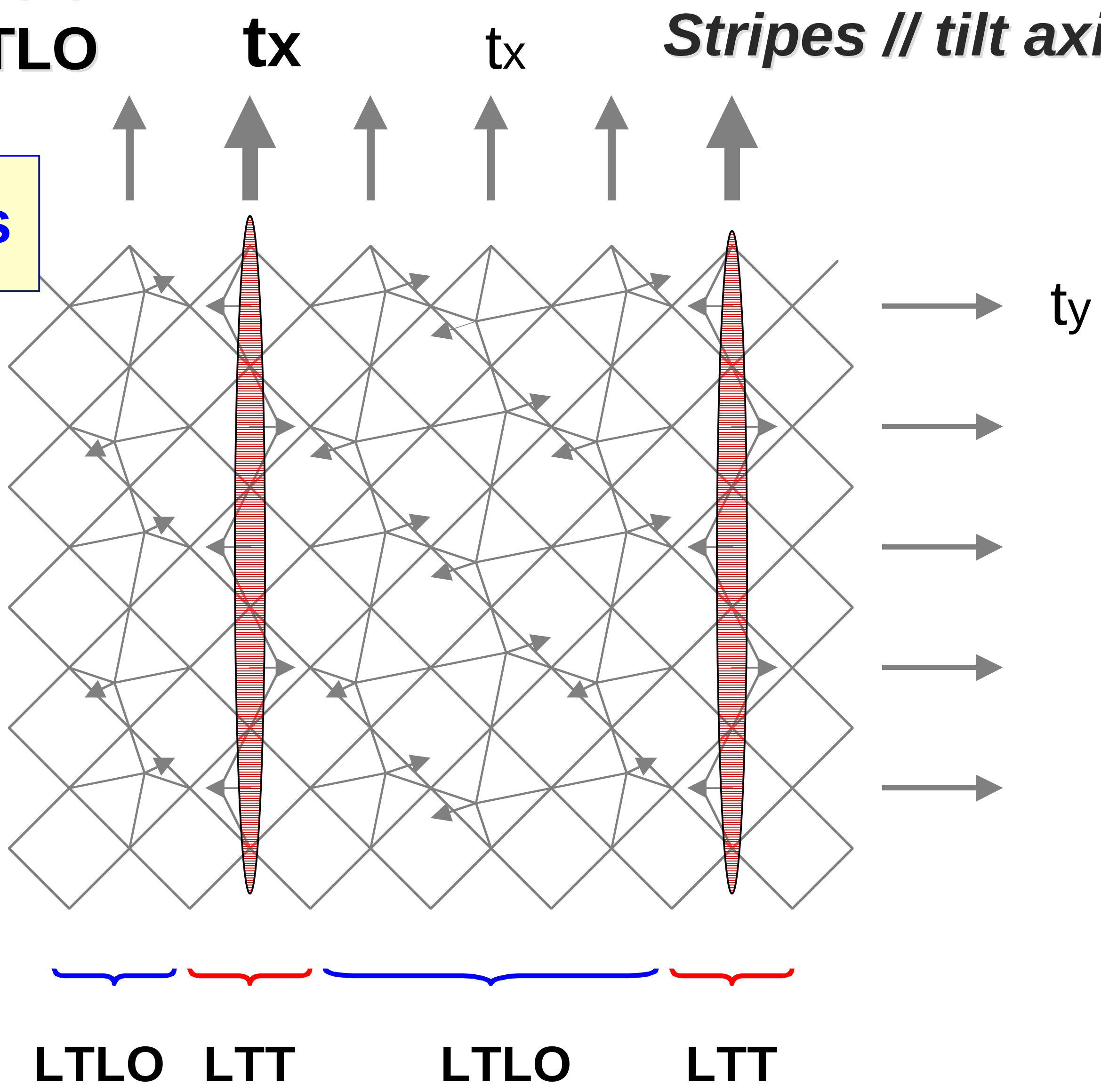
Mixed phase of LTT and LTLO

Stabilize stripes

M. K. Crawford et. al.



Stripes // tilt axis



Possible Stripe Structures 2

LTT and HTT

