Phase diagram of cuprate High-temperature superconductors

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Outline

1. Introduction

2. Optimization Variational Monte Carlo method

3. Electronic states of 2D Hubbard model
   - Antiferromagnetism
   - Superconductivity
   - Phase separation
   - Stripes
   - Kinetic energy driven mechanism
   - Phase diagram

4. Summary

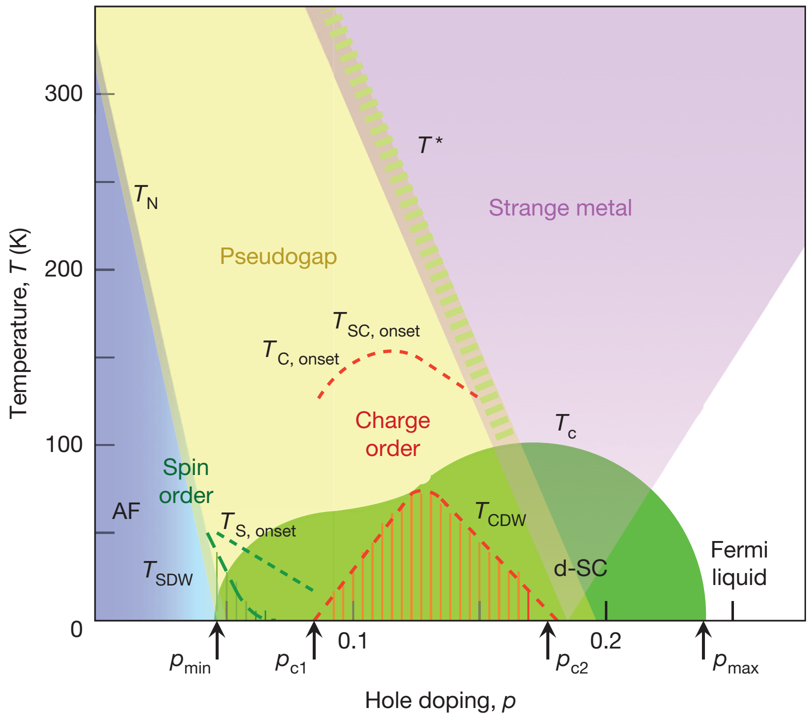
1. Introduction

High-T_c Cuprates

High-T_c cuprates

Correlated electron systems

- Parent materials are insulators.
  Mott insulator
- d-wave symmetry
- anomalous metallic phase
- near antiferromagnetic phase



B. Keimer et al., Nature 518, 179 (2015)

Electron Correlation and High T_c

We can expect higher T_c if superconductivity is induced by the interaction with large energy scale.

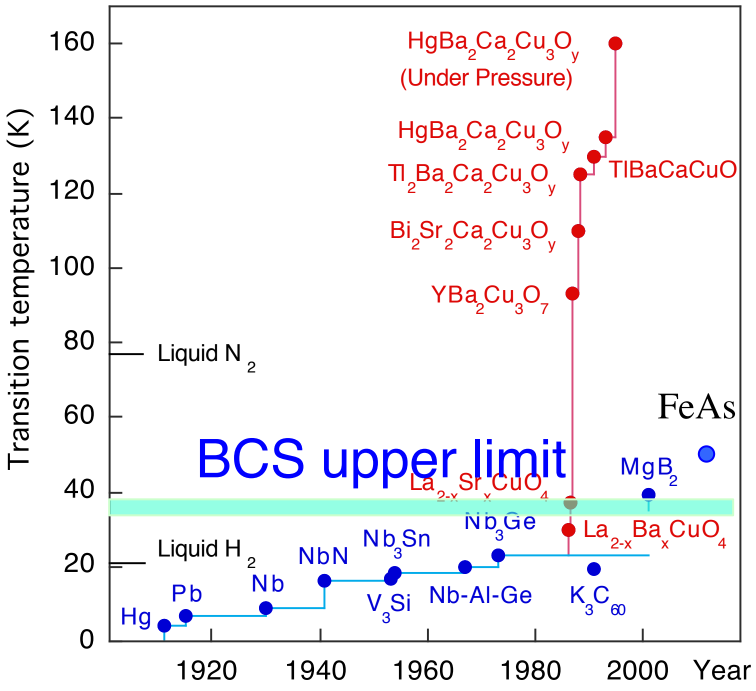
Electron-Electron Interaction

Energy scale ~ eV ~ 10,000K

Electron-phonon interaction

Energy scale ~ Debye Freq. ~ 300K

Upper bound of T_c ~ 30-40K (McMillan)



Electron-Correlation Mechanism

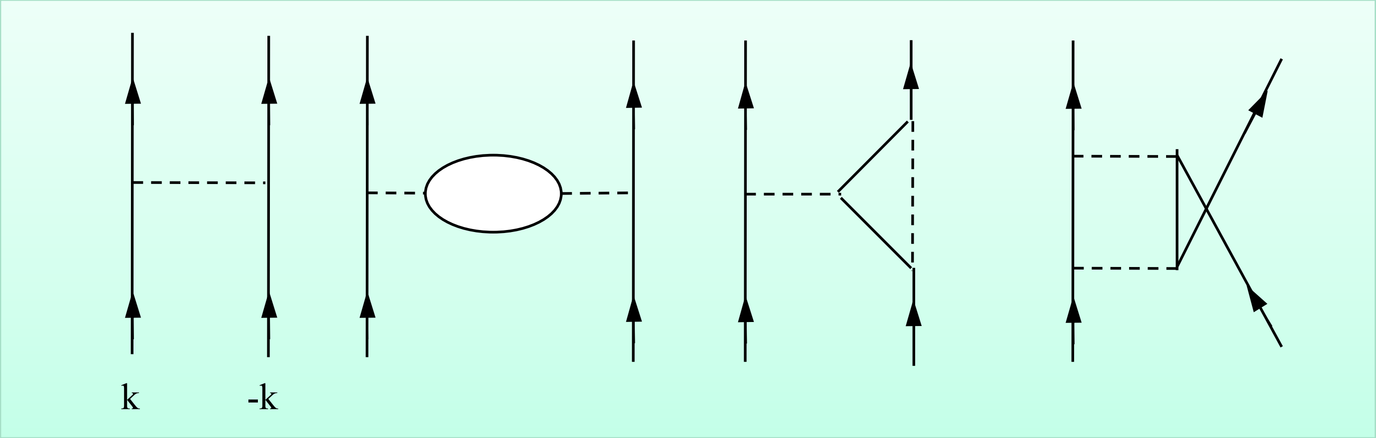
Kohn-Luttinger (1965)

Gap equation

$$\Delta_k = -\frac{1}{N}\sum_{k'} V_{kk'}\Delta_{k'}\frac{1-2f\left(E_{k'}\right)}{2E_{k'}} \qquad E_k = \sqrt{\xi_k^2 + \Delta_k^2}$$

$$\Delta(\theta) = \sum_{\ell}\Delta_{\ell}P_{\ell}(\cos\theta) \qquad -\frac{1}{2}N(\varepsilon_F)V_{\ell} = \lambda_{\ell} \qquad k_B T_c = \omega_{c,\ell}\exp\left(-1/\lambda_{\ell}\right)$$

Gap equation has a solution when *l* is large even for repulsive interaction.



