Theoretical Study of High Temperature Superconductivity

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Outline

1. Introduction
2. Superconductivity
3. High Temperature Superconductivity
4. Hubbard Model
5. Variational Monte Carlo method
6. Stripes in high-Tc cuprates
7. Spin-orbit coupling and Lattice distortion
8. Summary

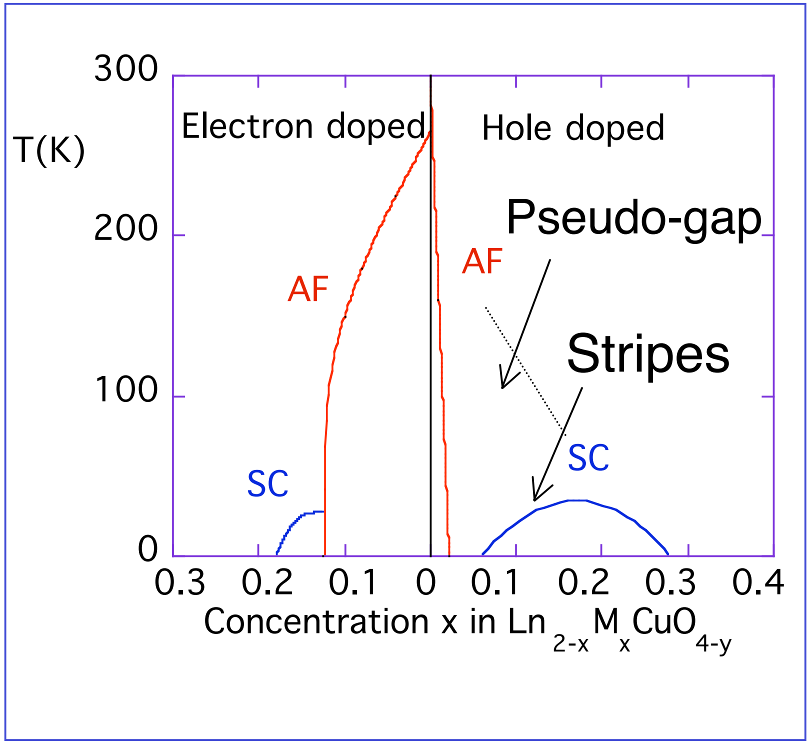
1. Introduction

Key words: Physics from U (Coulomb interactions)

- A possibility of superconductivity
  Superconductivity from U

- Competition of AF and SC

- Incommensurate state
  Stripes and SC
  Compete and Collaborate



- Stripes in the lightly-doped region

- Singular Spectral function

Purpose of Theoretical study

1. Origin of the superconductivity
   - Symmetry of Cooper pairs
   - Mechanism of attractive interaction

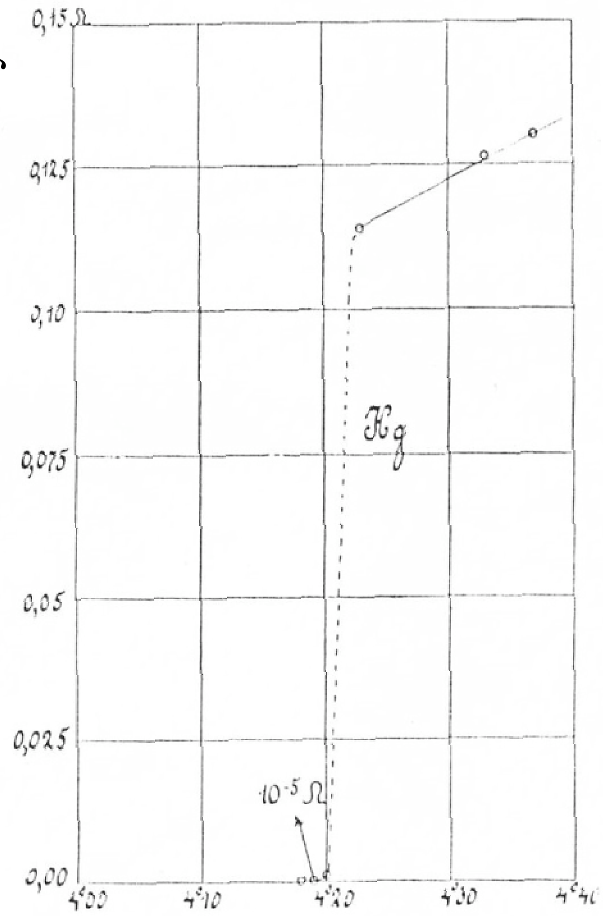
     Coulomb interaction U, Exchange interaction J

2. Physics of Anomalous Metallic behavior
   - Inhomogeneous electronic states: stripe
   - Pseudogap phenomena
   - Structural transition LTO, LTT

2. Superconductivity

1911 Kamerlingh Onnes

Resistivity



Temperature K

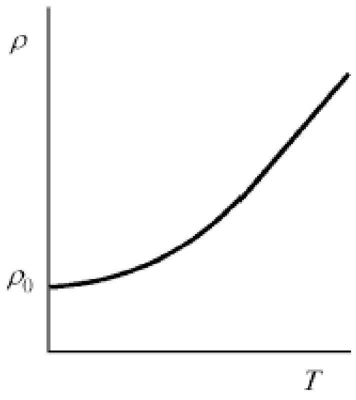
Elements that become superconducting

Superconductive at low temperatures

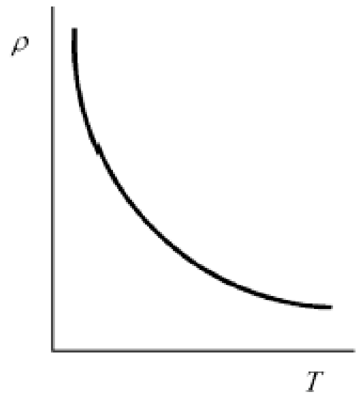
Superconductive under pressure

Characteristics of Superconductivity

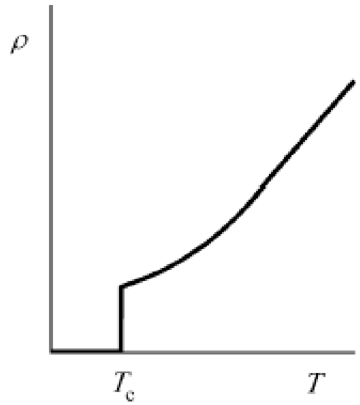
Electrical Resistivity



Metal

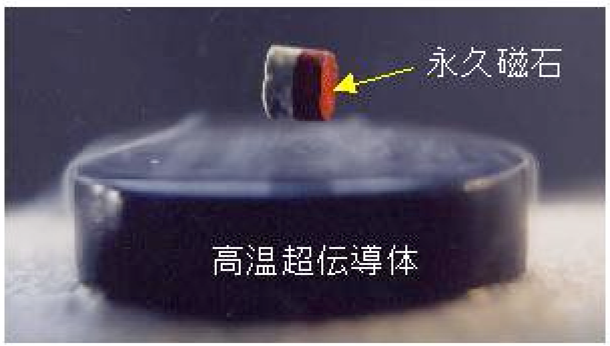


Semiconductor



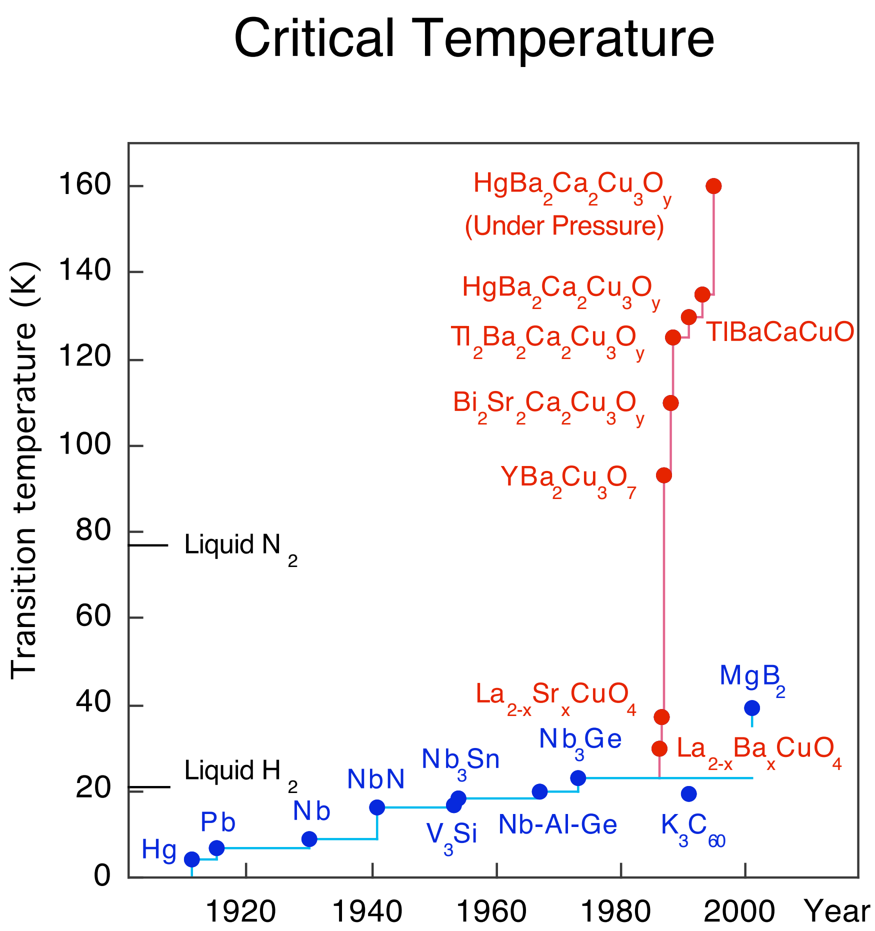
Superconductor

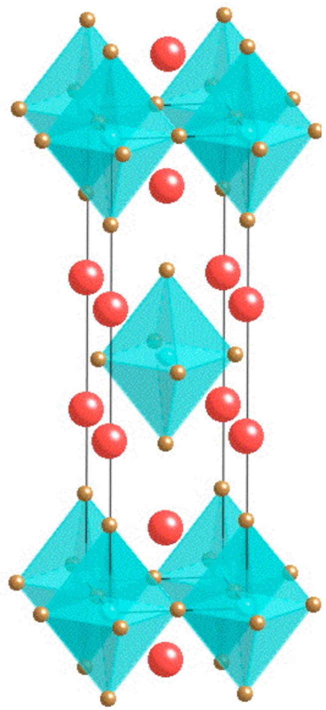
Meissner effect



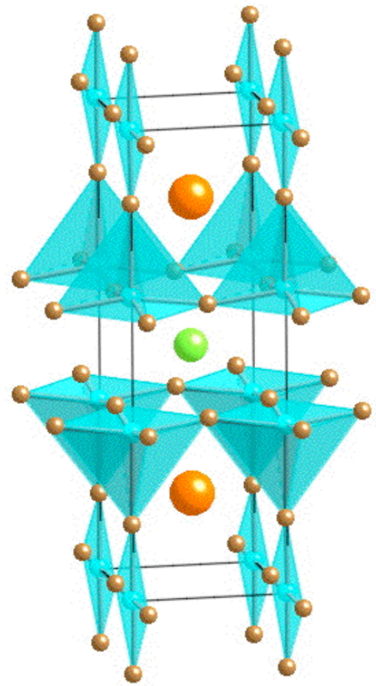
Exclusion of a magnetic field from a superconductor