Oscillation of tilt angle

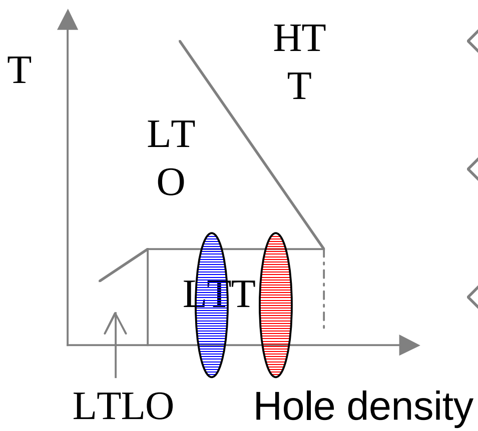
B.Buchner et. al. PRL 73(1994)1841

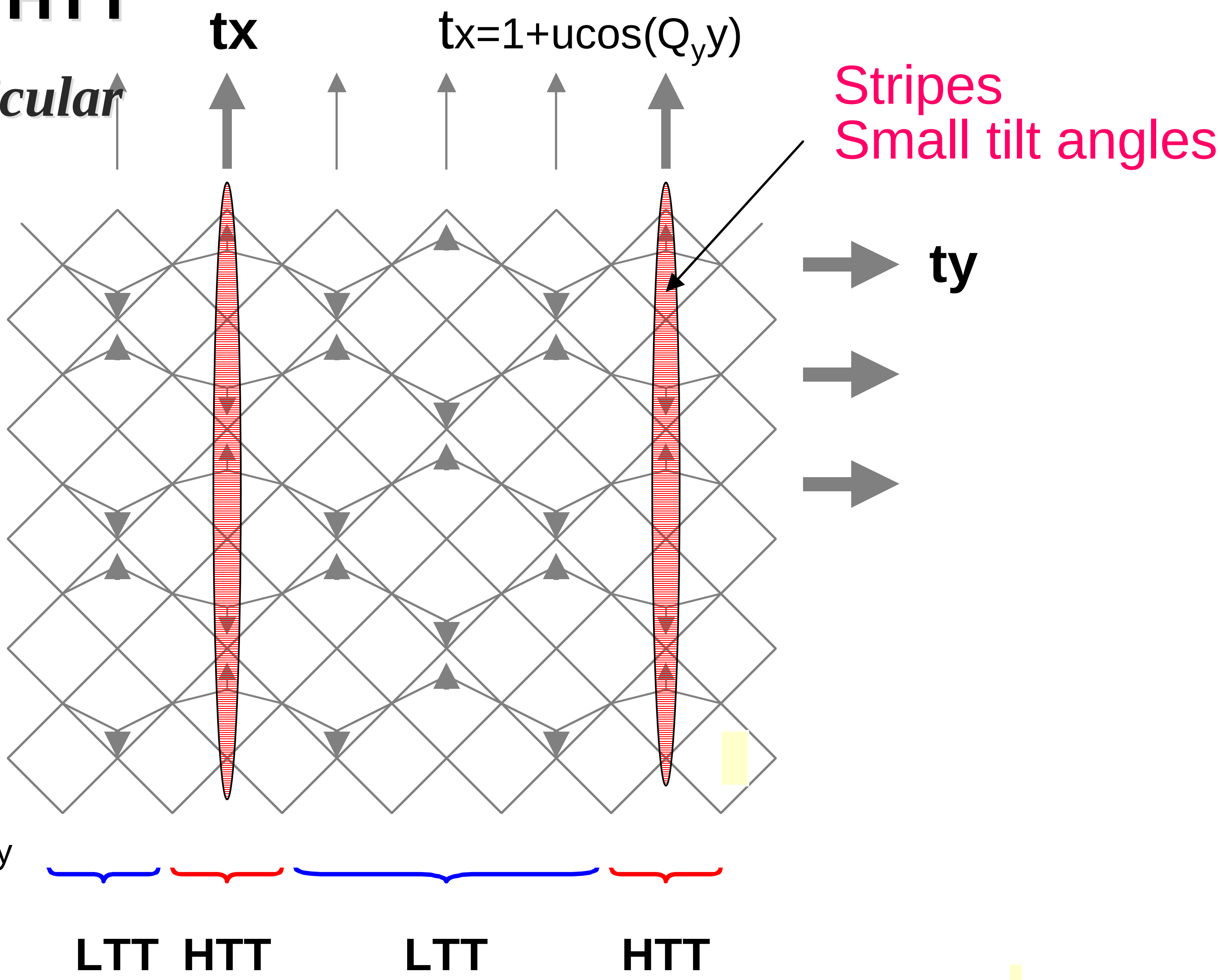
H.Oyanagi et al., T.Y.et al. LT23 Proc.