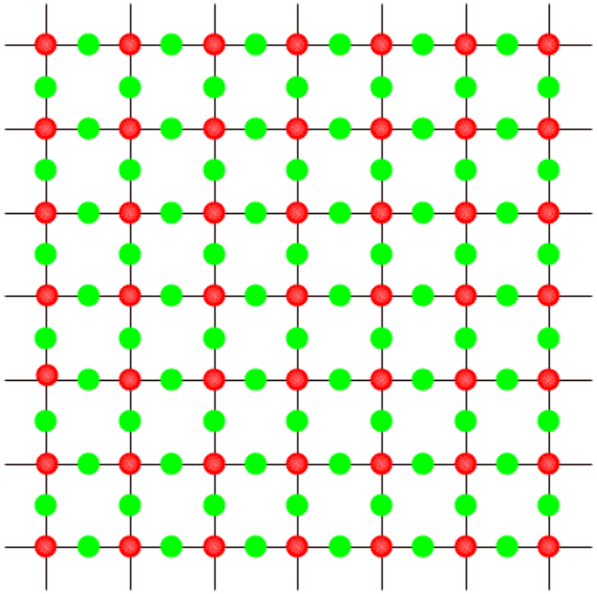
Energy scales and T_c

$T_c \sim 0.1t/(m^*/m)$ Empirical relation

	t	m*/m = r	t/r	T_c
Cuprates	5000K	5	1000	100K
Fe based	1000K	~ 2	500	50K
Heavy electrons	10000K	100 ~ 1000	10 ~ 100	1 ~ 10K ~ T_K (Kondo)
Organics	200 ~ 500K	2 ~ 5	100	10K
YBCO	5000K	5	1000	100K
KFe_2As_2	300K	7	30	3K
Hydrides H_3S	1000K	1	1000	100K

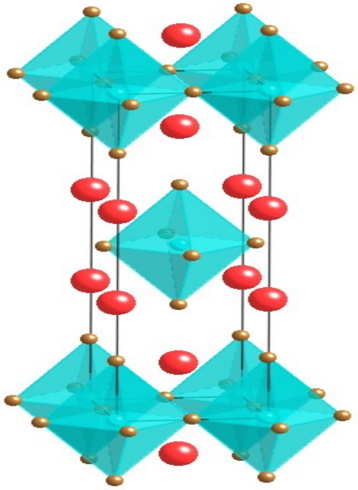
T.Y. Condensed Matter 4, 57 (2019)