3. High Temperature Superconductors





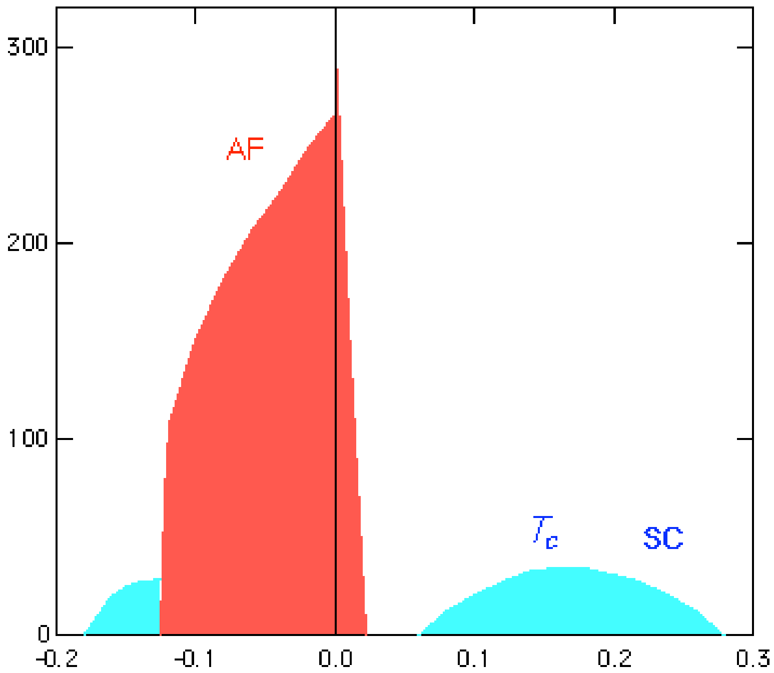
La_2CuO_4



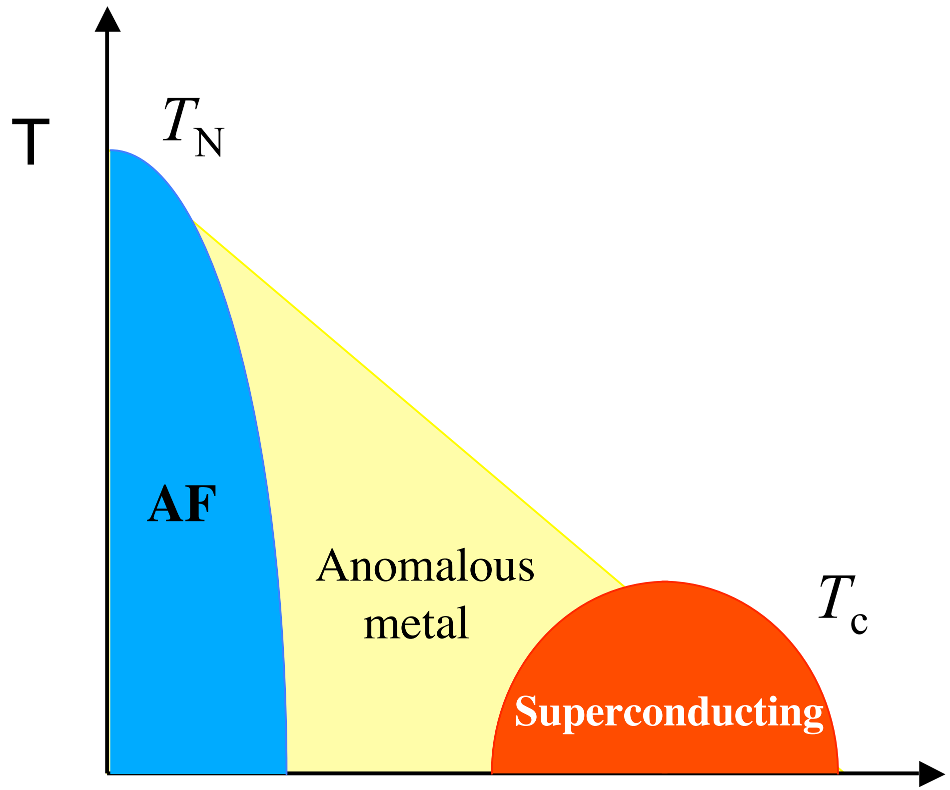
$YBa_2Cu_3O_7$

Phase Diagrams

Phase diagram of HTSC



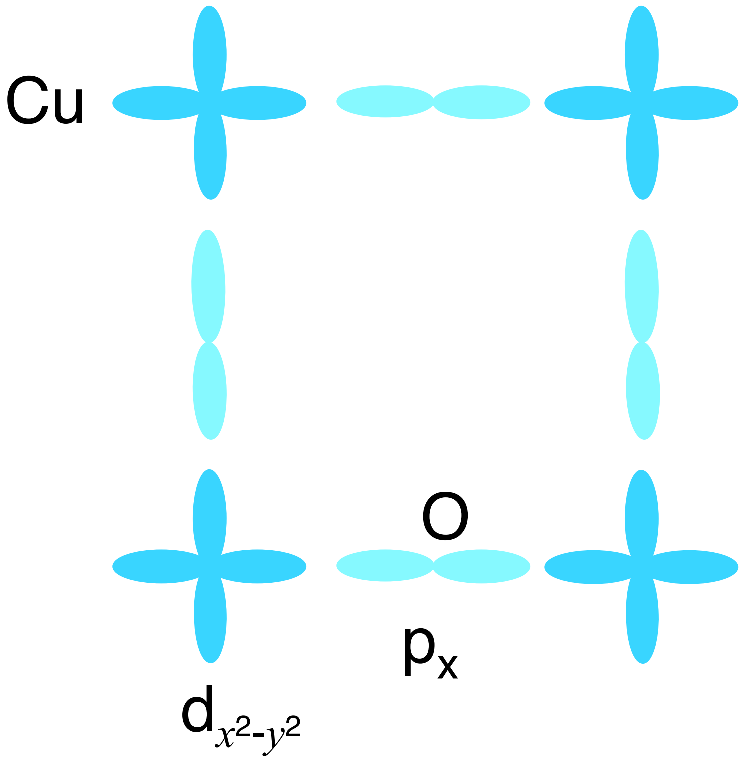
Hole density Electron density

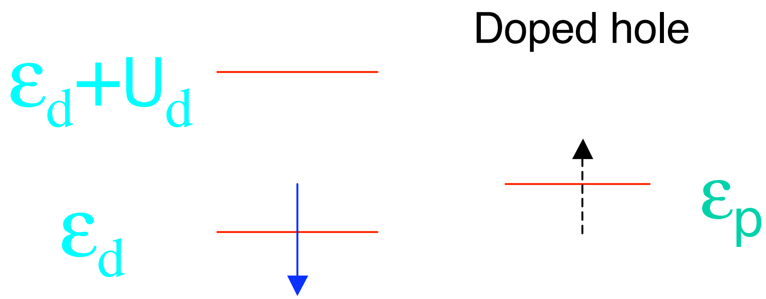


Carrier density

Model of HTSC

Two-Dimensional Plane





Characteristics

- Two dimensional
- Low spin 1/2
- O level is very closed to Cu level.

Temperature dependence of Resistivity

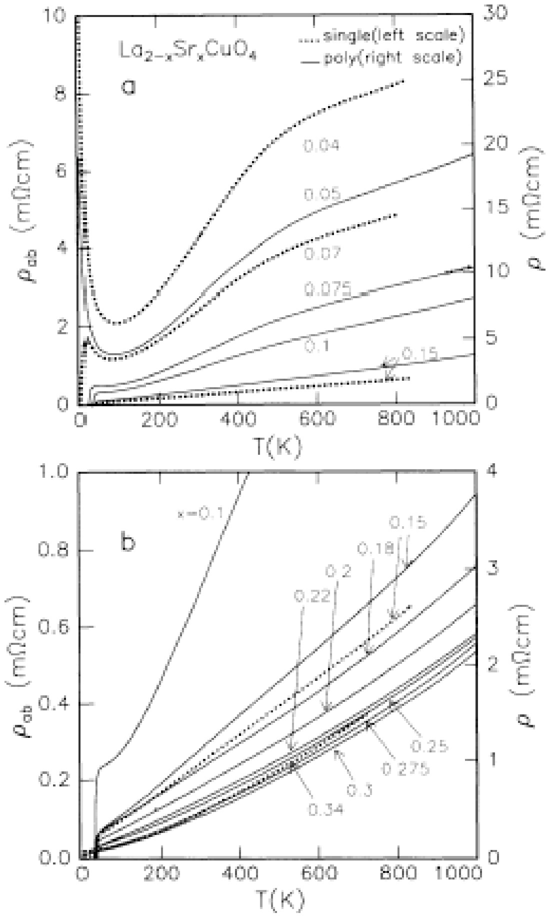


FIG. 1. The temperature dependence of the resistivity for $La_{2-x}Sr_xCuO_4$. (a) $0 < x \leq 0.15$, (b) $0.1 \leq x < 0.35$. Dotted lines, the in-plane resistivity (ρ_{ab}) of single-crystal films with (001) orientation; solid lines, the resistivity (ρ) of polycrystalline materials. Note, $\rho_M = (h/e^2)d = 1.7$ mΩ cm.

H. Takagi et al.

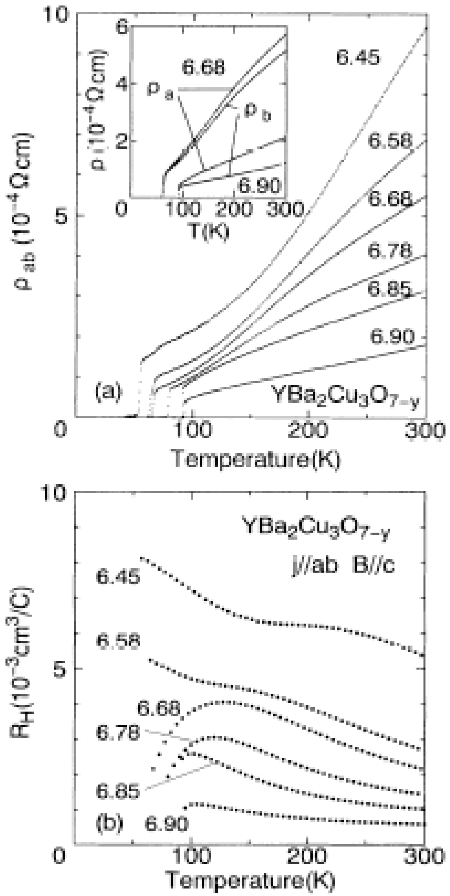


FIG. 1. (a) Temperature dependence of in-plane resistivity of twinned $YBa_2Cu_3O_{7-y}$ crystals with oxygen concentration $7-y$ ~6.90, 6.85, 6.78, 6.68, 6.58, and 6.45. Inset: Temperature dependence of ρ_a and ρ_b for detwinned crystals of T_c=90 and 60 K. (b) Temperature dependence of R_H of twinned crystals measured under j ∥ ab plane and **B** ∥ c axis at $B = 5$ T.

T. Ito et al.

Specific Heat

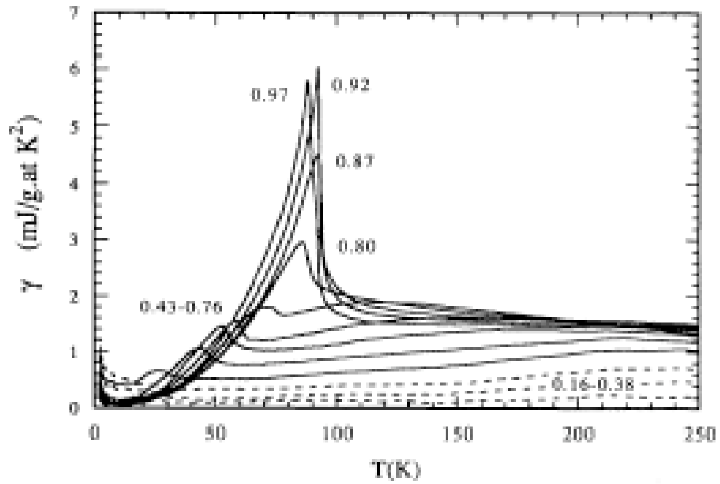


FIG. 4. Electronic specific heat coefficient $\gamma(x,T)$ vs T for $YBa_2Cu_3O_{6+x}$ relative to $YBa_2Cu_3O_6$. Values of x are 0.16, 0.29, 0.38, 0.43, 0.48, 0.57, 0.67, 0.76, 0.80, 0.87, 0.92, and 0.97.

Loram et al., Phys. Rev. Lett. 71, 1740 (1993)

LSCO

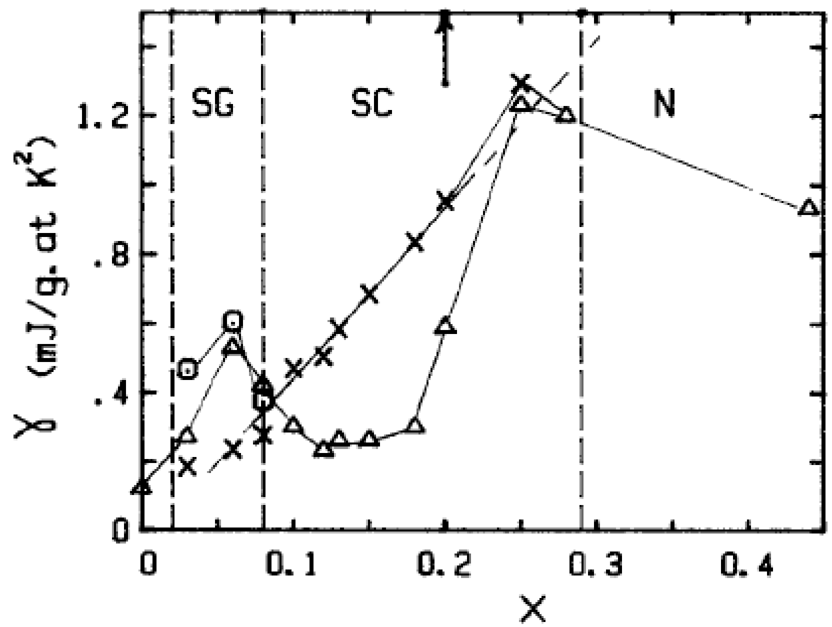


FIGURE 2

γ vs x. for x≤.08 Δ,γ (2K); o,γ (8K); x,γ (40K)
for x≥.1 Δ,γ(0); x, γ_n

Loram et al., Physica C162-164, 498 (1989)

Nuclear Magnetic Resonance

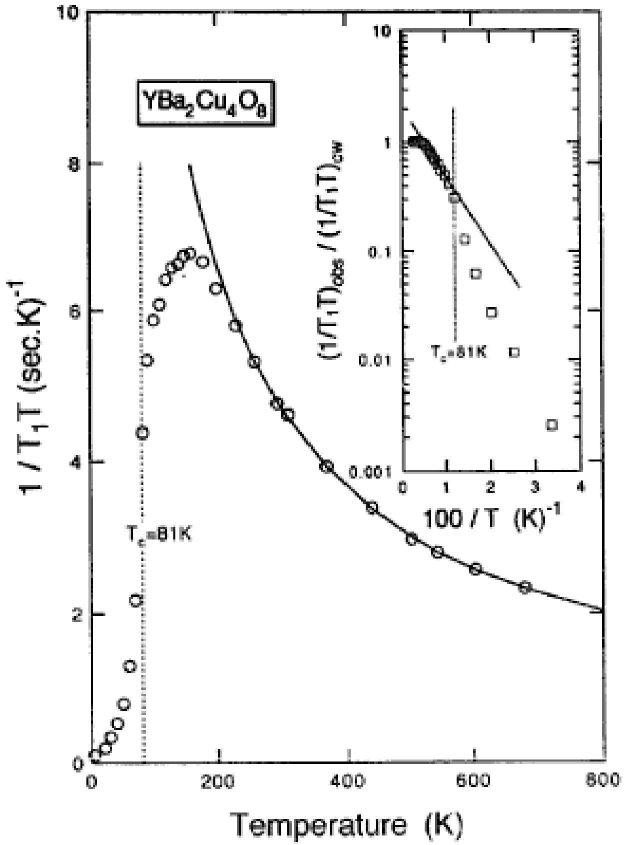


Fig. 1. Temperature dependence of the nuclear spin-lattice relaxation rate $1/T_1T$ for Cu(2) sites of $YBa_2Cu_4O_8$. The solid curve shows the best fit of the data to Eq. (1) for $T > 250$ K. The inset shows the Arrhenius plots for the ratio of the observed $(1/T_1T)_{obs}$ to the expected $(1/T_1T)_{cw}$ from Eq. (1), and the best fit of the data to Eq. (2) is shown by the solid line.

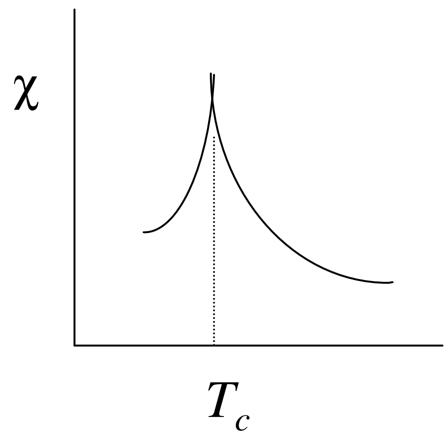
Yasuoka et al., Physica B199 (1994)278

$YBa_2Cu_4O_8$

T_c= 81K

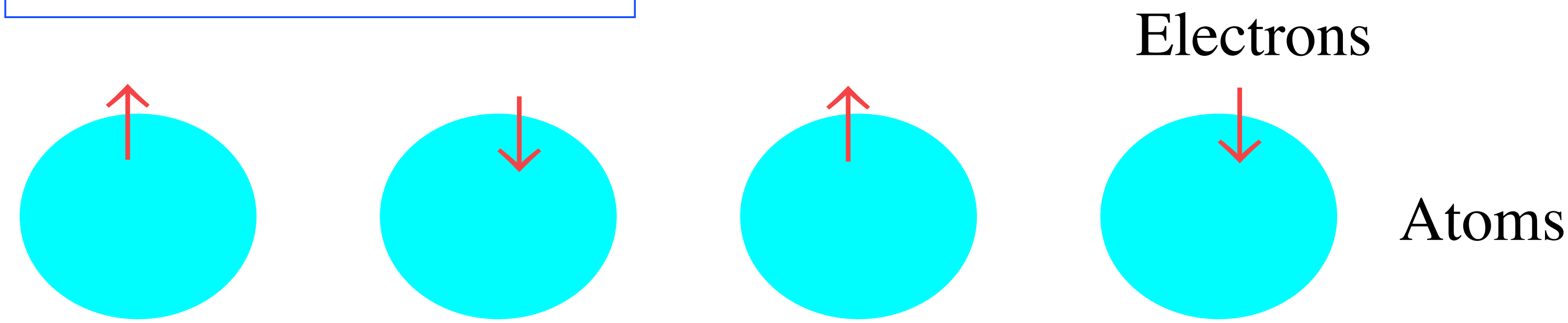
The decrease of $1/TT_1$ above T_c suggests the existence of the pseuo-gap.