Stripes perpendicular to tilt axis

stable

M. K. Crawford et. al.





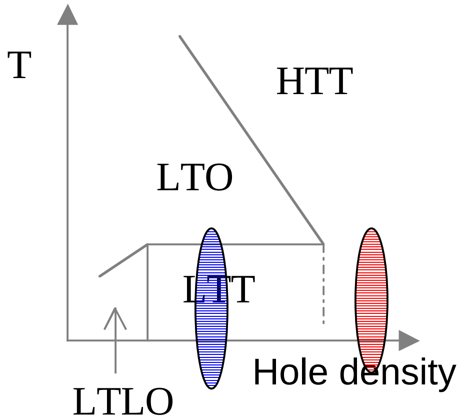
Possible Stripe Structures 3

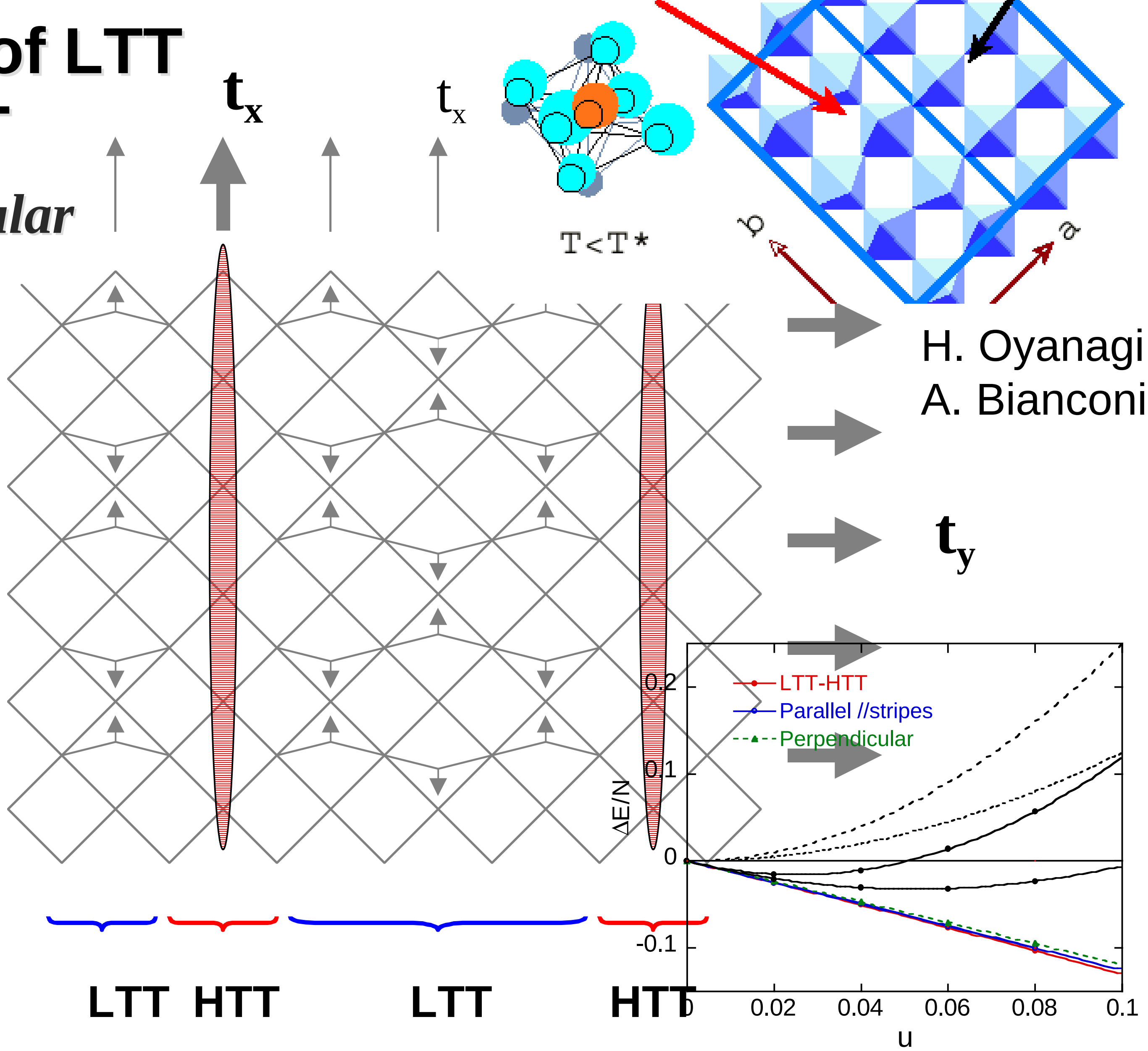
Mixed phase of LTT and HTT