Model of High-Tc Cuprates

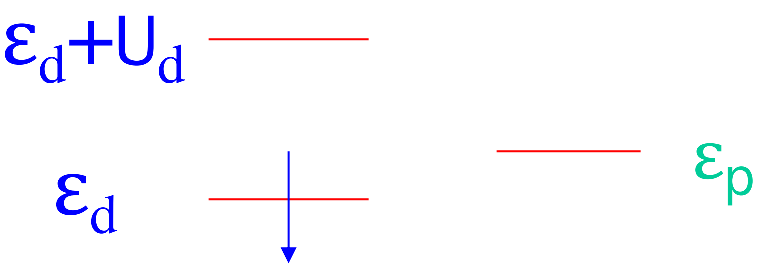


Two-Dimensional plane

CuO_2 plane →

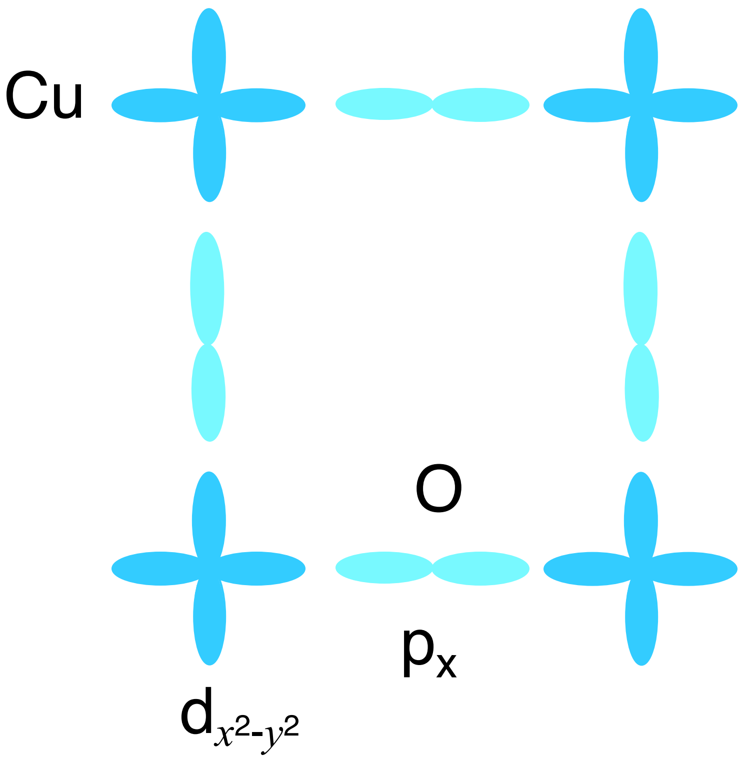


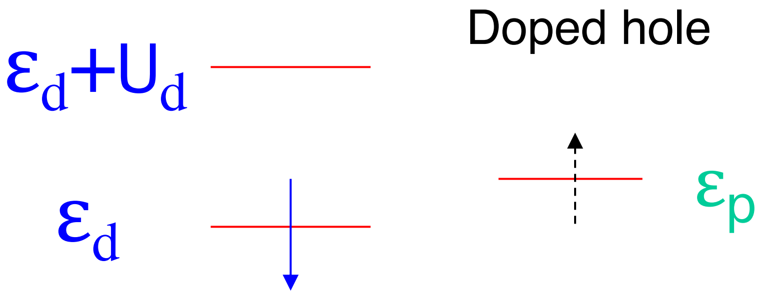
- Copper atoms
- Oxygen atoms



Model of Cuprates

Two-Dimensional Plane



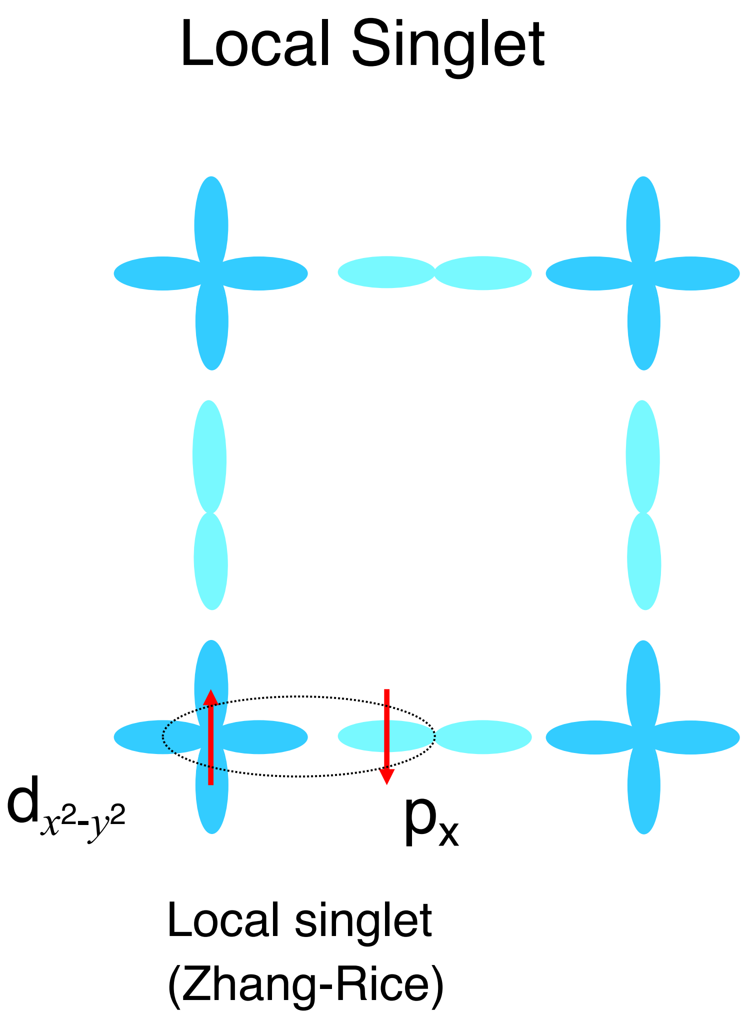


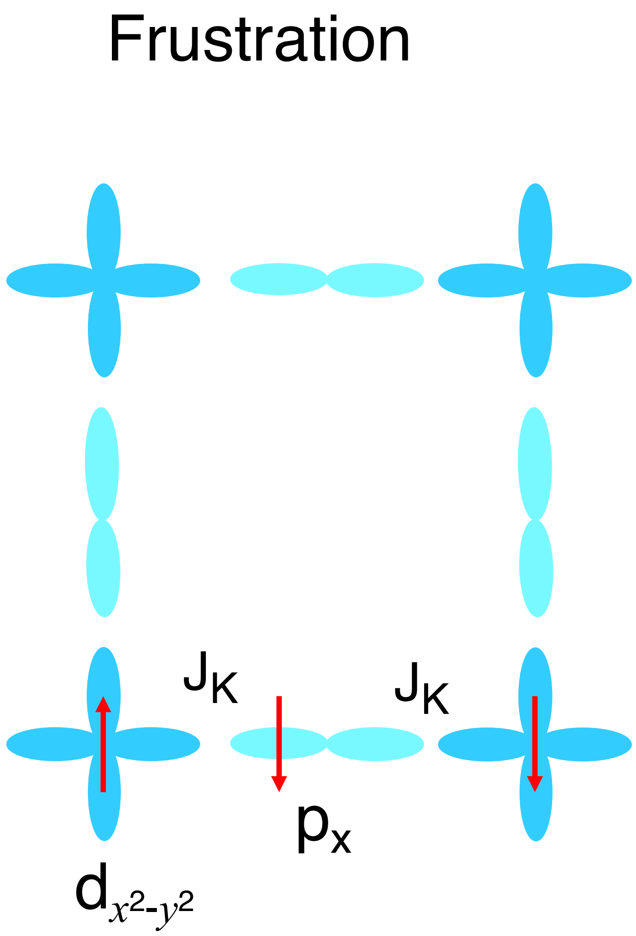
(Hole picture)