In the conventional case



4. Hubbard Model

Itinerant Electrons



Mott insulators

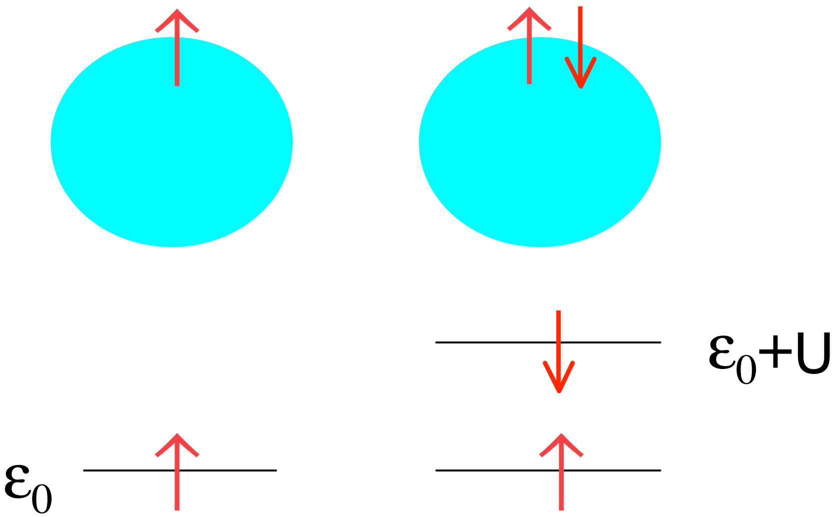
MnO, FeO, CoO, Mn_3O_4, Fe_3O_4,
NiO, CuO

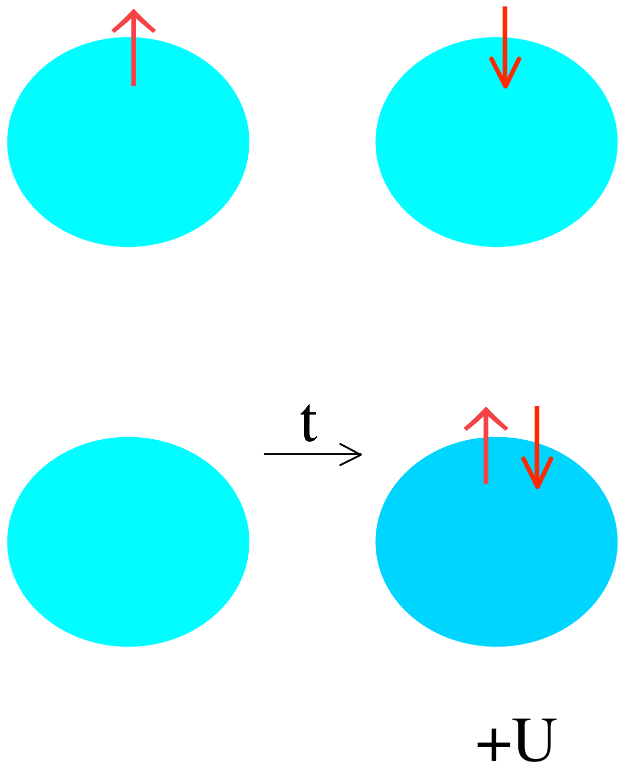
Insulators due to the Coulomb interaction

(Note: Antiferromagnets such as MnO and NiO are not Mott insulators in the strict sense.)

On-site Coulomb Interaction

Coulomb interaction





U >> t → Insulator

Gap in the Hubbard Model

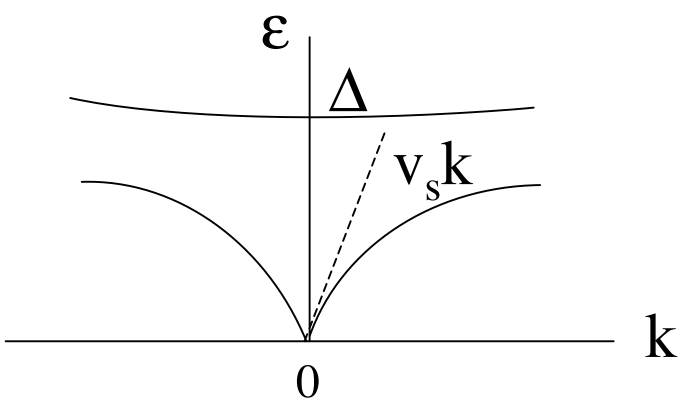
Hartree-Fock theory (Half-filling)

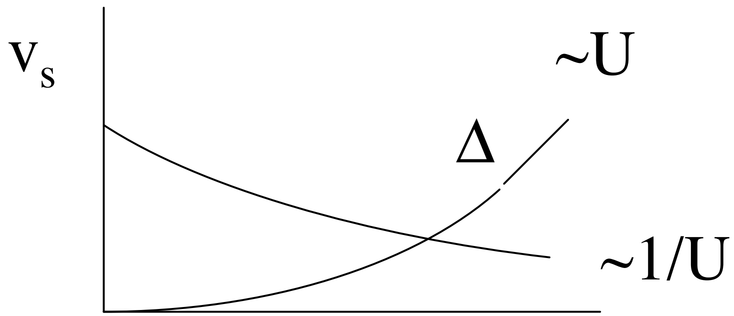
AF Gap $\Delta = Um$ $\quad \Delta \sim t\, e^{-2\pi t/U}$ $\quad d = 1, 3$

$\sim t\, e^{-2\pi (t/U)^{1/2}}$ $\quad d = 2$

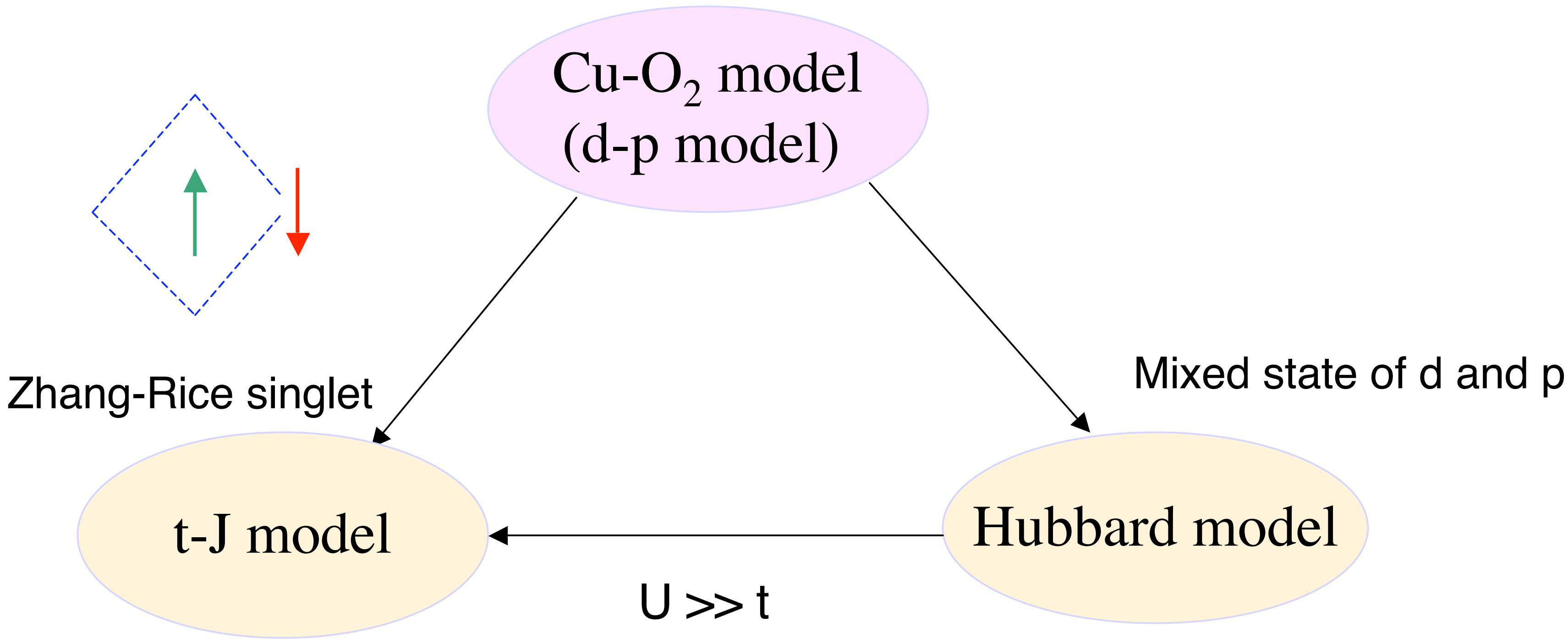
1D Hubbard model

		U << t	U >>t
Hubbard gap	Δ	$(16/\pi)\sqrt{tU}e^{-\pi/(2U)}$	U
Spin-wave velocity	$2v_s/\pi = J$	$(4t/\pi)(1 - U/4\pi t)$	$4t^2/U$





Cu-O_2 Model and Hubbard Model



$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^{+} c_{j\sigma} + h.c.) + J \sum_{\langle ij \rangle} S_i \cdot S_j$$

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^{+} c_{j\sigma} + h.c.) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$t_{pd} \ll U_d - (\varepsilon_p - \varepsilon_d)$
$t_{pd} \ll \varepsilon_p - \varepsilon_d$
$\varepsilon_p - \varepsilon_d \ll U_d$

$\varepsilon_p - \varepsilon_d \sim 0(t_{pd})$

5. Variational Monte Carlo method

We evaluate the expectation values using the Monte Carlo method.

Gutzwiller function $$\psi_G = P_G \psi_0$$

ψ_0 : trial wave function Fermi sea, AF state, or BCS state

$$P_G = \prod_j \left(1 - (1-g) n_{j\uparrow} n_{j\downarrow}\right)$$ Gutzwiller operator

$$0 \leq g \leq 1$$

Control the on-site correlation in terms of g

weight g
Coulomb +U

weight 1

Variational Monte Carlo Method

Normal state ψ_0 Slater determinant

$$\psi_0 = \sum_{l} a_l \psi_l$$

ψ_l : particles in the real space

Wave numbers: $k_1, k_2, \ldots, k_n$

Coordinate positions: $j_1, j_2, \ldots, j_n$

$$\det D_\uparrow = \begin{vmatrix} e^{ik_1 j_1} & e^{ik_1 j_2} & & e^{ik_1 j_n} \\ & & & \\ e^{ik_n j_1} & e^{ik_h j_2} & & e^{ik_n j_n} \end{vmatrix}$$

Slater determinant

Weight of this state $a_l = \det D_\uparrow \det D_\downarrow$

The large number of particle configurations $\rightarrow$ Monte Carlo method

Monte Carlo algorithm

Expectation value

$$\langle \psi Q \psi \rangle = \sum_{mn} a_m a_n \langle \psi_m Q \psi_n \rangle = \sum_m \frac{a_m^2}{\sum_l a_l^2} \sum_n \frac{a_n}{a_m} \langle \psi_m Q \psi_n \rangle$$

The appearance rate of ψ_m is proportional to $P_m = \dfrac{a_m^2}{\sum_l a_l^2}$ in M.C. steps,

$$\langle \psi Q \psi \rangle = \frac{1}{M} \sum_m \left(\sum_n \frac{a_n}{a_m} \langle \psi_m Q \psi_n \rangle \right) \qquad m = 1, \quad , M$$

Metropolis法 $\psi_j \rightarrow \psi_n$

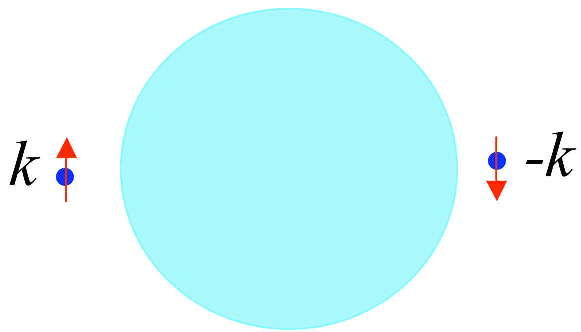
If $R = |a_n|^2 / |a_j|^2 \geq \xi$, adopt ψ_n

$< \xi$ ψ_j again

ξ: random numbers $0 \leq \xi < 1$

Superconducting state

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



Gutzwiller Projection P_G

To control the on-site strong correlation

Weight g
Coulomb +U

Weight 1
Parameter 0<g<1

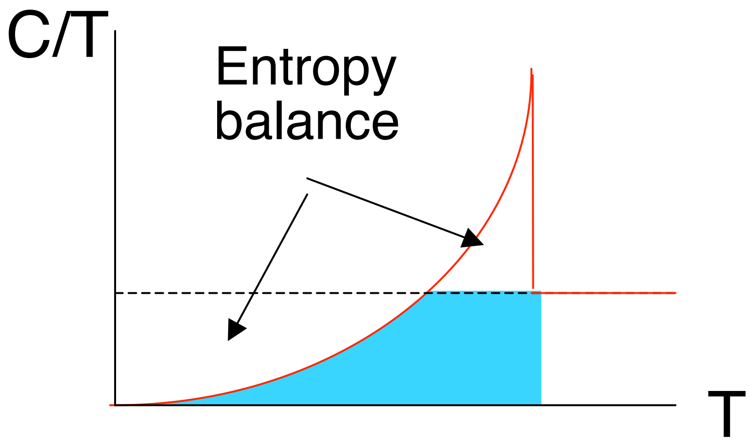
Equivalent
to
RVB state (Anderson)

Superconducting condensation energy

SC Condensation energy

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

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



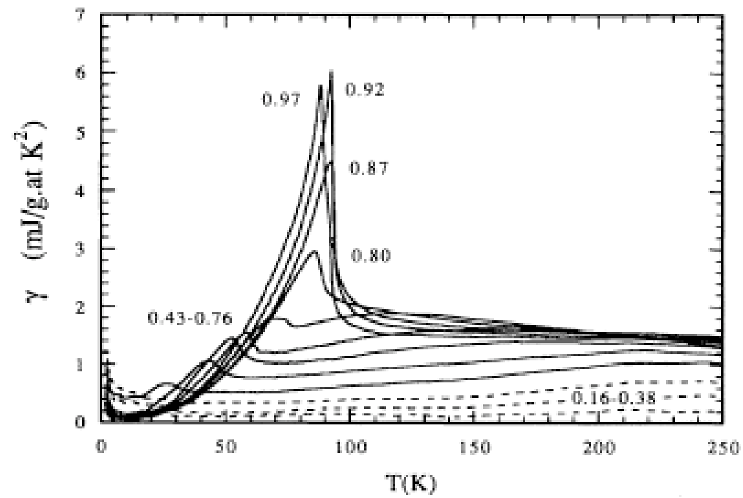


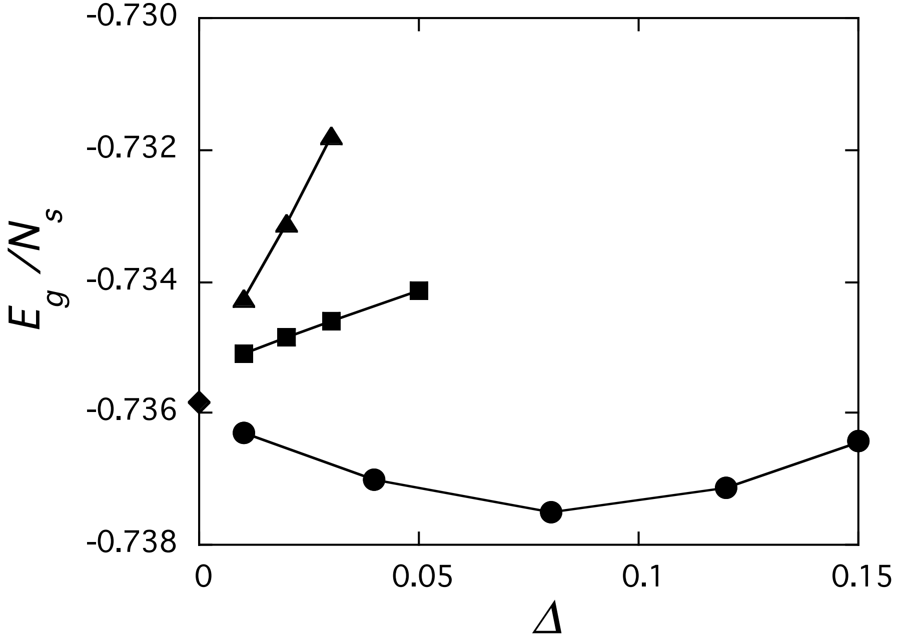
FIG. 4. Electronic specific heat coefficient $\gamma(x,T)$ vs T for $YBa_2Cu_3O_{6+x}$ relative to $YBa_2Cu_3O_6$. Values of x are 0.16, 0.29, 0.38, 0.43, 0.48, 0.57, 0.67, 0.76, 0.80, 0.87, 0.92, and 0.97.