Stripes perpendicular to tilt axis

Stable

M. K. Crawford et. al.





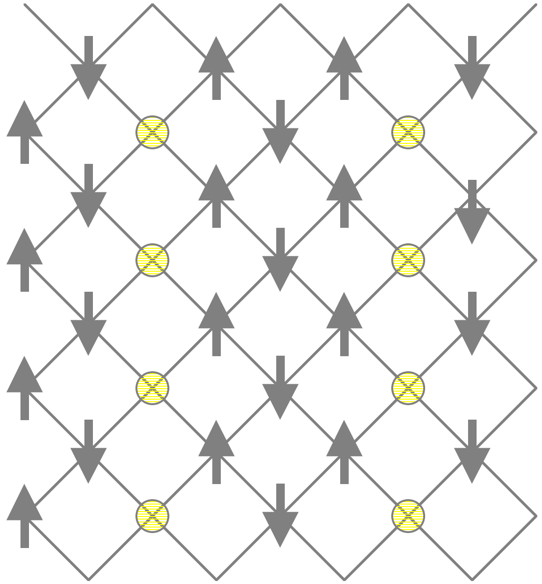
H. Oyanagi
A. Bianconi

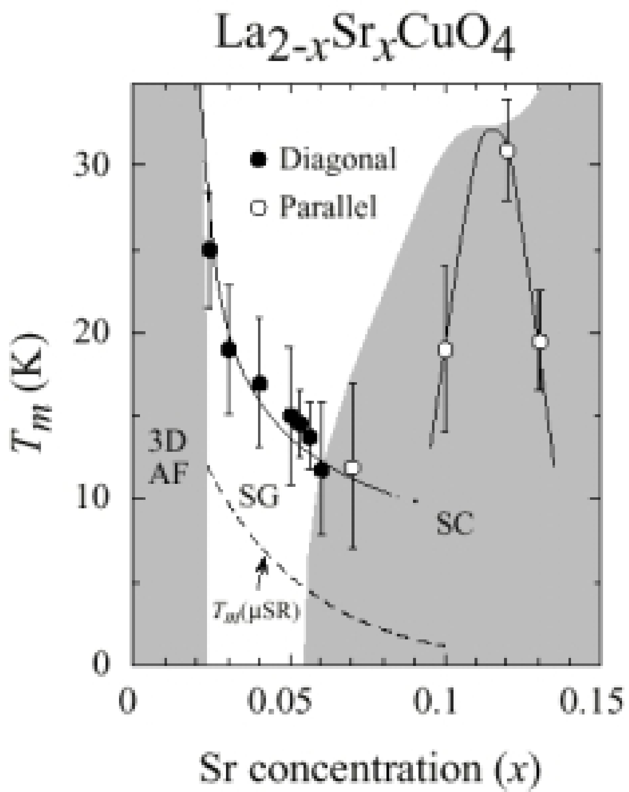
Diagonal stripes in lightly doped region