Characteristics

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

Holes in the CuO_2 plane

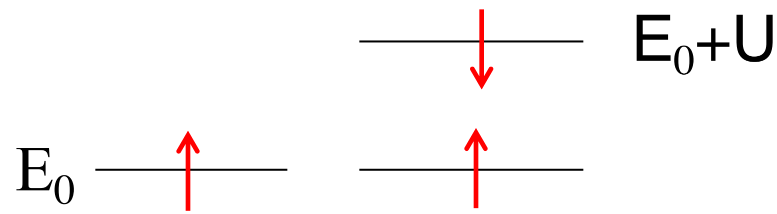


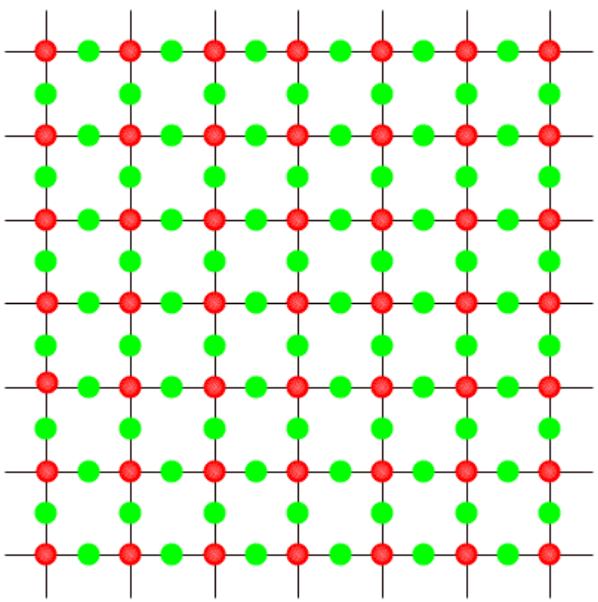


Hubbard model

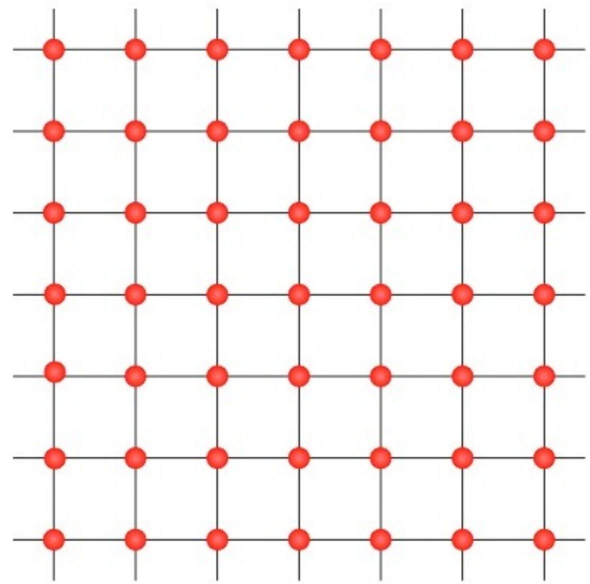
— One-band effective model —

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





Two-Dimensional plane



Hubbard model

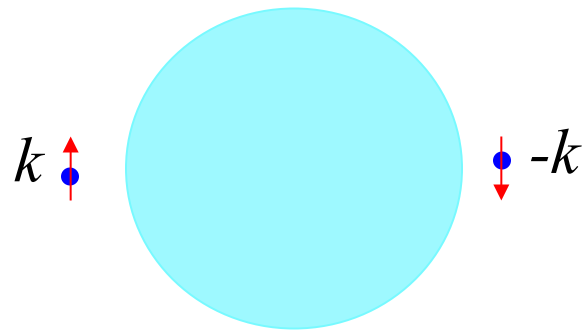
2. Optimization Variational Monte Carlo method

Optimized many-body wave function

Superconducting state with correlation

Pairing state in correlated electron systems

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



Gutzwiller Projection P_G

To control the on-site strong correlation

Weight g
Coulomb +U

Weight 1
Parameter 0<g<1

BCS state
in
Correlated Electrons

Off-Diagonal Wave Function

Off-diagonal wave functions

Gutzwiller wave function $\psi_G = P_G \psi_0$

Off-diagonal wave functions

$$\psi_\lambda = e^{-\lambda K} P_G \psi_0 = \psi_\lambda^{(2)}$$

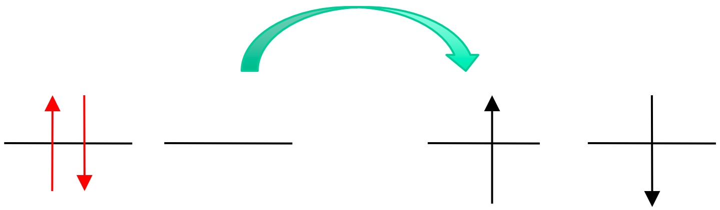
$$\psi_\lambda^{(3)} = P_G e^{-\lambda K} P_G \psi_0$$

$$\psi_\lambda^{(4)} = e^{-\lambda' K} P_G e^{-\lambda K} P_G \psi_0$$

$\lambda, g, \ldots$: parameters

Site-diagonal operator

Site-off-diagonal



T. Y. et al., JPSJ 67, 3867 (1998)
T. Y. JPSJ 85, 147017 (2016)
T. Y. JPSJ 88, 054702 (2019)

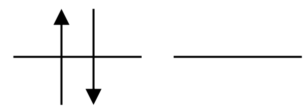
The wave function approaches an exact one.

Electron Correlation Operator

Site-diagonal correlation operator

$\psi = \sum_j a_j \varphi_j$ a_j modified

Gutzwiller P_G



Jastrow factor P_J

Doublon-holon P_{d-h}

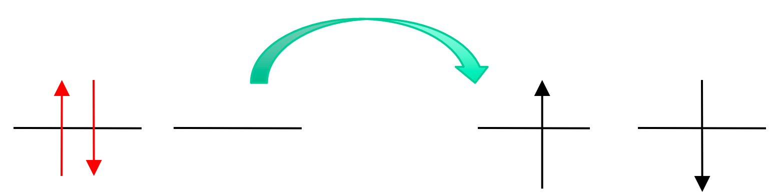
H. Yokoyama et al. JPSJ

Site off-diagonal correlation operator

a_j, a_k mixing effect

Kinetic operator K

Off-diagonal Mixing
in configuration space $e^{-\lambda K}$



Comparison of Variational Energy

$4 \times 4 \;\; t'/t = 0$

	$N_e = 16 \;\; U/t = 5$	$N_e = 12 \;\; U/t = 4$	$N_e = 12 \;\; U/t = 10$	
$P_G \psi_{FS}$	-11.654	-18.239	-13.960	
$P_J P_{d-h} P_G \psi_{FS}$	-11.856		-14.031	
$P_J P_{d-h} P_G \psi_{pair}$	-12.459	-18.406	-14.435	many-parameter wave function
$e^{-\lambda K} P_G \psi_{FS}$	-12.366	-18.481	-14.544	
$P_G e^{-\lambda K} P_G \psi_{FS}$	-12.479	-18.528	-14.647	
$e^{-\gamma K} P_G e^{-\lambda K} P_G \psi_{FS}$	-12.487	-18.536	-14.685	
Exact	-12.530	-18.571	-14.808	

Comparison of Variational Energy 2

	10×10 $t'/t = -0.3$ $N_e = 92$ $U/t = 12$		10×10 $t'/t = -0.0$ $N_e = 88$ $U/t = 18$
$P_G \psi_{FS}$	–0.3650		-0.4218
$P_G \Psi_{AF}$	-0.3771		-0.4259
$P_{d-h} P_G \Psi_{FS}$	-0.4259		-0.4634
$P_J P_{d-h} P_G \Psi_{FS}$	-0.4265		-0.4642
$P_{d-h} P_G \Psi_{AF-d}$	-0.4915	Yokoyama et al	
$e^{-\lambda K} P_G \psi_{FS}$	-0.4956		-0.5115
$P_G e^{-\lambda K} P_G \psi_{FS}$	-0.5095		-0.5175