Loram et al. PRL 71, 1740 (‘93)

optimally doped YBCO

SC Condensation energy
~ 0.2 meV

Evaluations in the superconducting state

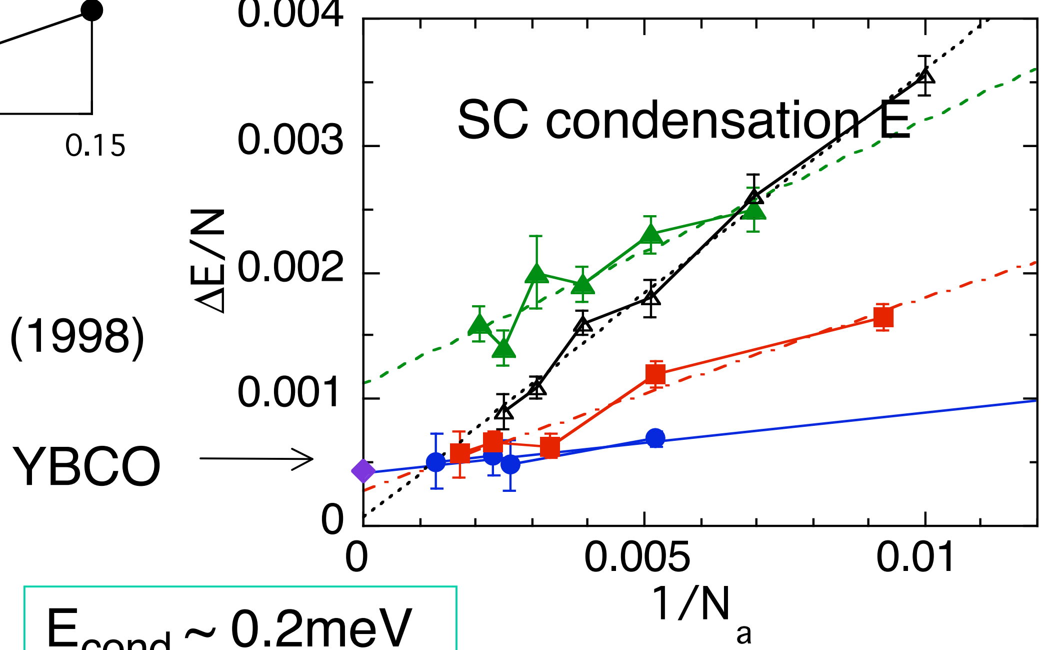


Variational Monte Carlo method

10x10 Hubbard model U= 8

T. Nakanishi et al. JPSJ 66, 294 (1997)

K. Yamaji et al., Physica C304, 225 (1998)
T. Yanagisawa et al.,
Phys. Rev. B67, 132408 (2003)

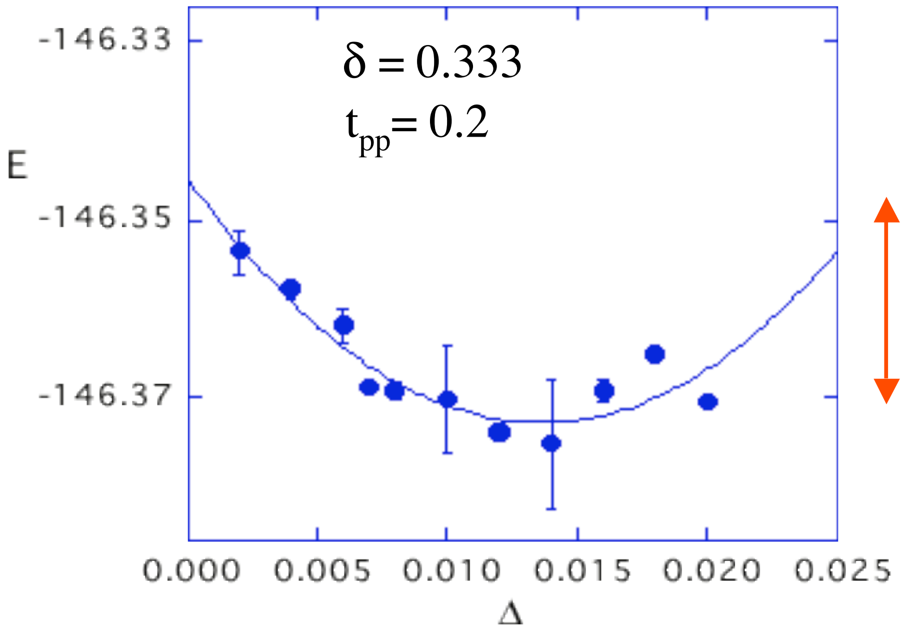


$E_{cond} \sim 0.2$meV

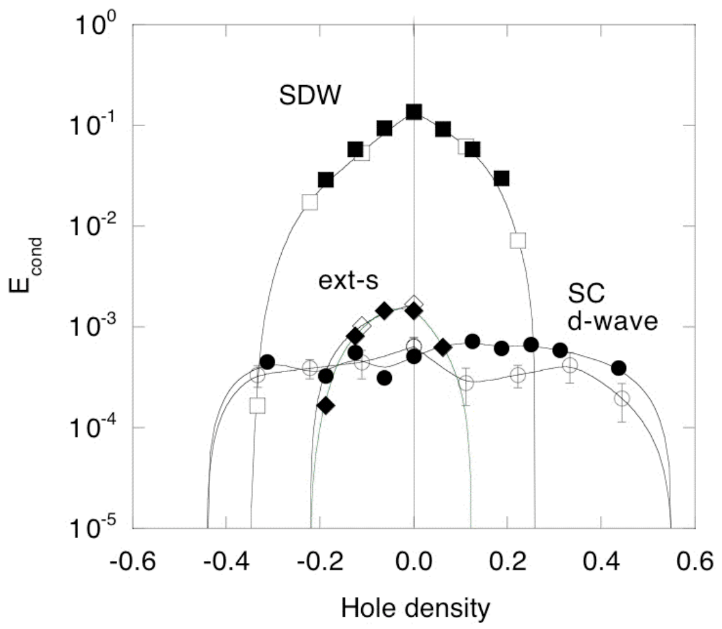
Condensation Energy for d-p model

Condensation energy

$E_{cond} \sim 0.00038 t_{dp}$
$= 0.56$ meV/site



2D d-p model
6x6 and 8x8

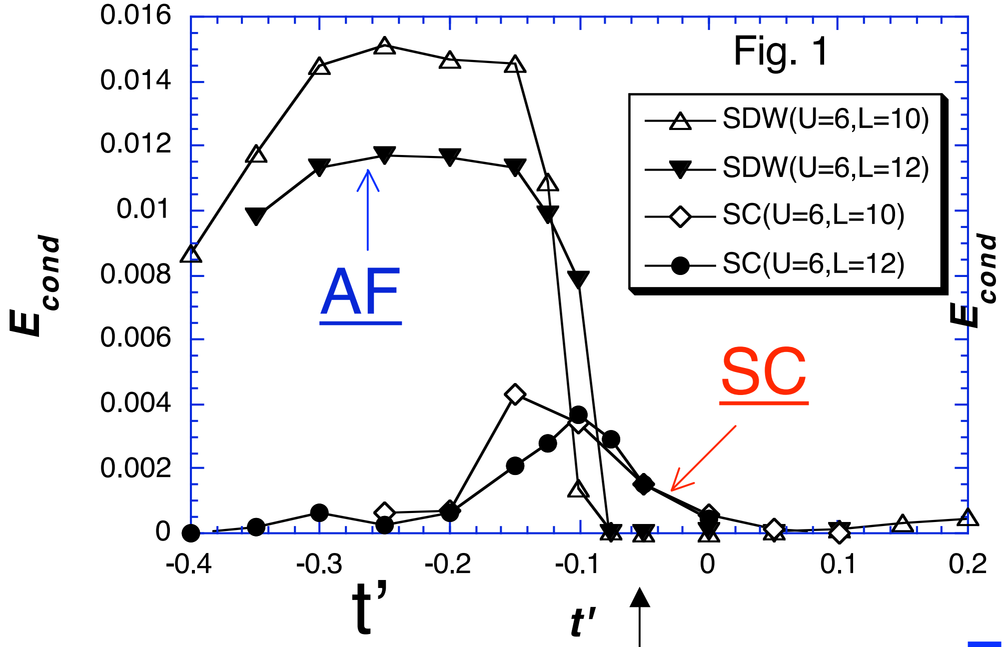


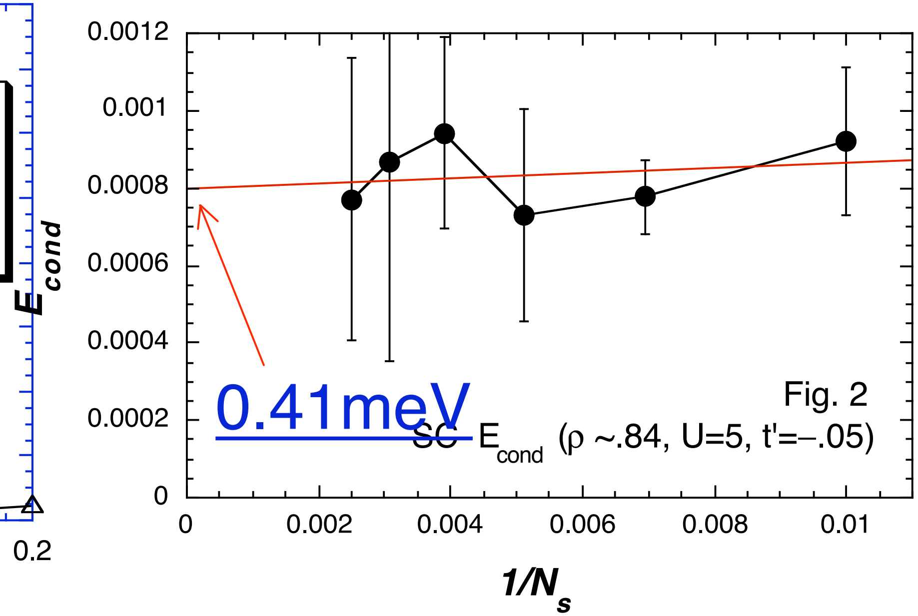
T.Yanagisawa et al., PRB64, 184509 ('01)

Superconductivity and Antiferromagnetism

Competition

Size dependence of SC condensation energy





t'

Pure d-wave SC

Experiments

0.26 meV/site (critical field H_c)

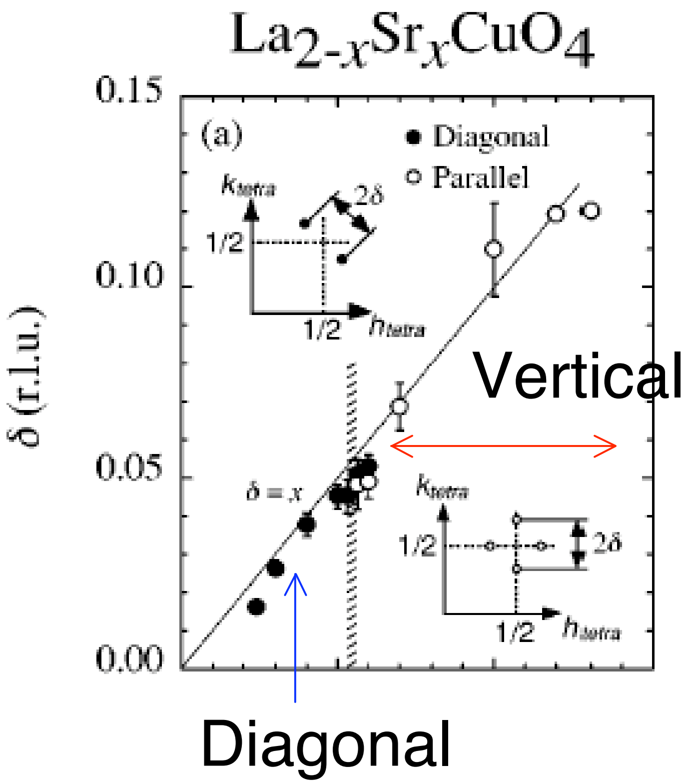
0.17~0.26 (C/T)

6. Stripes in high-Tc cuprates

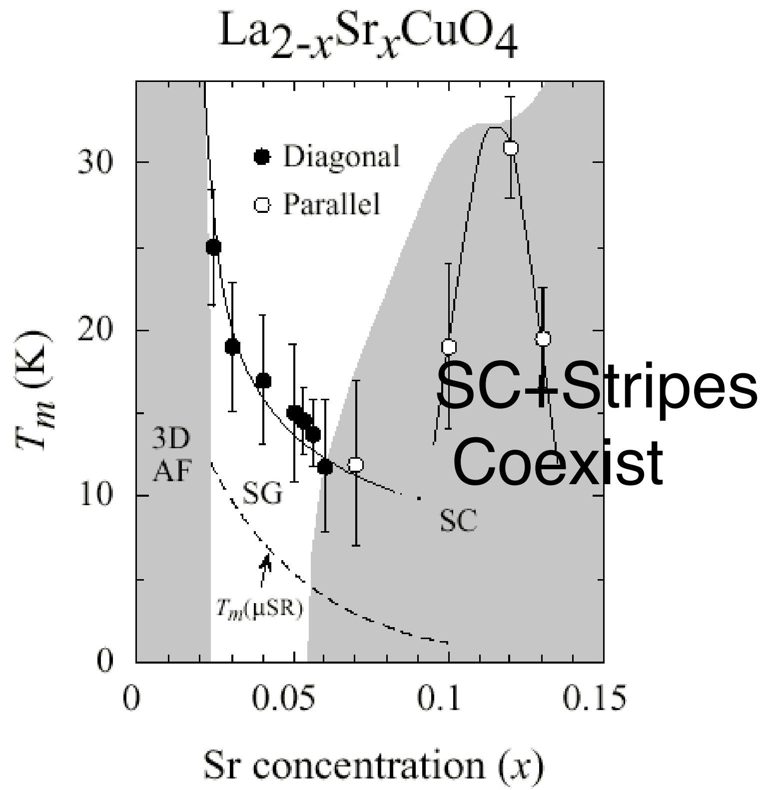
- Vertical stripes for x > 0.05
- Diagonal stripes for x < 0.05

AF coexists with SC?