Diagonal stripes are observed for

$La_{2-x}Sr_xNiO_4$
$La_{2-x}Sr_xCuO_4$
$La_{2-x-y}Nd_ySr_xCuO_4$

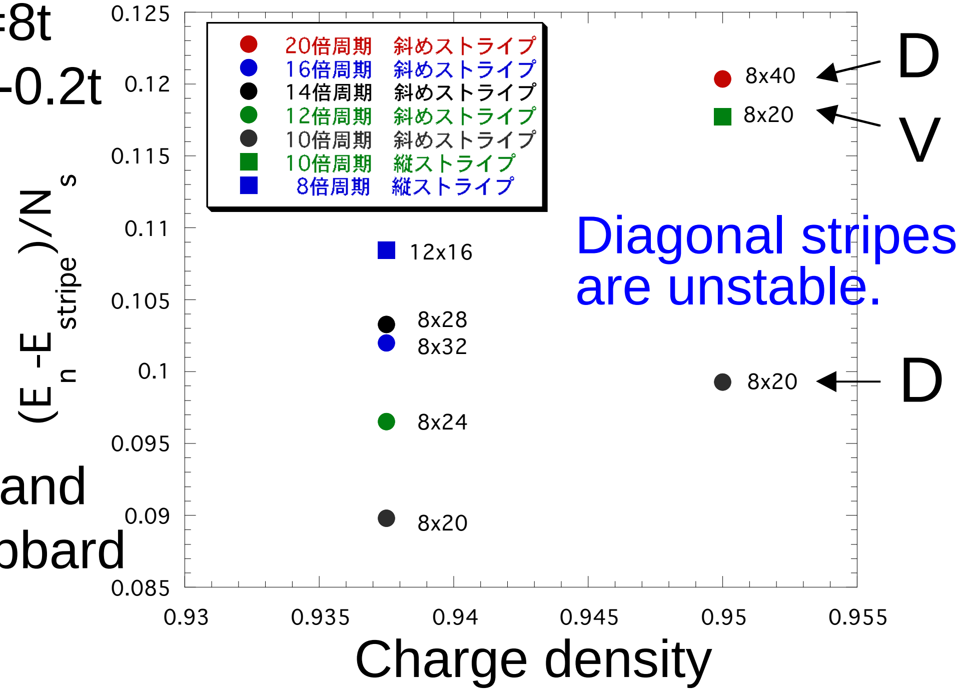
in the lightly doped region.