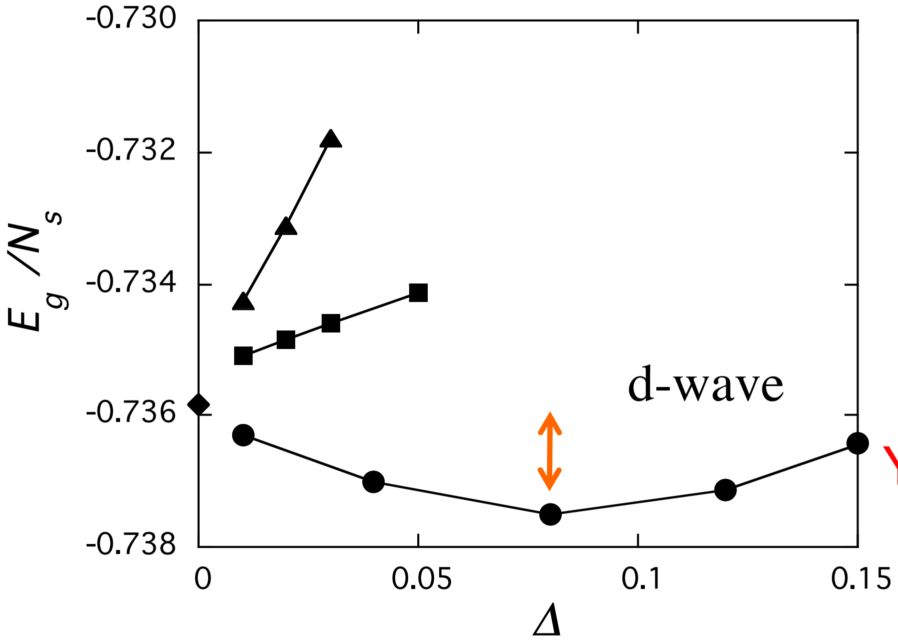
3. Electronic States of Hubbard model

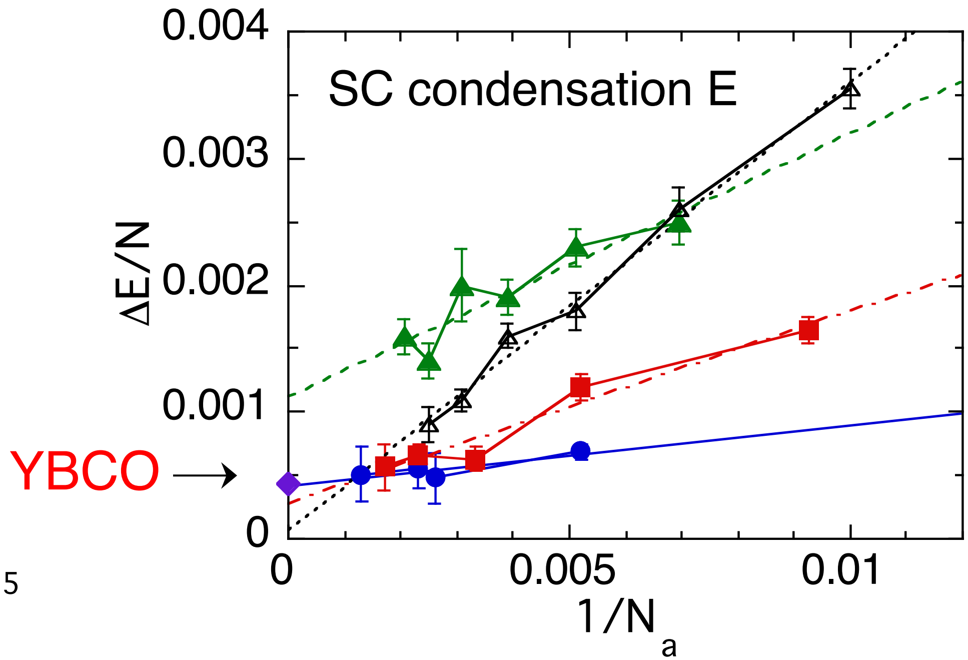
Research for the Hubbard model

Two-dimensional Hubbard model

1. Optimized wave function   kinetic energy effect
2. Antiferromagnetic (AF) correlation
3. Superconductivity (SC)   d-wave
4. Effect of t' (nearest-neighbor transfer)
5. Phase separation
6. Phase diagram

Condensation Energy: Gutzwiller function





2D Hubbard model

10x10 Hubbard model U = 8

Extrapolation N = ∞

$E_{cond} \sim 0.2$meV

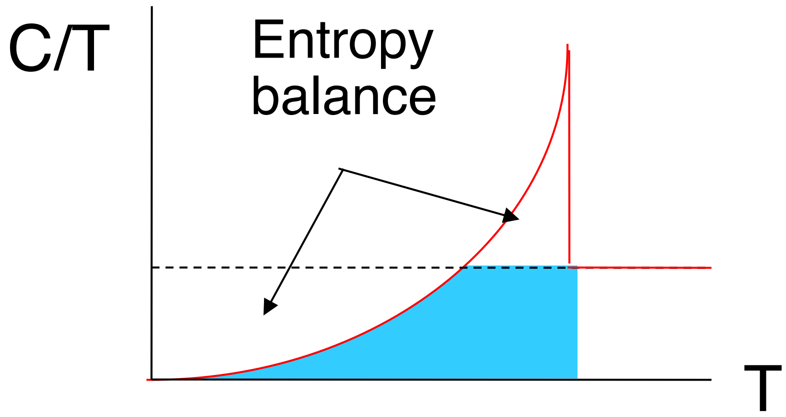
Agrees with experiments!

Superconducting Condensation Energy

SC Condensation energy

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

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



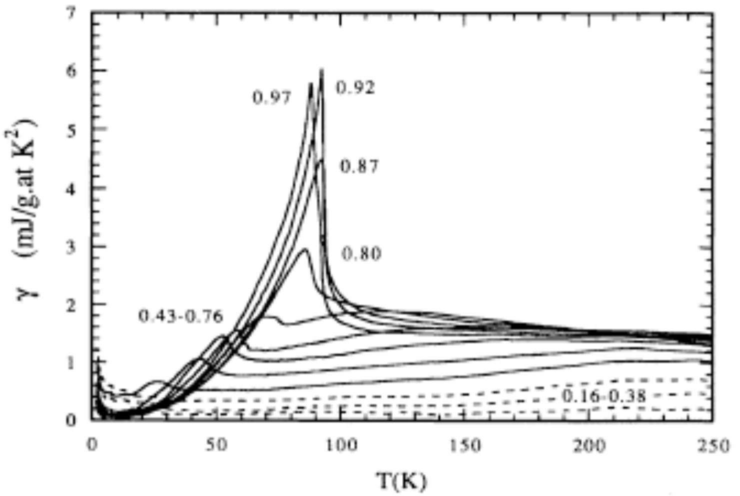


FIG. 4. Electronic specific heat coefficient $\gamma(x,T)$ vs T for $YBa_2Cu_3O_{6+x}$ relative to $YBa_2Cu_3O_6$. Values of x are 0.16, 0.29, 0.38, 0.43, 0.48, 0.57, 0.67, 0.76, 0.80, 0.87, 0.92, and 0.97.