Neutron scattering



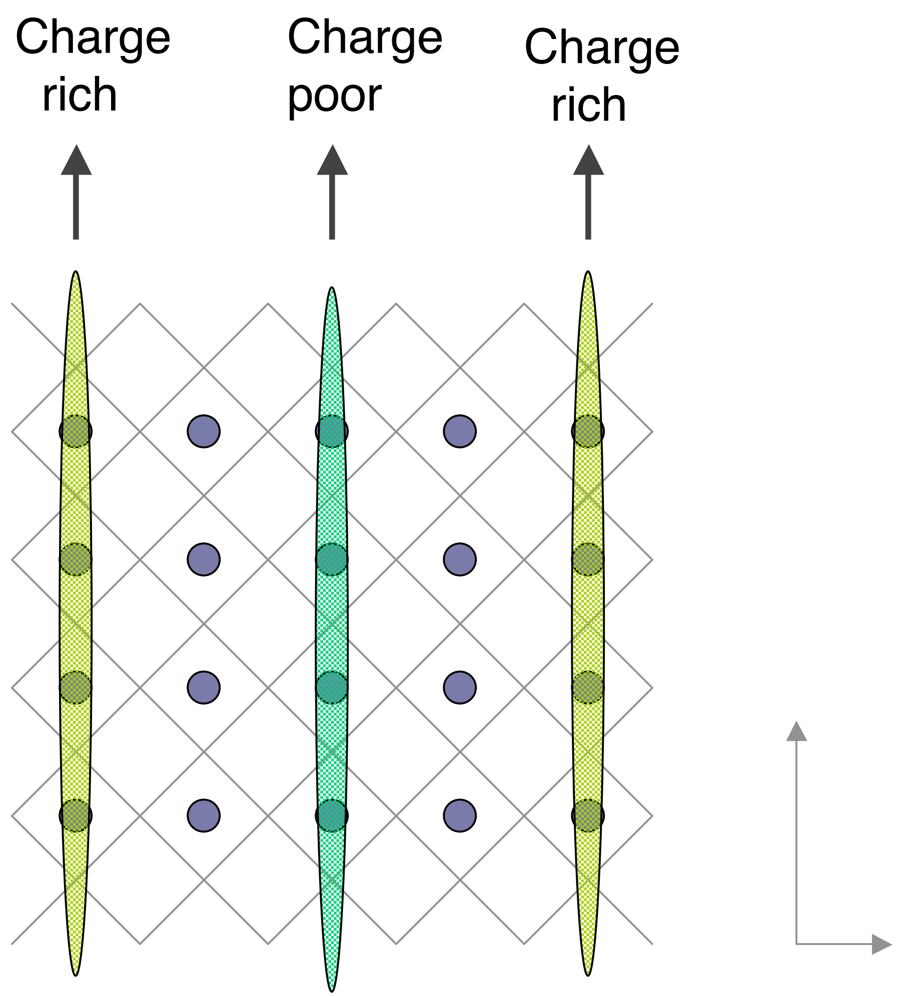
M.Fujita et al. Phys. Rev.B65,064505('02)



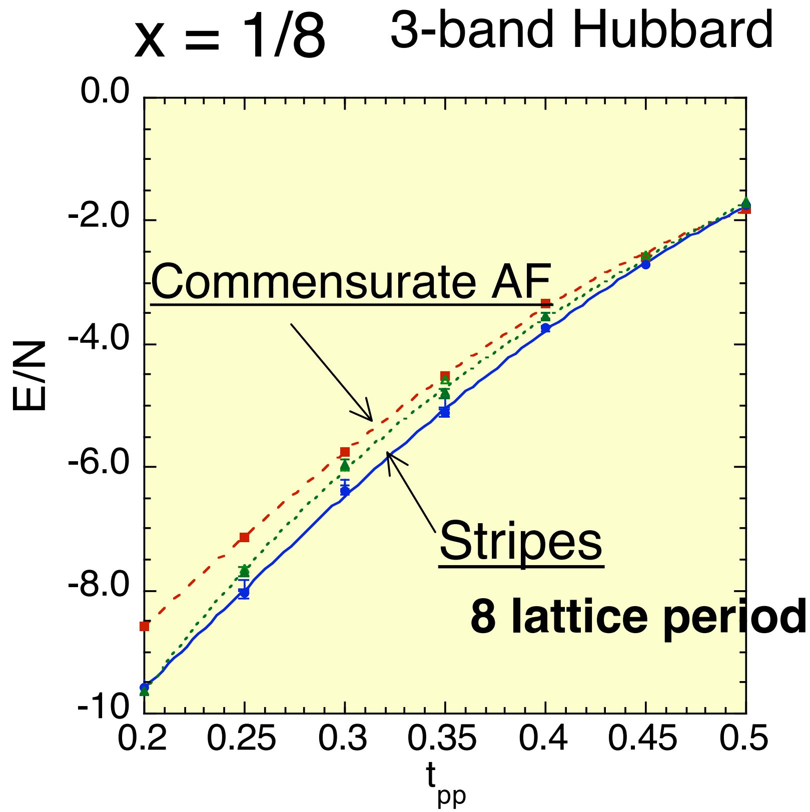
S.Wakimoto et al. PRB61, 3699('00)

Vertical Stripes in the under-doped region

Vertical stripes: 8 lattice periodicity (Tranquada)



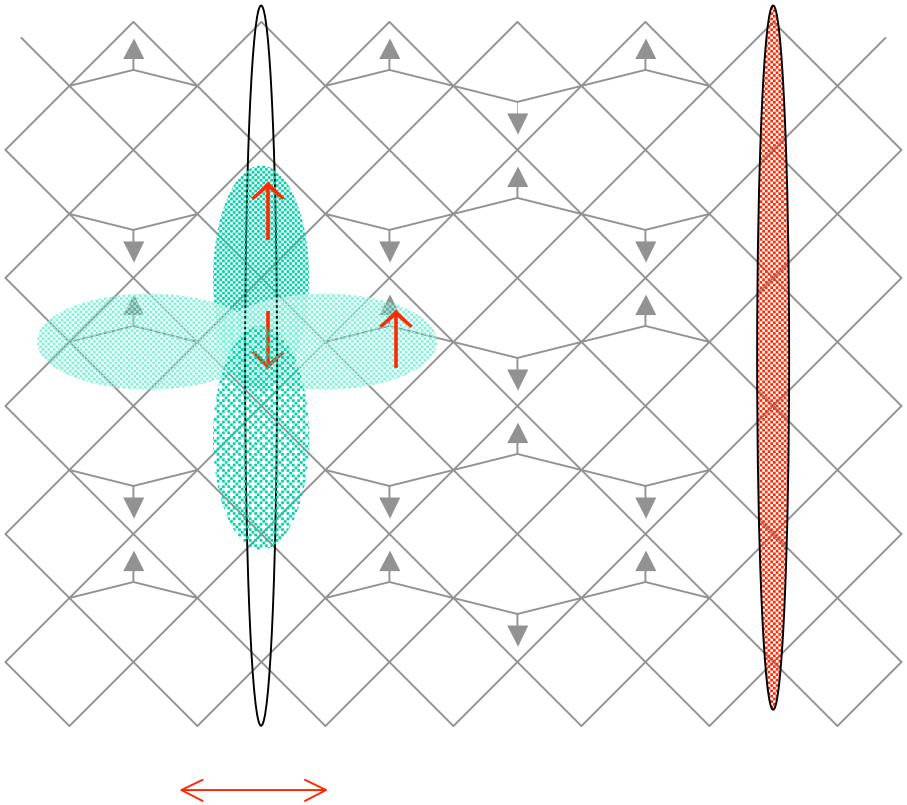
VMC



T.Y. et al., J.Phys.C14,21('02)

Stripes and Superconductivity

Compete and Collaborate



Nano-scale SC

SC coexists with stripes (AF)

Bogoliubov-de Gennes eq.

$$\begin{pmatrix} H_{ij\uparrow} + F_{ij} \\ F^{*}_{ji} - H_{ji\downarrow} \end{pmatrix} \begin{pmatrix} u_j^{\lambda} \\ v_j^{\lambda} \end{pmatrix} = E^{\lambda} \begin{pmatrix} u_i^{\lambda} \\ v_i^{\lambda} \end{pmatrix}$$

$$\alpha_{\lambda} = u_i^{\lambda} a_{i\uparrow} + v_i^{\lambda} a^{+}_{i\downarrow}$$

$$\overline{\alpha_{\lambda}} = \overline{u}_i^{\lambda} a_{i\uparrow} + \overline{v}_i^{\lambda} a^{+}_{i\downarrow}$$

Wave function

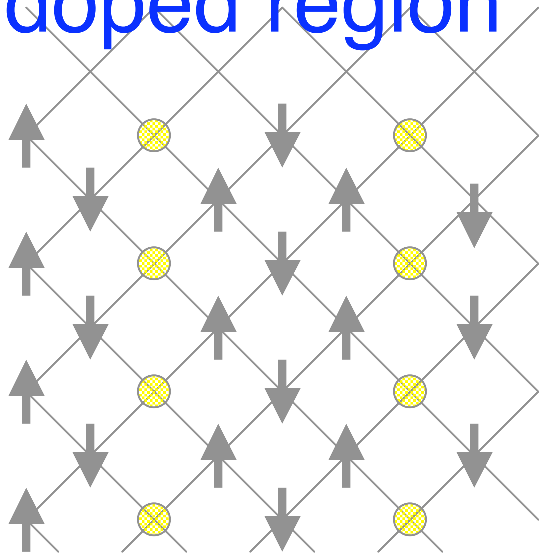
$$V_{\lambda j} = v_j^{\lambda} \qquad (\overline{U})_{\lambda j} = \overline{u}_j^{\lambda}$$

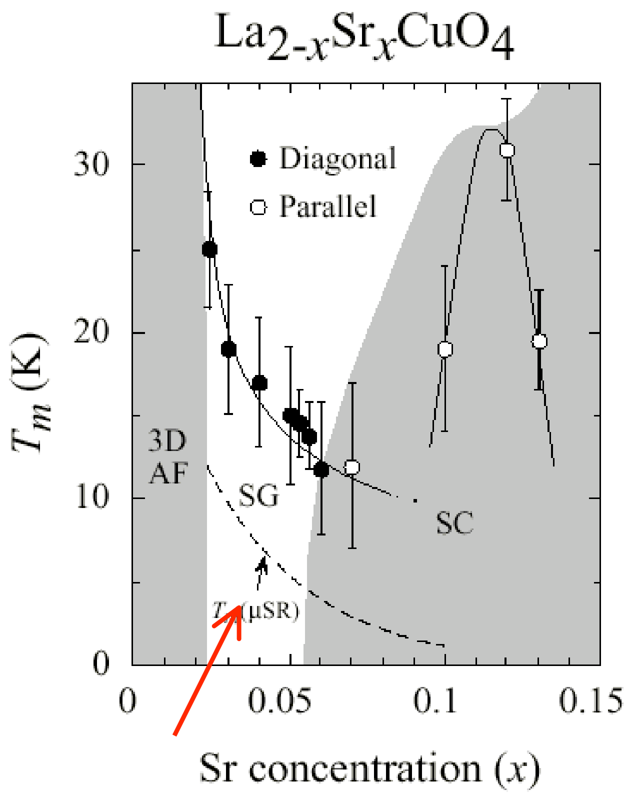
$$\psi_{SC} = P_G P_{N_e} \prod_{\lambda} \alpha_{\lambda} \overline{\alpha}^{+}_{\lambda} |0\rangle \propto P_G \left(\sum_{ij} (U^{-1}V)_{ij} a^{+}_{i\uparrow} a^{+}_{j\downarrow} \right)^{N_e/2} |0\rangle$$

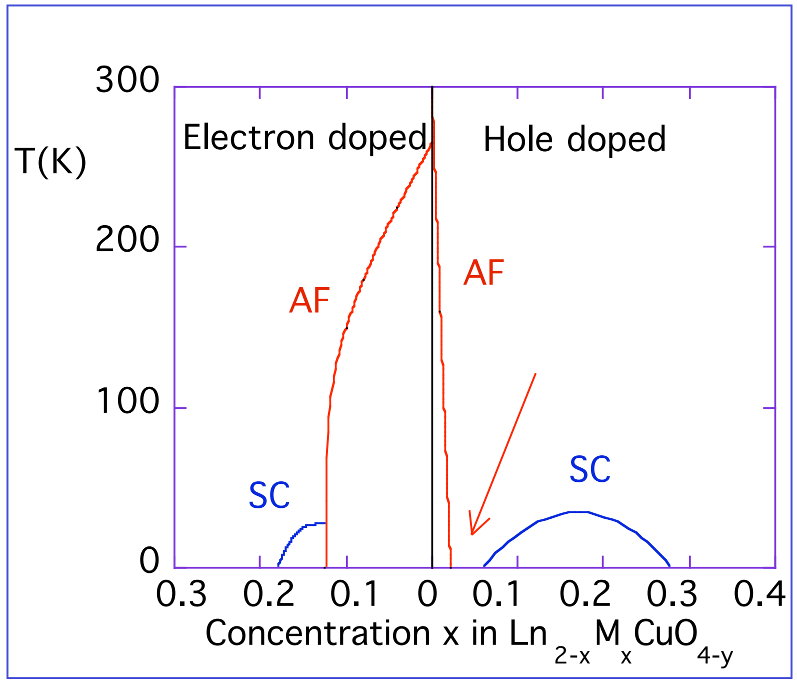
Diagonal stripes in lightly doped region

Diagonal stripes are observed for

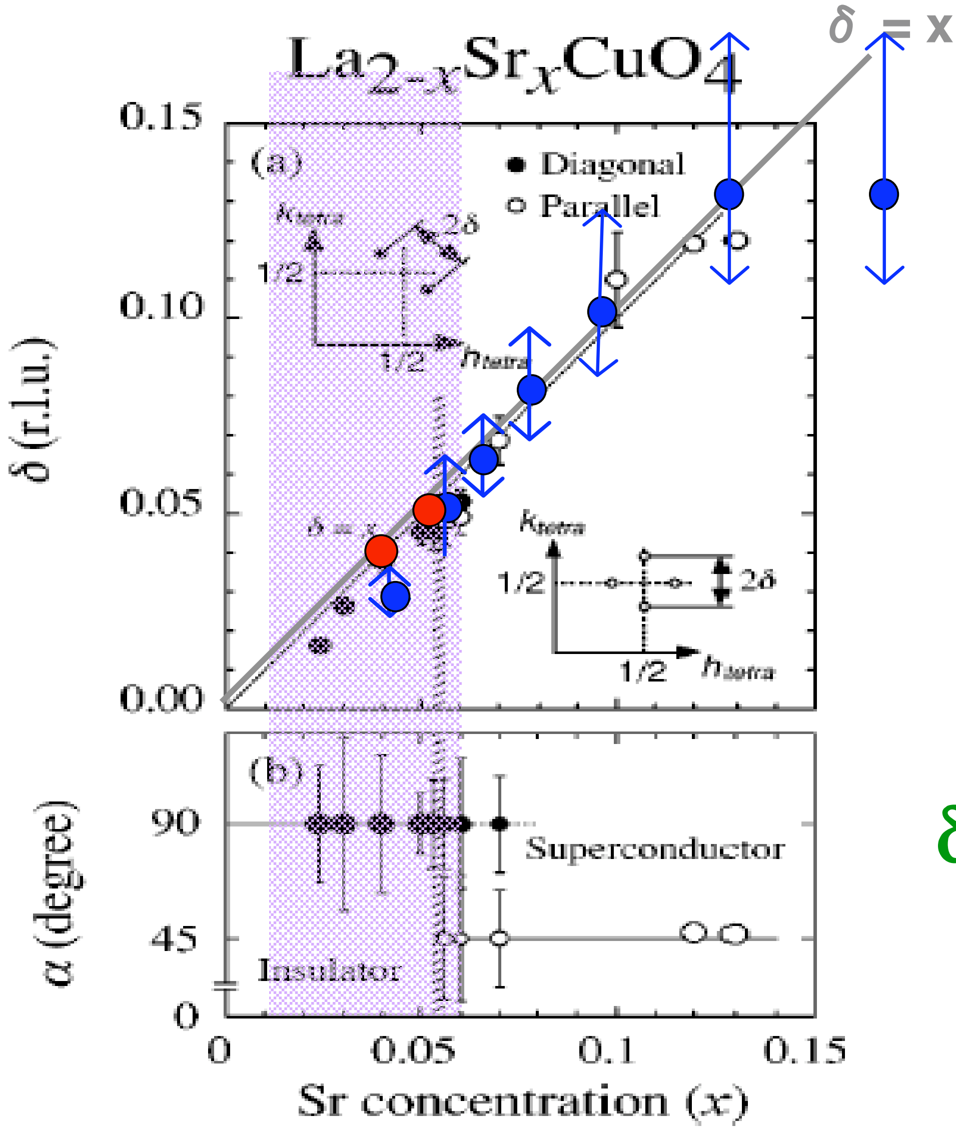
$La_{2-x}Sr_xNiO_4$
$La_{2-x}Sr_xCuO_4$
$La_{2-x-y}Nd_ySr_xCuO_4$







Incommensurability: Comparison with Experiments



Vertical stripes

Diagonal stripes

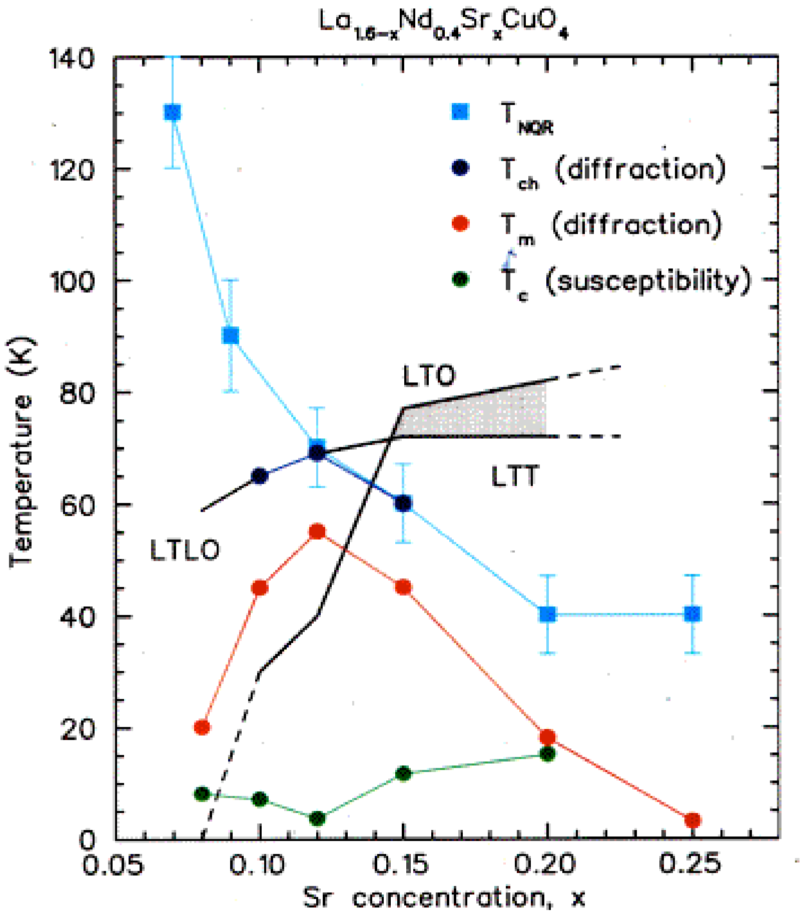
U=8.0 t'= -0.2

δ can be explained by 2D Hubbard model.