U=8t
t'=-0.2t

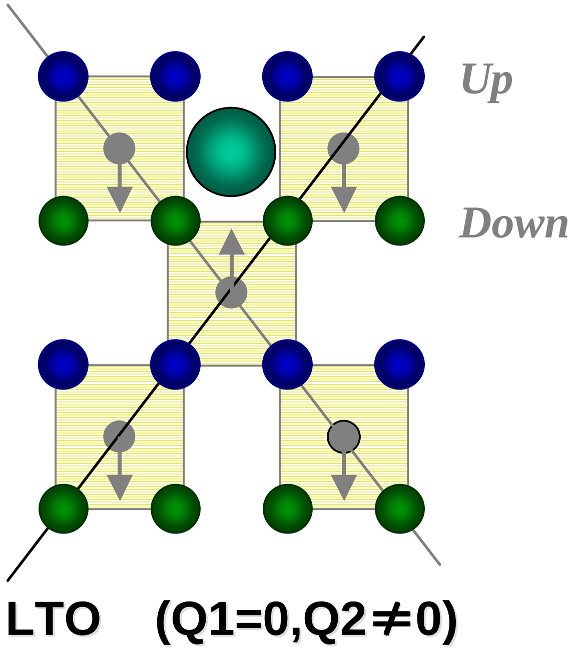
1-band Hubbard

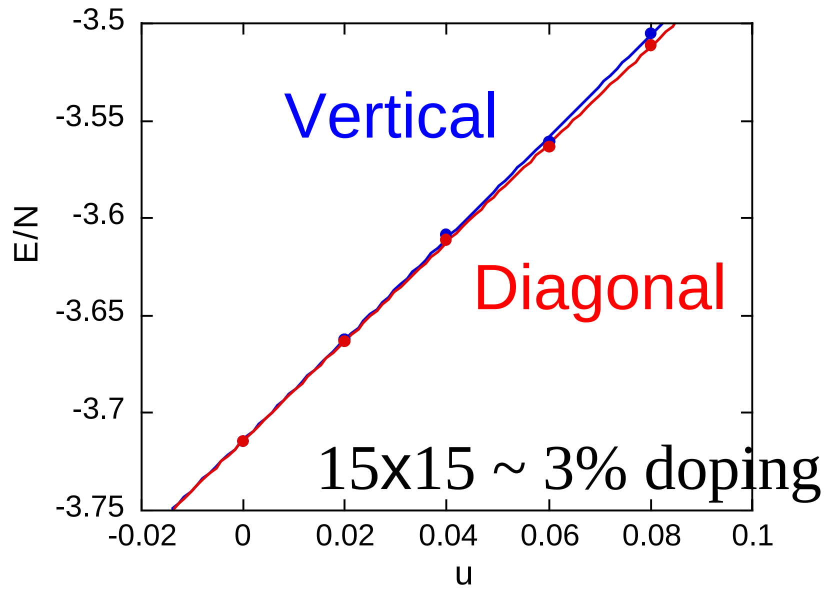


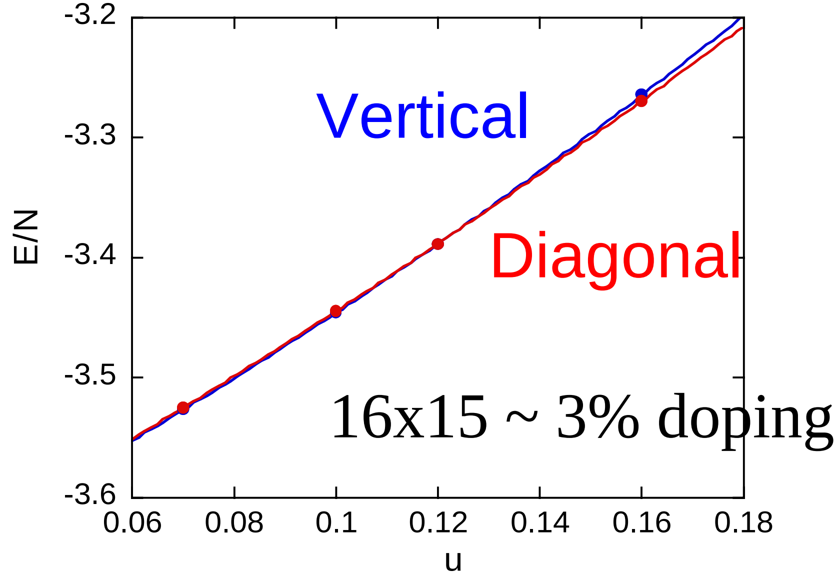
Diagonal Stripes in LTO structure

Anisotropy in t_{pp} transfer stabilizes diagonal stripes.