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

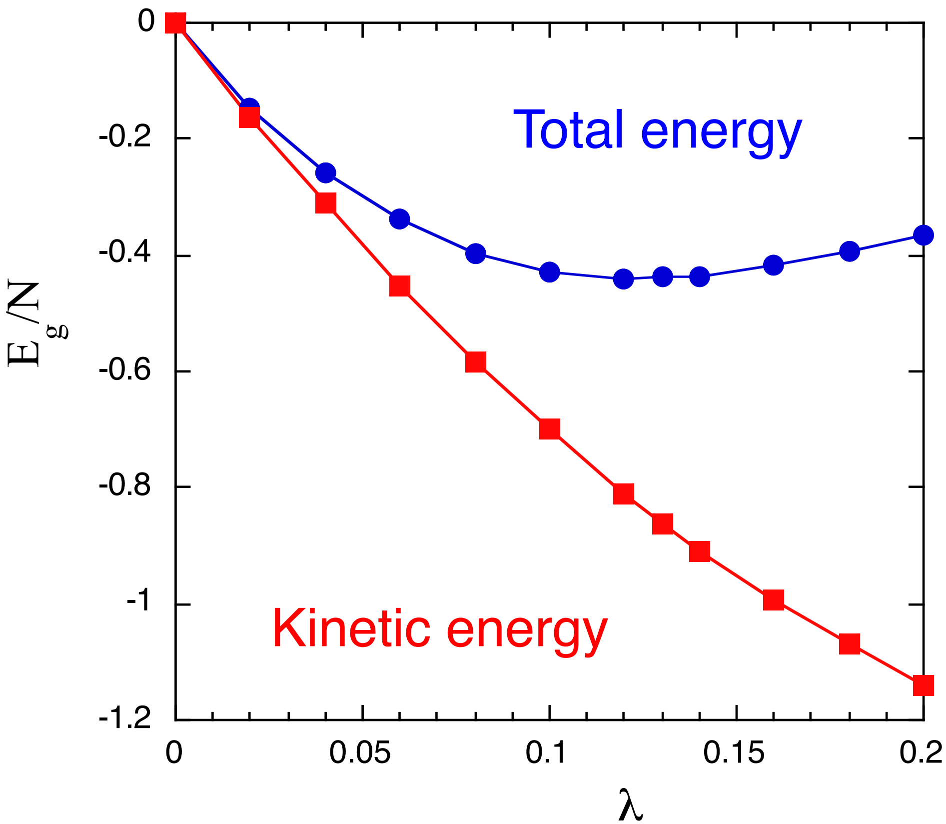
optimally doped YBCO

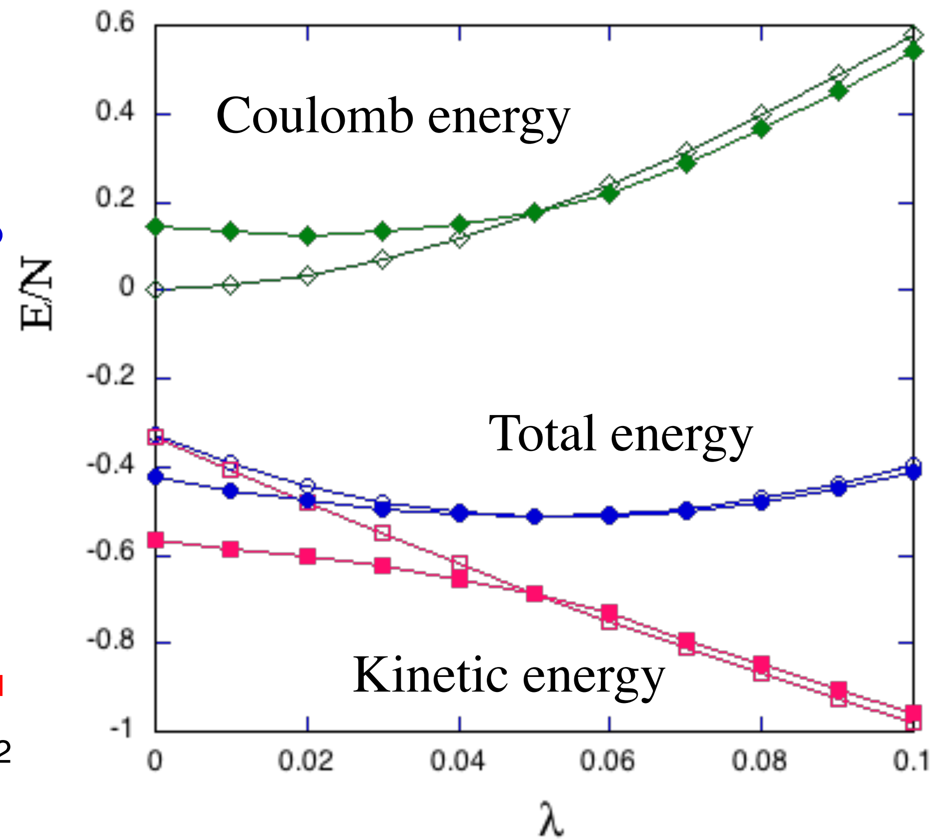
SC Condensation energy
~ 0.2 meV/site

Off-diagonal wave function

$$\psi_\lambda = e^{-\lambda K} P_G \psi_0$$

$e^{-\lambda K}$ lowers the energy.