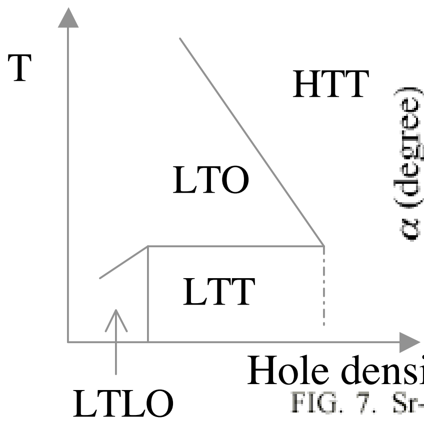
Stripes and Structural transition

Structural transitions: Lattice distortions
LTT,LTO,LTLO,HTT

Stripes: suggested by Incommensurability



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



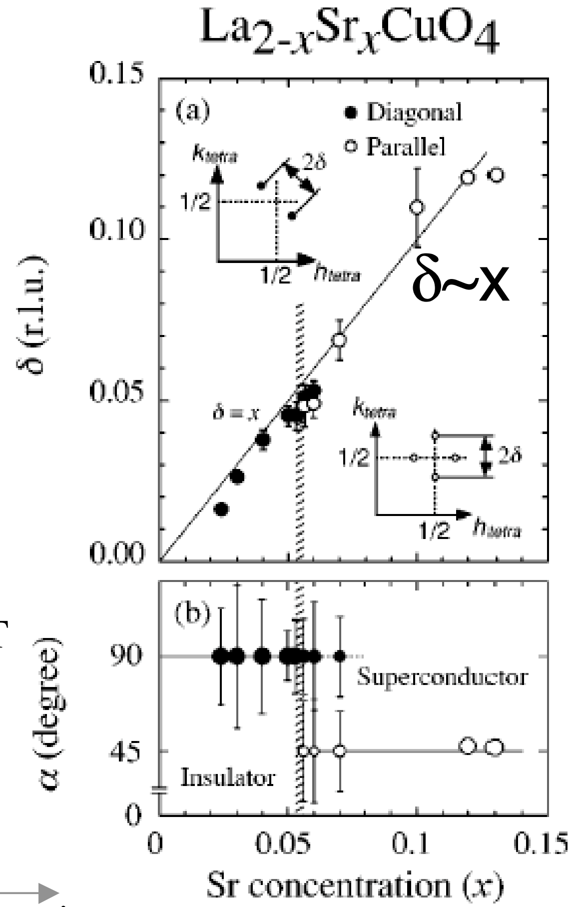


FIG. 7. Sr-concentration dependence of (a) the incommensurability δ and (b) the angle a defined in Fig. 3. Previous results for $x=0.024$ (Ref. 11), 0.04 (Ref. 10), 0.05 (Ref. 10), 0.12 (Ref. 5), 0.1 (Ref. 15), and 0.13 (Ref. 15) are included. In both figures, the solid and open symbols represent the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

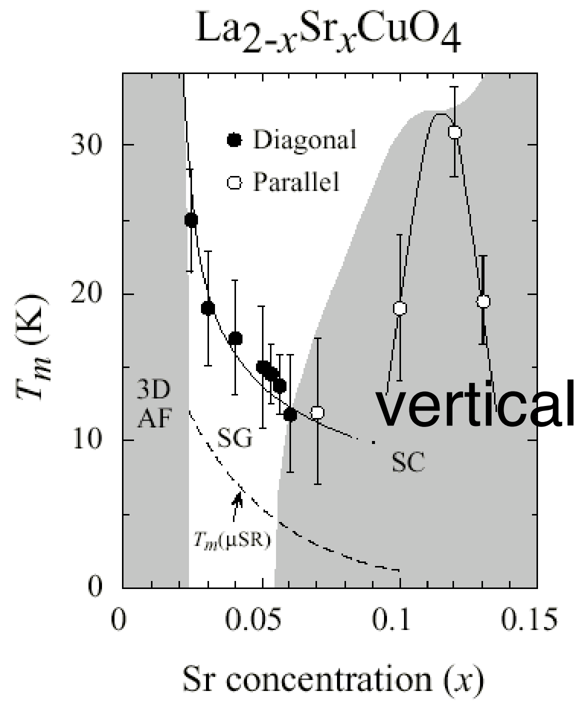
M.Fujita et al. Phys. Rev.B65,064505('02)

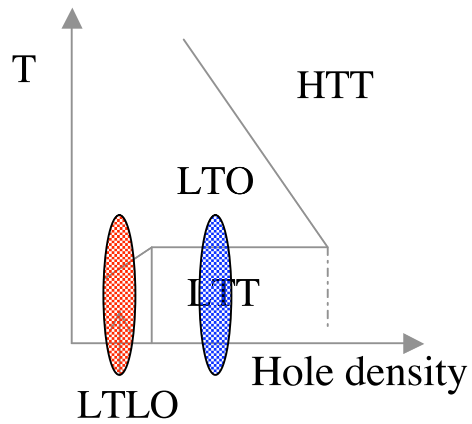
What happens under lattice distortions

1. Anisotropy of the transfer integrals
   Anisotropic electronic state
   vertical stripes
   Diagonal stripes x<0.05

2. Spin-Orbit Coupling induced from
   lattice distortions

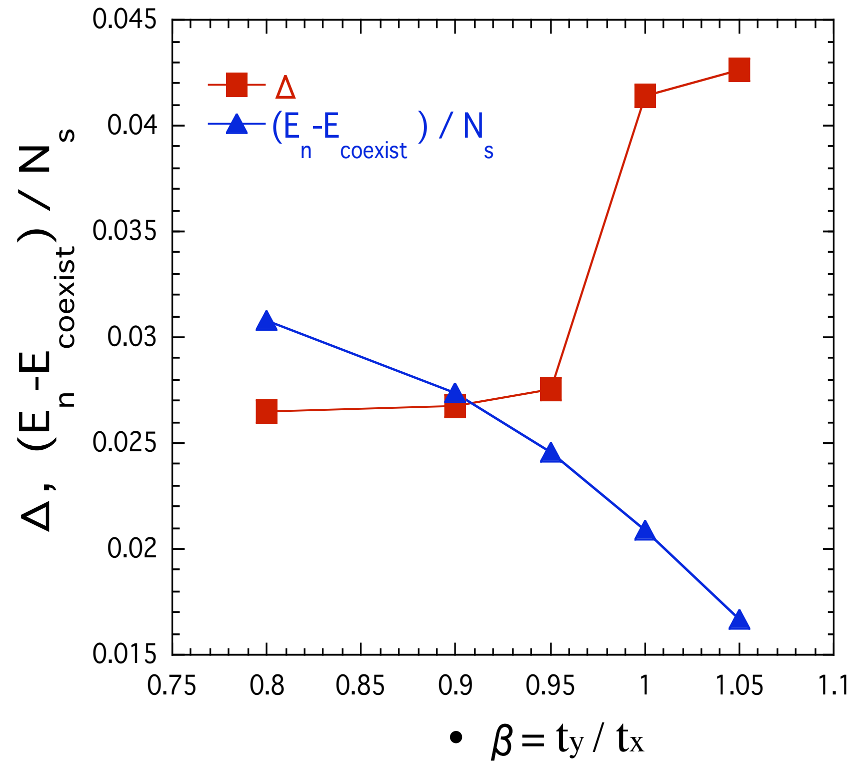
3. Electron-phonon interaction

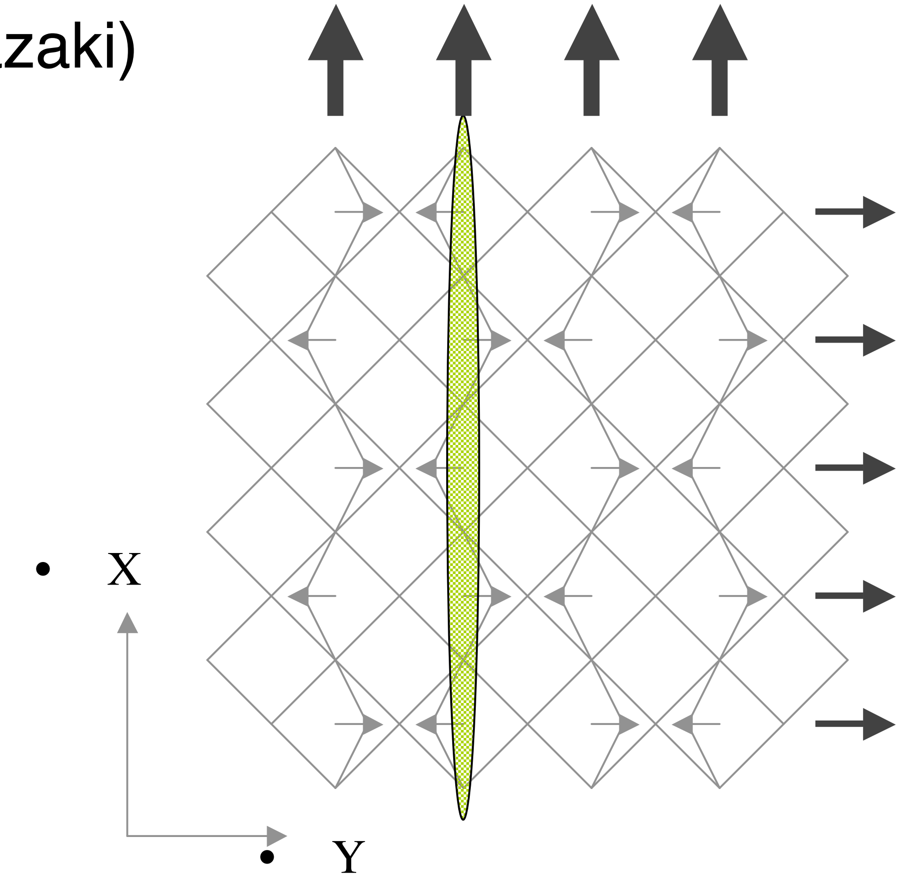




Anisotropy of the transfer integrals in LTT phase

One-band Hubbard model (Miyazaki)





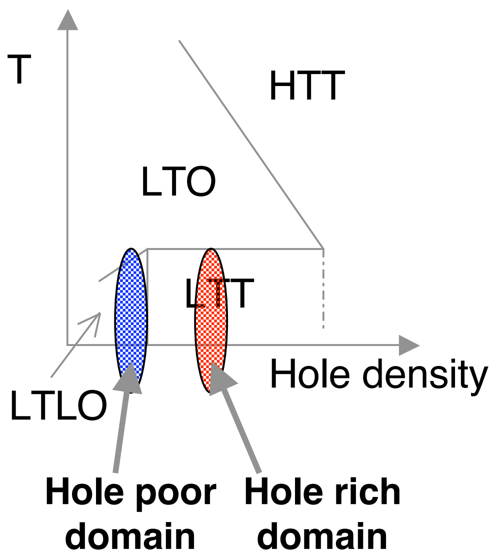
LTT structural transitions stabilize stripes.