$t_{pd} \rightarrow t_{pd}$ (1-u) $t_{pp} \rightarrow t_{pp}$ (1-u) (one direction)







4. Spin-Orbit Coupling

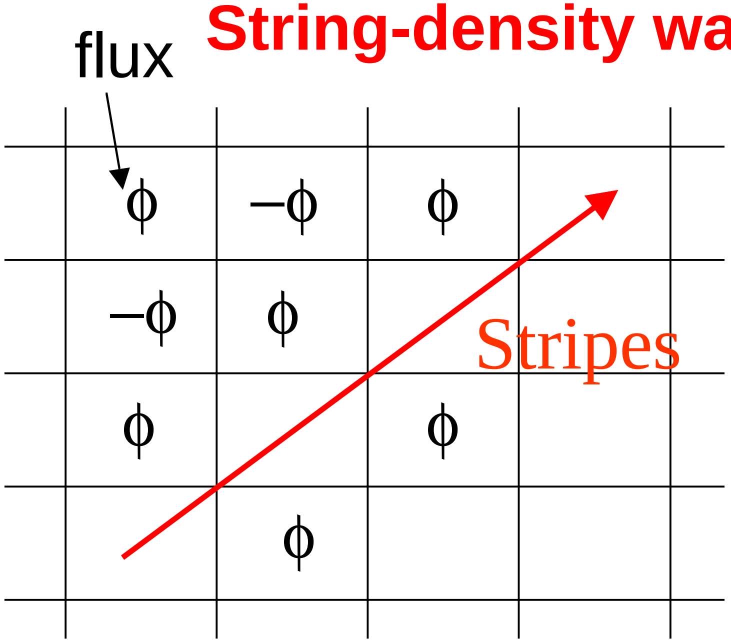
Buckling in the Cu-O plane
Induces spin-orbit coupling.

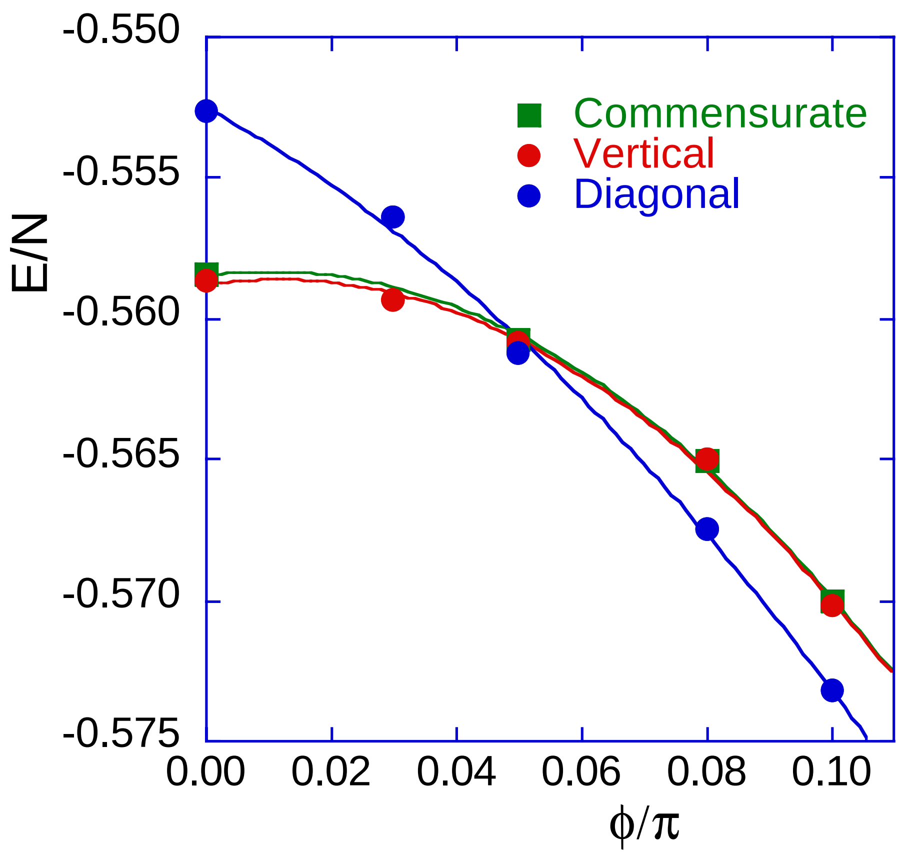
$$H_{kin} = -\sum_{ij\sigma}(t_{ij} + ic\sigma\theta_{ij})d_{i\sigma}^{+}d_{j\sigma}$$