Spin Correlation Function

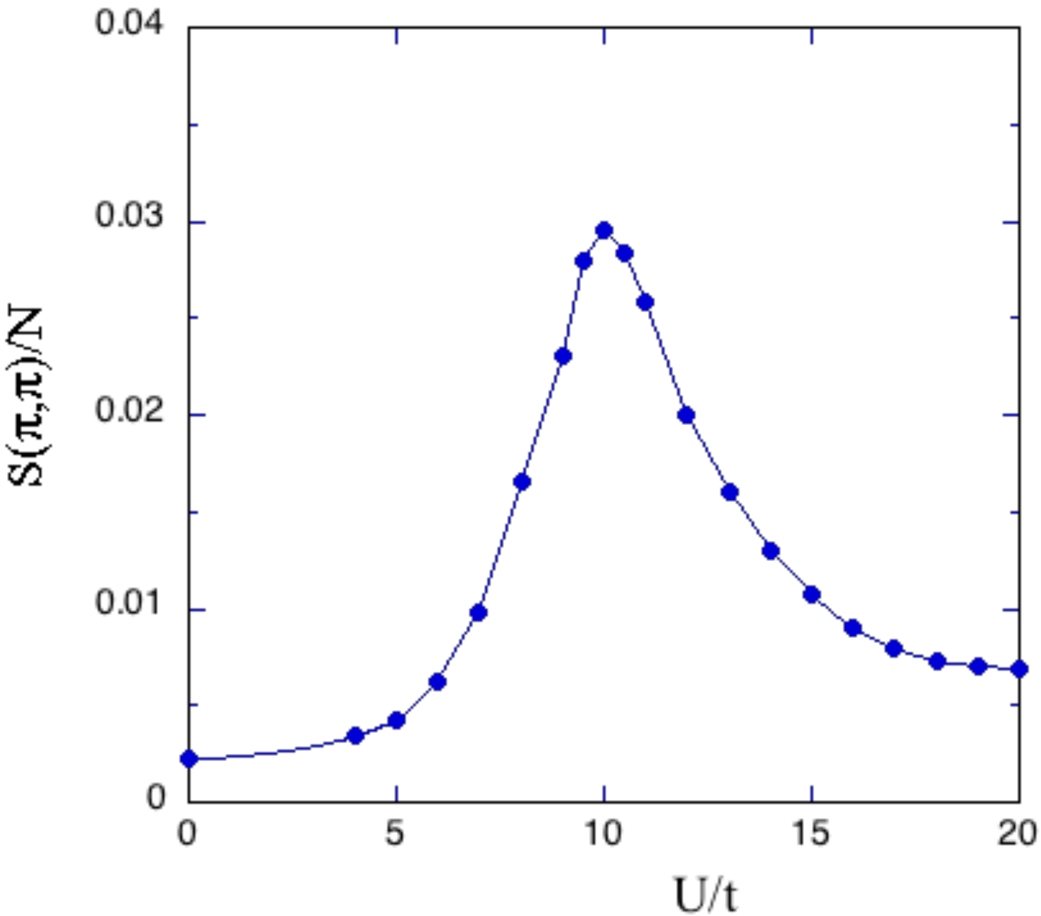
$$S(q)=\frac{1}{4N}\sum_{ij}e^{iq\cdot(r_i-r_j)}\left\langle\left(n_{i\uparrow}-n_{i\downarrow}\right)\left(n_{j\uparrow}-n_{j\downarrow}\right)\right\rangle$$

$$q=(\pi,\pi)$$

10×10 $N_e=88$ $t'=0$

S(q) shows a peak as a function of U.

AF correlation decreases in the strongly correlated Region.