Possible Stripe Structure 1

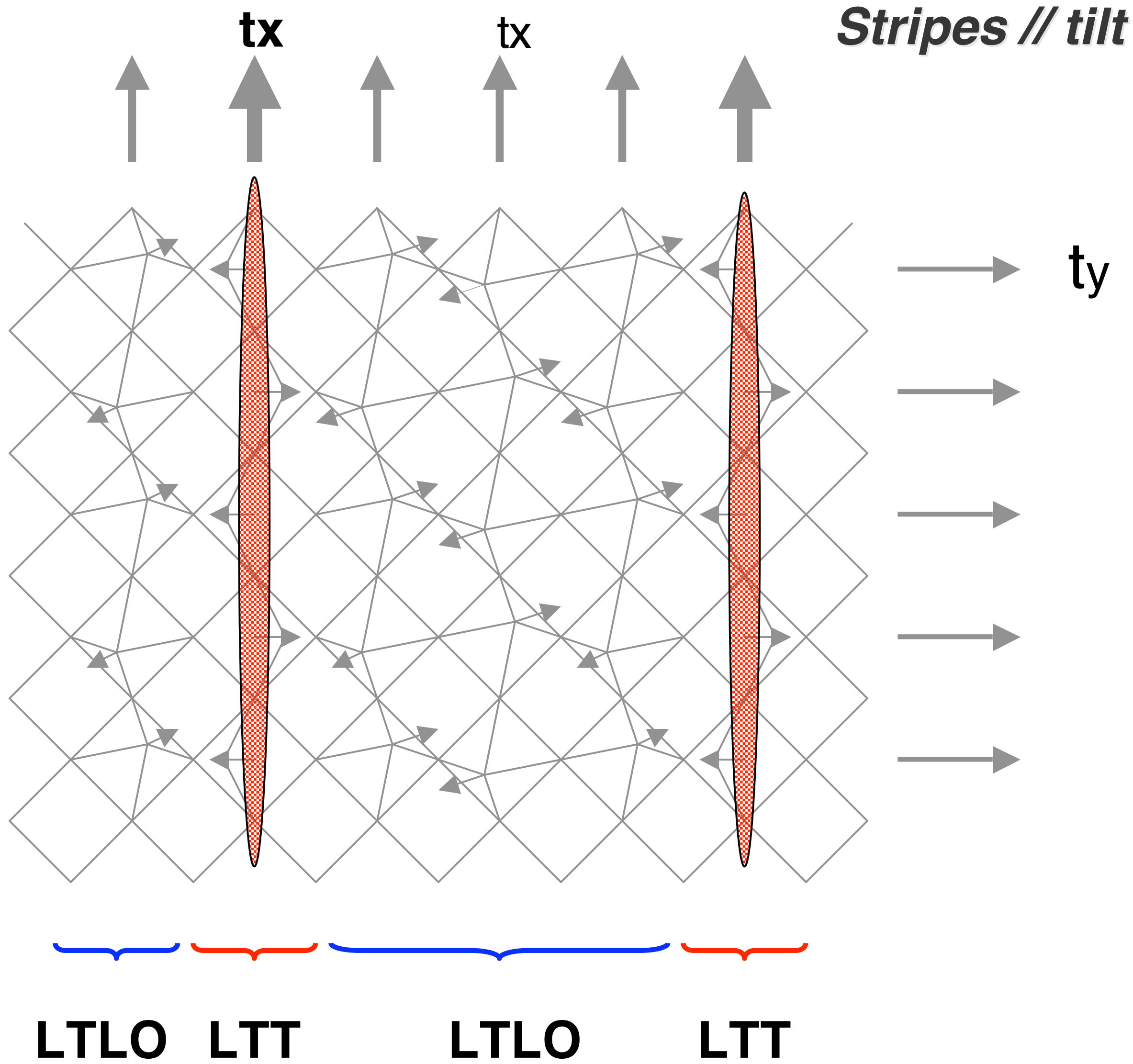
Mixed phase of LTT and LTLO

Stabilize stripes

M. K. Crawford et. al.



Stripes // tilt axis

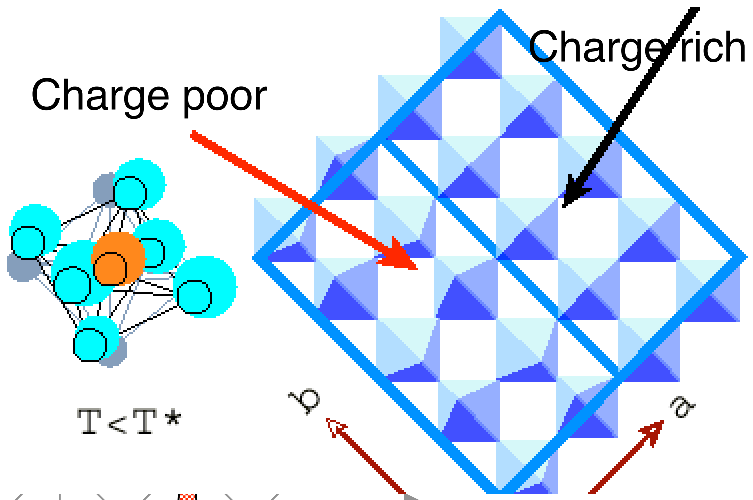


Possible Stripe Structure

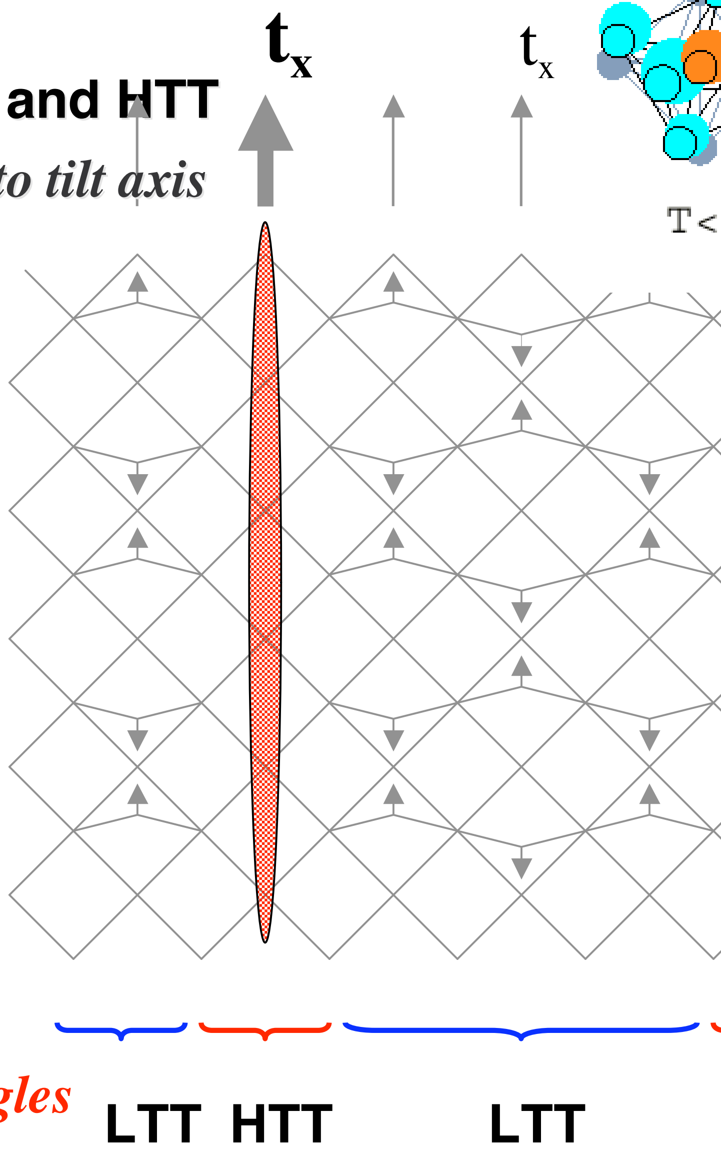
Mixed phase of LTT and HTT

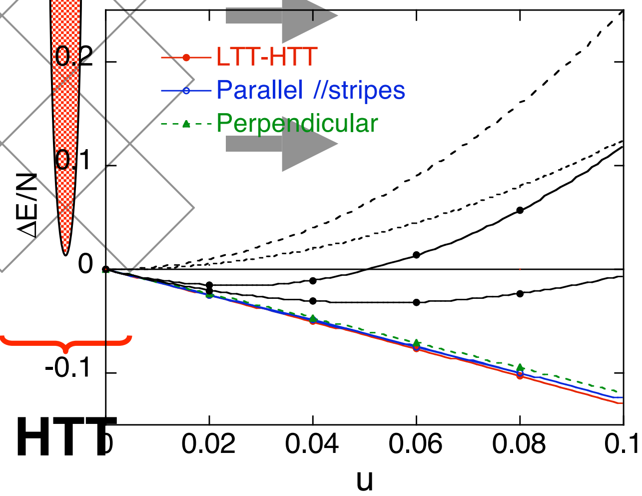
Stripes perpendicular to tilt axis

Stable

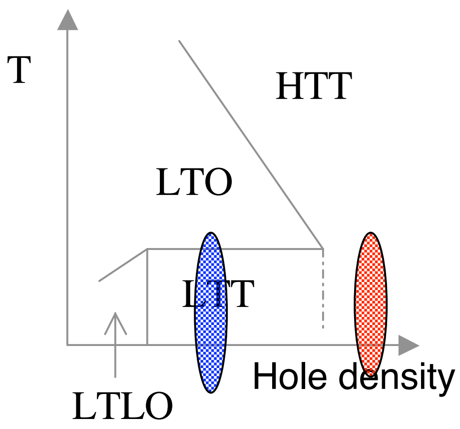


H. Oyanagi
A. Bianconi





M. K. Crawford et. al.



Oscillation of tilt angles

7. Spin-orbit coupling and Lattice distortion

Spin-Orbit Coupling induced by the Lattice distortion

Tilting

Friedel et al., J.Phys.Chem.Solids 25, 781 (1964)

$$\langle p_x(x-a/2, y)\uparrow | H_{dp} | d_{xz}(r)\uparrow\rangle = -t_{xz}e^{-ik_x/2\cdot a}$$

$$\langle p_y(x, y-a/2)\uparrow | H_{dp} | d_{yz}(r)\uparrow\rangle = -t_{yz}e^{-iky/2\cdot a}$$

$$H_{SO} = \xi(r)L\cdot S$$

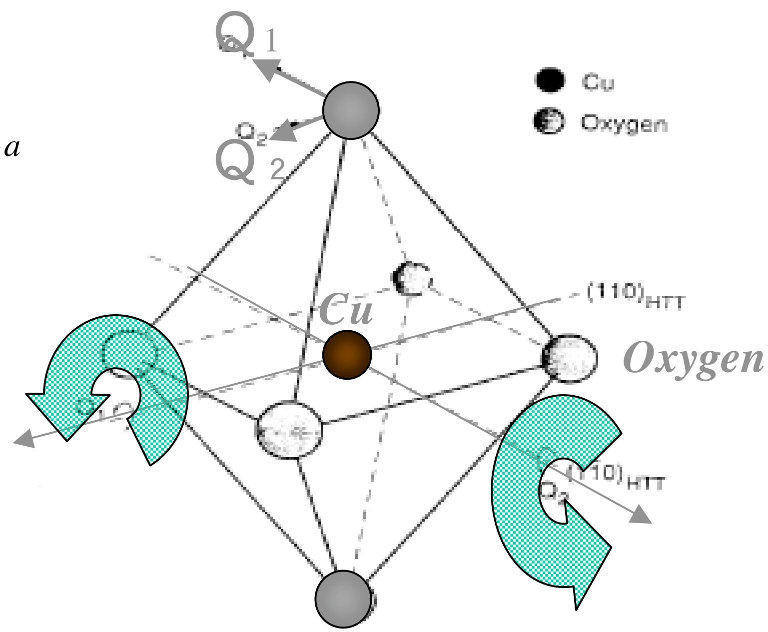
$$\langle d_{xz}(r)\uparrow | H_{SO} | d_{yz}(r)\uparrow\rangle = -\frac{i}{2}\xi$$

$$\langle d_{yz}(r)\uparrow | H_{SO} | d_{xz}(r)\uparrow\rangle = \frac{i}{2}\xi$$

$$\langle d_{x^2-y^2}(r)\uparrow | H_{SO} | d_{yz}(r)\downarrow\rangle = \frac{i}{2}\xi$$

$$\langle d_{x^2-y^2}(r)\uparrow | H_{SO} | d_{xz}(r)\downarrow\rangle = \frac{1}{2}\xi$$

Effective iξ term for p-p transfer



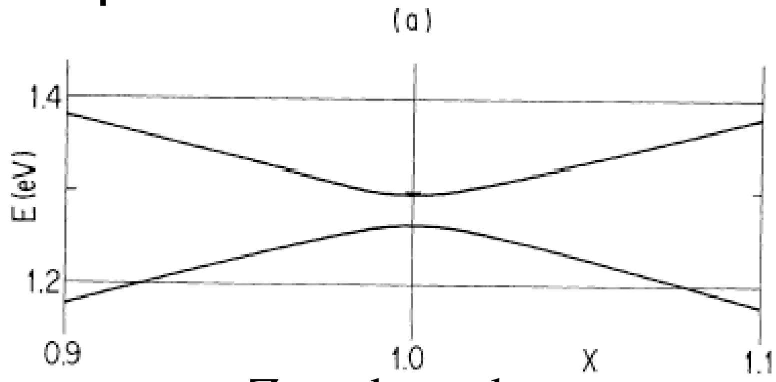
t_{xz}, t_{yz} $\neq 0 \sim$ tilt angle

Five orbitals $\times$ ($\uparrow\downarrow$):

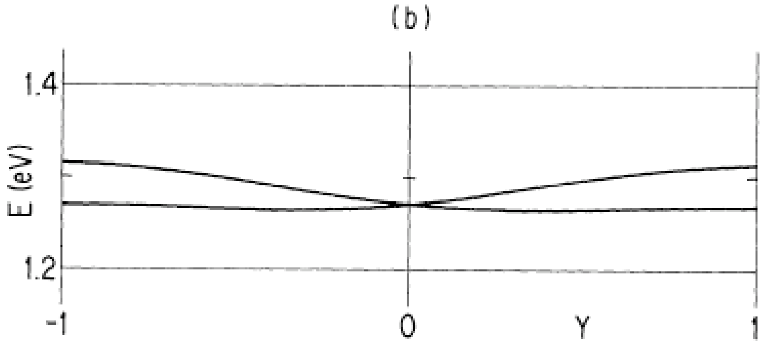
($d_{x^2-y^2}$, d_{xz}, d_{yz}, p_x, p_y)

Dispersion in the presence of spin-orbit coupling

d-p model



Zone boundary



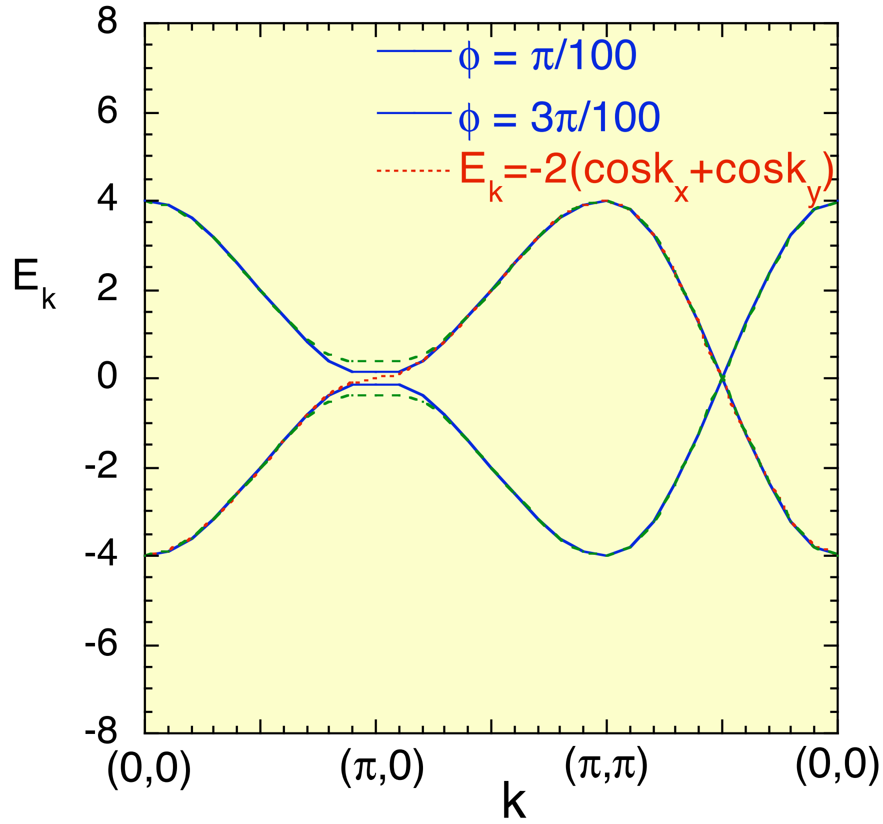
$\xi = 0.4$ $(\pi/2,\pi/2)$

K.Yamaji, JPSJ 57 (1988) 2745.
T.Y. et al., JPSJ 74 (2005) 835.