(Bonesteal et al.,PRL68,2684('92))

Flux state and Diagonal Stripes in underdoped (lightly) region

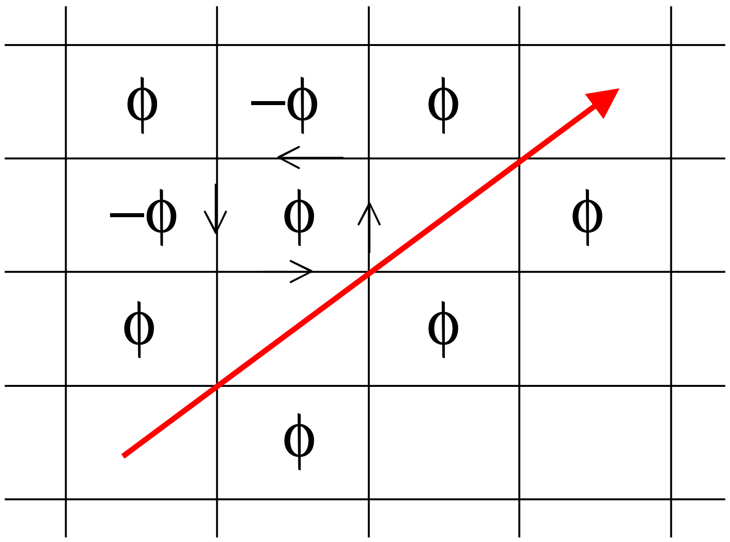
String-density wave



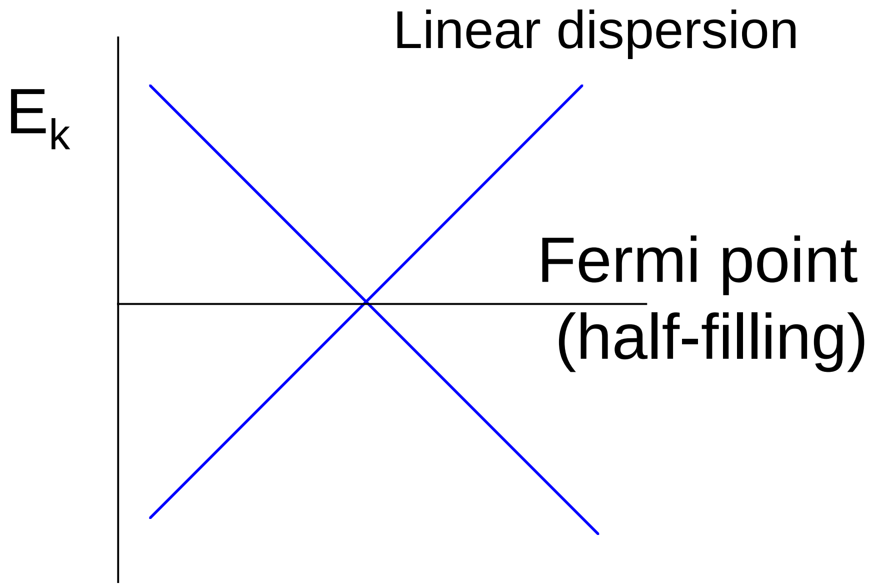


Flux state

$$E(k_x,k_y)=\pm\left|e^{i\phi/4}e^{ik_x}+e^{-i\phi/4}e^{ik_y}+e^{i\phi/4}e^{-ik_x}+e^{-i\phi/4}e^{-ik_y}\right|$$



Excitation: Dirac fermion



Insulating or
Bad metal state
(small Fermi surface)

5. Summary

1. SC condensation energy agrees with experiments based on the Correlated d-wave SC function (Gossamer state).
2. Vertical stripes are stable in the LTT phase.
   Mixed LTT-HTT is most stable.

	lightly	under	optimal	over
LTT	Vertical	Vertical	(V?)	Comm.
LTO	Diagonal	Vertical	(V?)	Comm.

ΔE_{sc} ~ 0.2 meV

(optimally doped)