One-band effective model

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

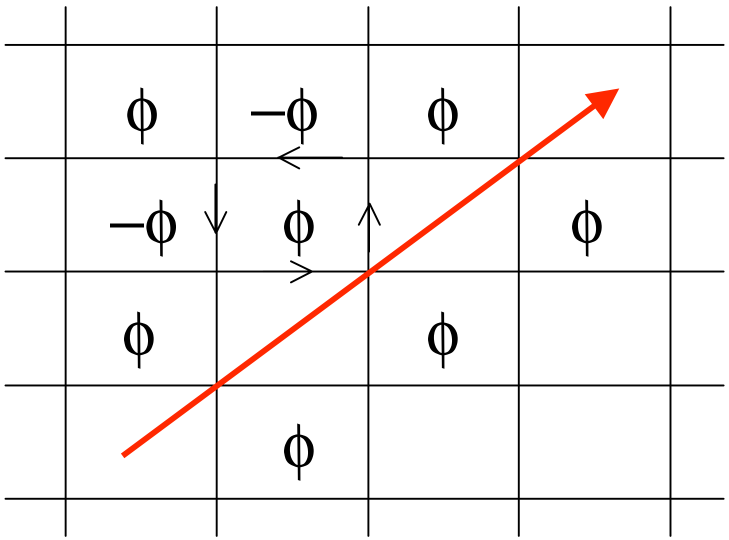
(Bonesteal et al.,PRL68,2684('92))

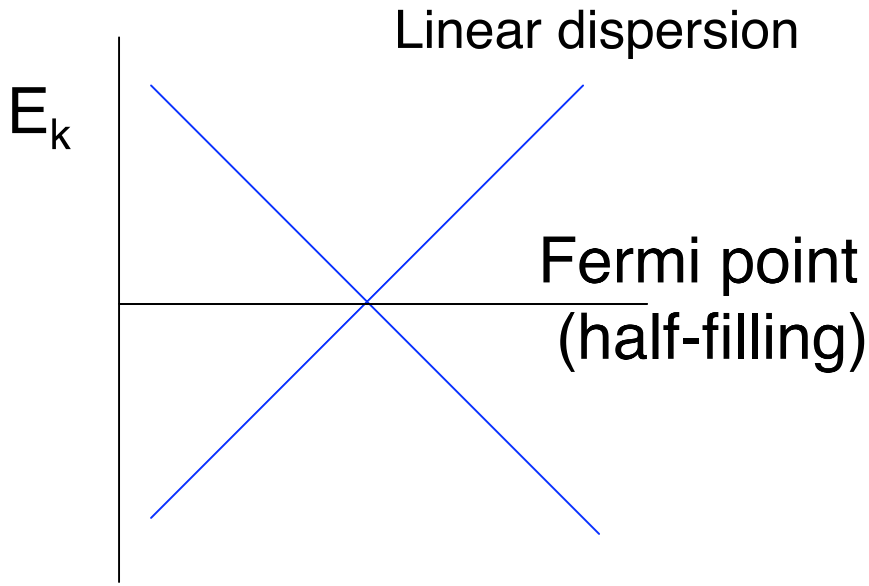


Flux state

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

Excitation: Dirac fermion





Small Fermi surface

Inhomogeneous d-density wave

Pseudo-gap in the density of states

Flux state

⟶ Pseudo-gap

An origin of pseudo-gap

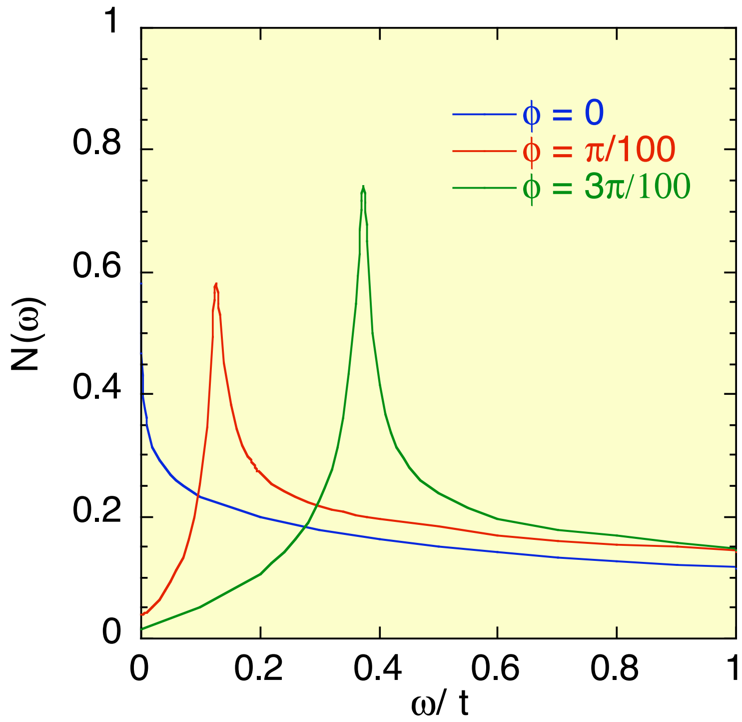
Density of states

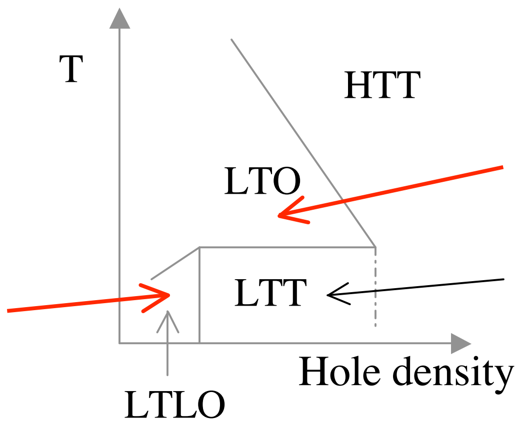
$$N_\sigma(k,\varepsilon) = -\frac{1}{\pi}\,\mathrm{Im}\,G_\sigma(k,\varepsilon+i\delta)$$

Eigenfunction $\varphi_{\sigma m}(r)$

$$H\varphi_{\sigma m}(r) = E_{\sigma m}\varphi_{\sigma m}(r)$$

$$G_\sigma(r,r',i\omega) = \sum_m \frac{\varphi_{\sigma m}(r)\varphi^*_{\sigma m}(r')}{i\omega - E_{\sigma m}}$$

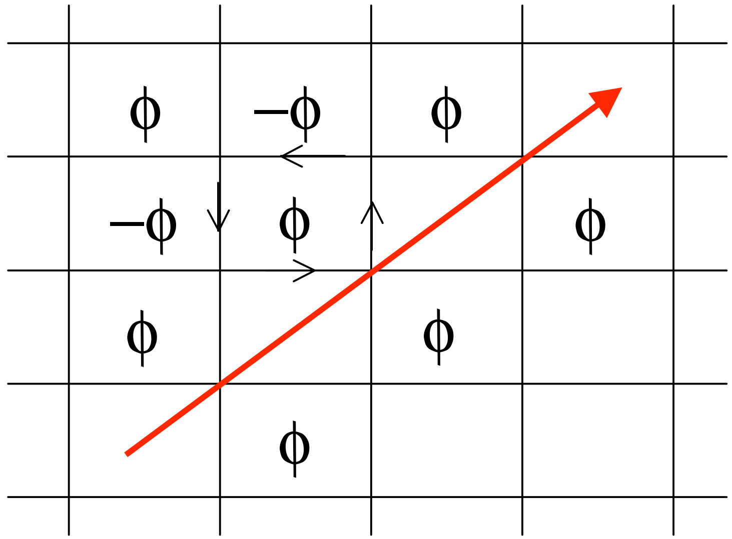


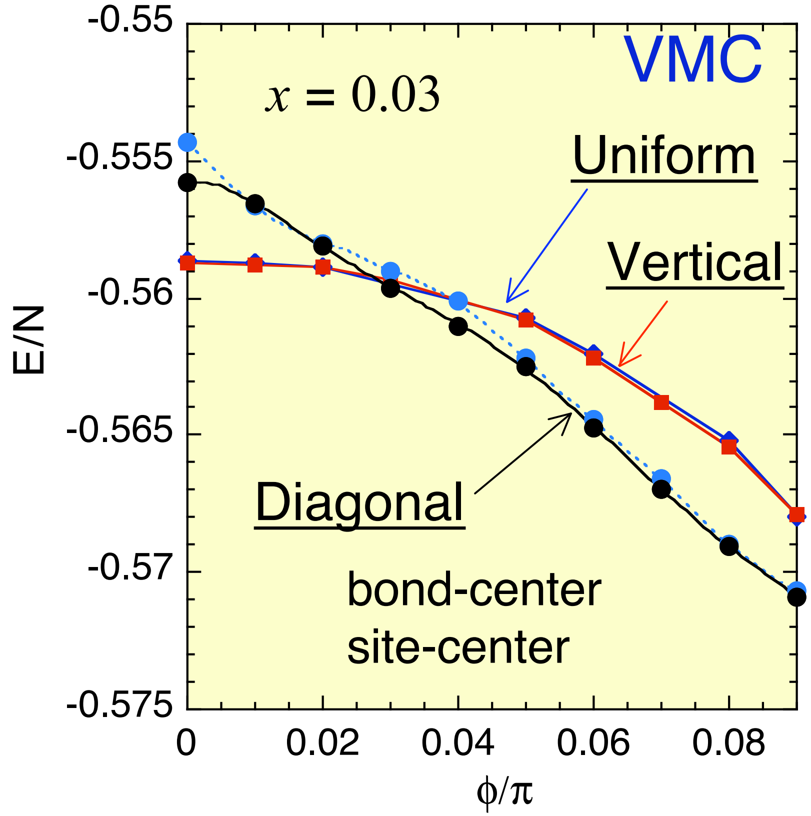


Diagonal stripes with Spin-orbit coupling

Spin-orbit coupling induces flux.

Spin-orbit coupling stabilizes the diagonal stripes.





$\Phi = 4\phi$

Diagonal Stripe & d-density wave

T.Y. et al., JMMM 272 (2004) 183.

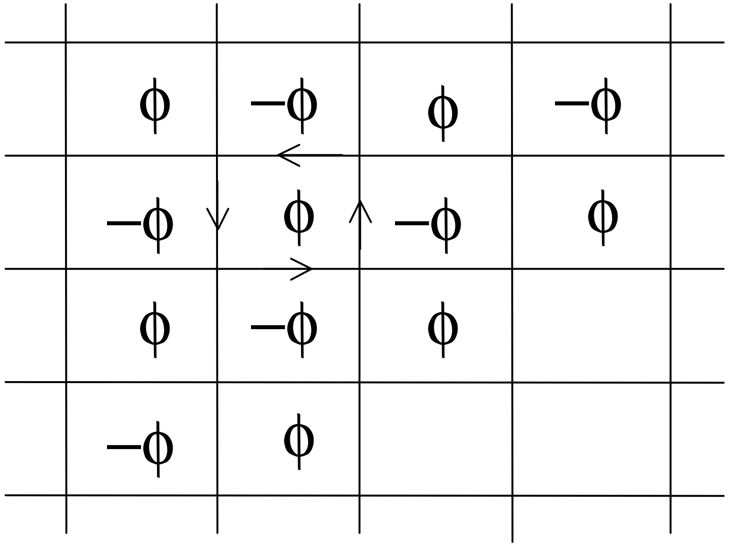
d-density wave

d-density wave

$$i\Delta_Q Y(k) = \left\langle c^{+}_{k+Q\sigma} c_{k\sigma} \right\rangle \quad Q = (\pi, \pi)$$

$$Y(k) = \cos(k_x) - \cos(k_y)$$

Nayak, Phys. Rev. B62, 4880 (‘00)
Chakravarty et al., PRB63, 094503 (‘01)



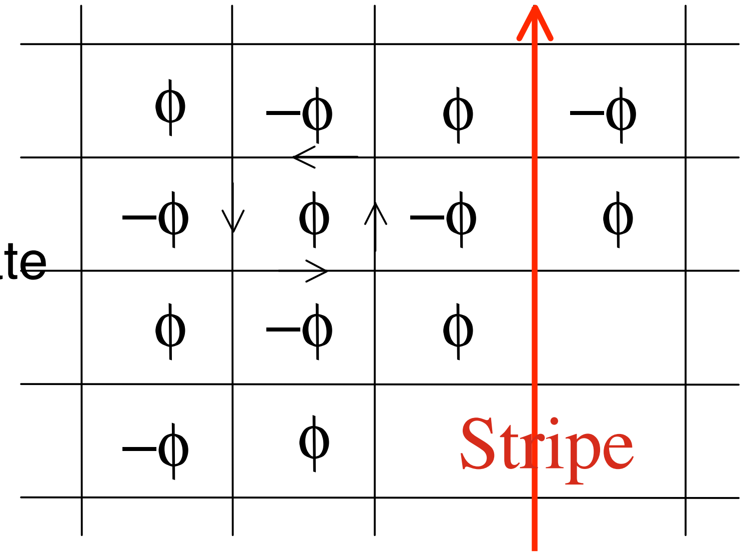
Inhomogeneous density wave

$$i\Delta_Q Y(k) = \left\langle c^{+}_{k+Q\sigma} c_{k\sigma} \right\rangle \quad \text{d-symmetry}$$

$$\Delta_{lQ_s\sigma} = \sum_k \left\langle c^{+}_{k+lQ_s\sigma} c_{k\sigma} \right\rangle \quad \text{incommensurate}$$

$Q_s = (\pi+2\pi\delta, \pi)$ vertical

$Q_s = (\pi+2\pi\delta, \pi+2\pi\delta)$ diagonal



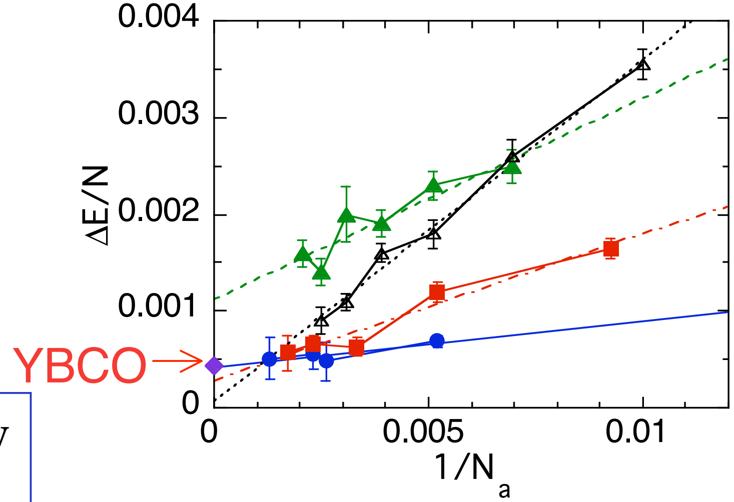
8. Summary

HTSC and Correlated Electrons

Variational Monte Carlo study of

BCS-Gutzwiller function

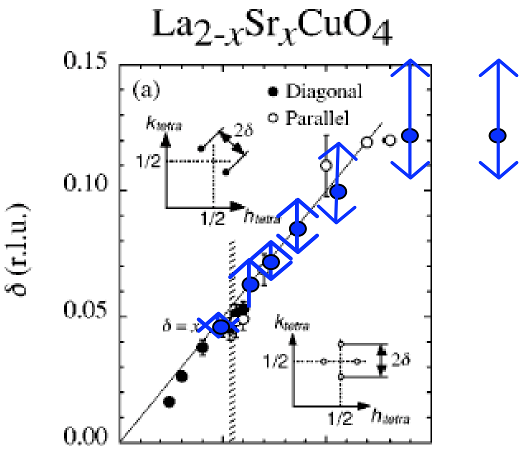
$$\psi_{CdS} = P_G \prod_k (u_k + v_k c^+_{k\uparrow} c^+_{-k\downarrow})|0\rangle$$



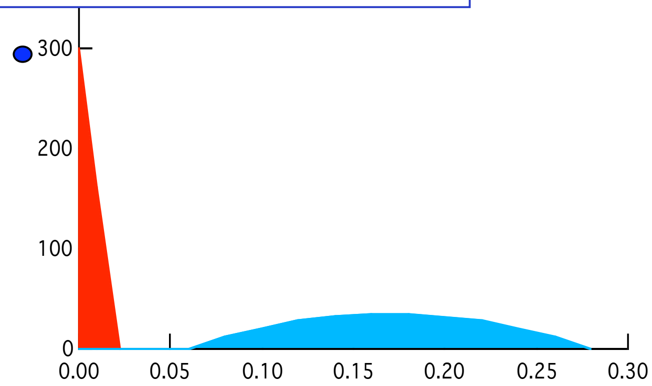
Theoretical estimate of
SC condensation energy

Agreement with Exp.

$E_{cond} \sim 0.2meV$



Incommensurability
Neutron scatterings



underdoped

overdoped