Superconducting state

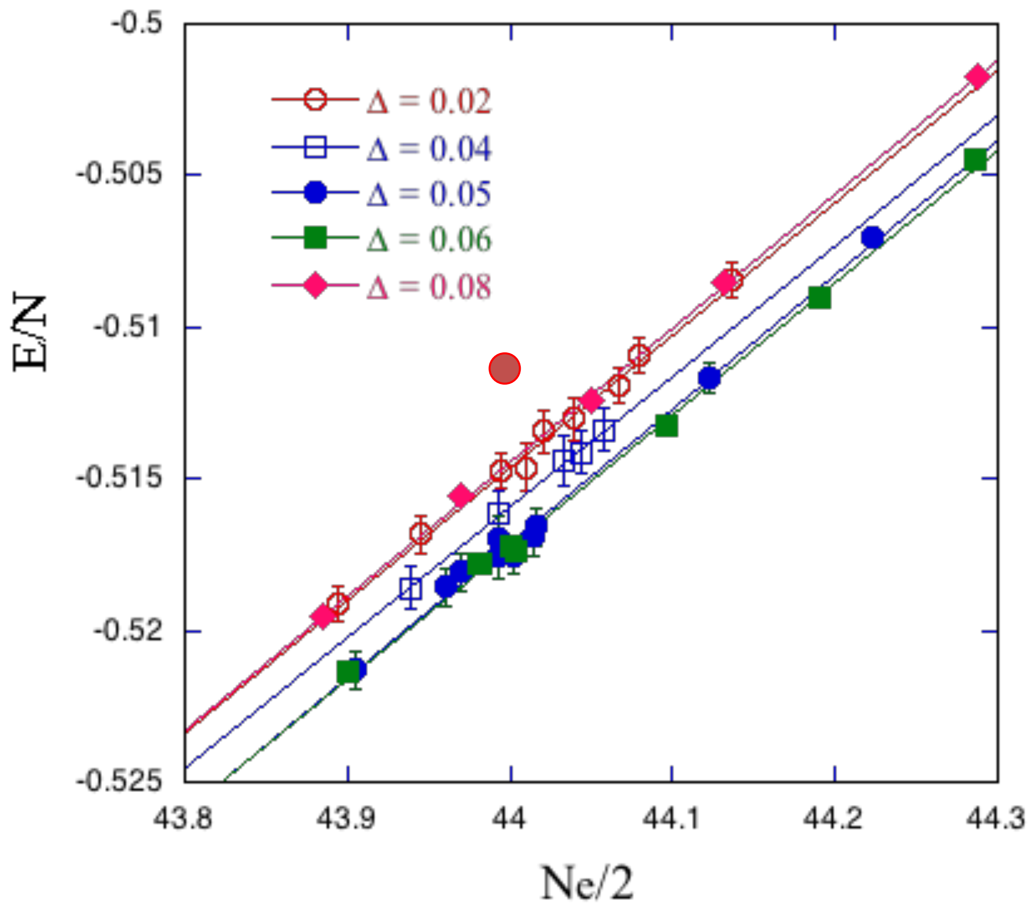
Correlated Superconducting state

d-wave SC

$$\psi = e^{-\lambda K} P_G \psi_{BCS}$$

BCS state ψ_{BCS}

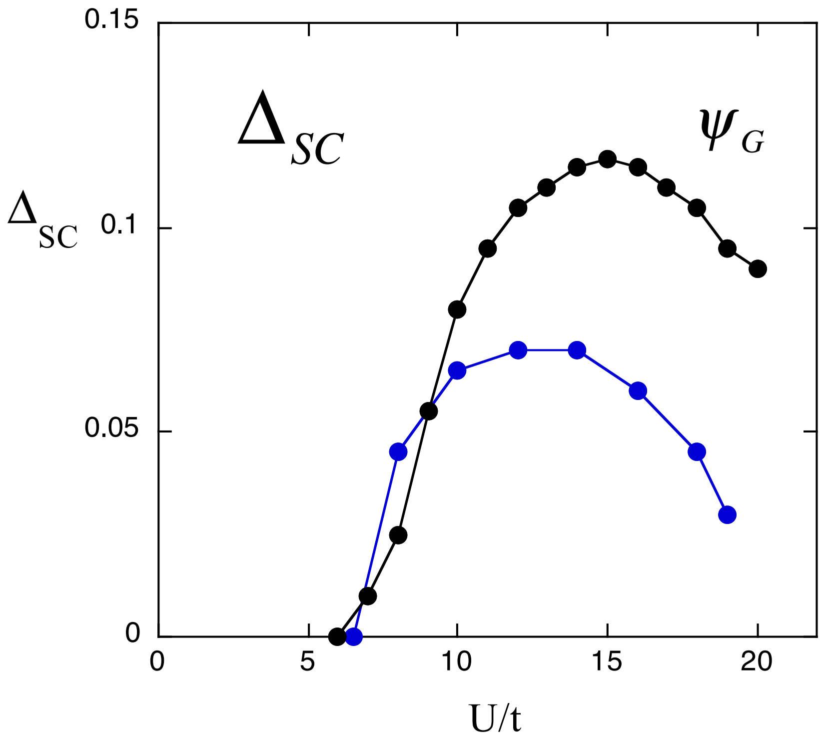
d-wave pairing



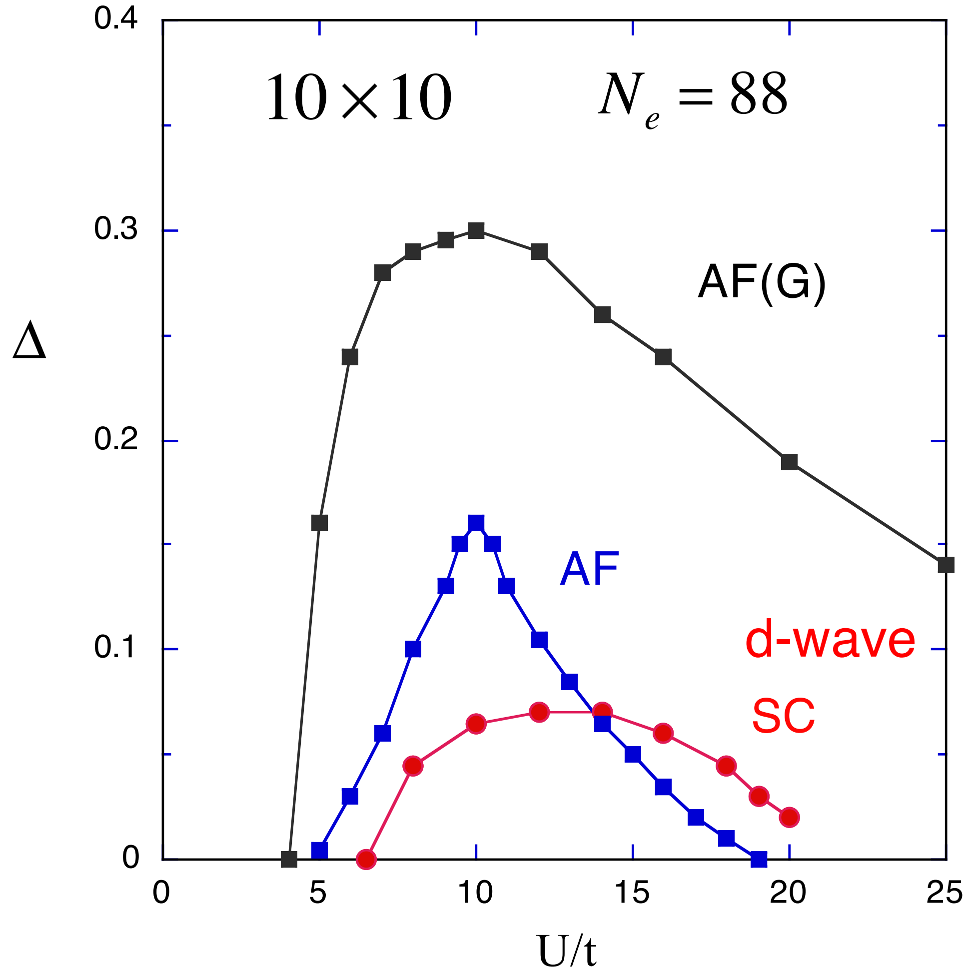
The minimum of the energy
at $\Delta > 0$

SC in Strongly Correlated Region

SC state is more stabilized in strongly-correlated region



U/t

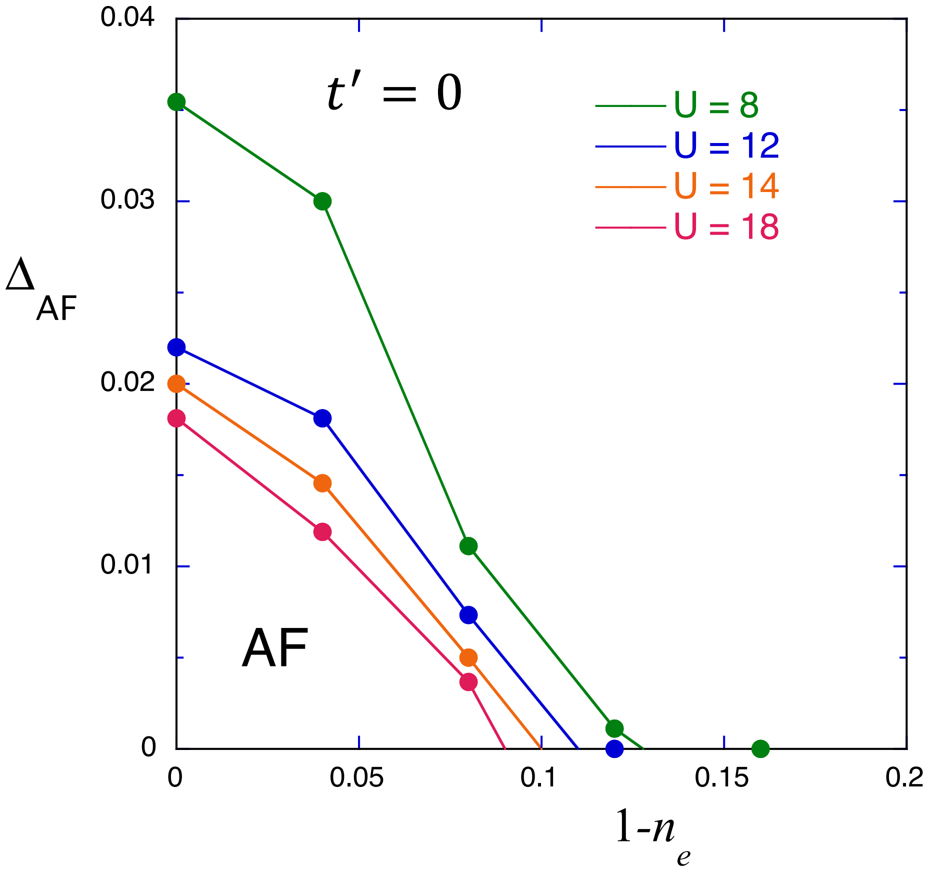


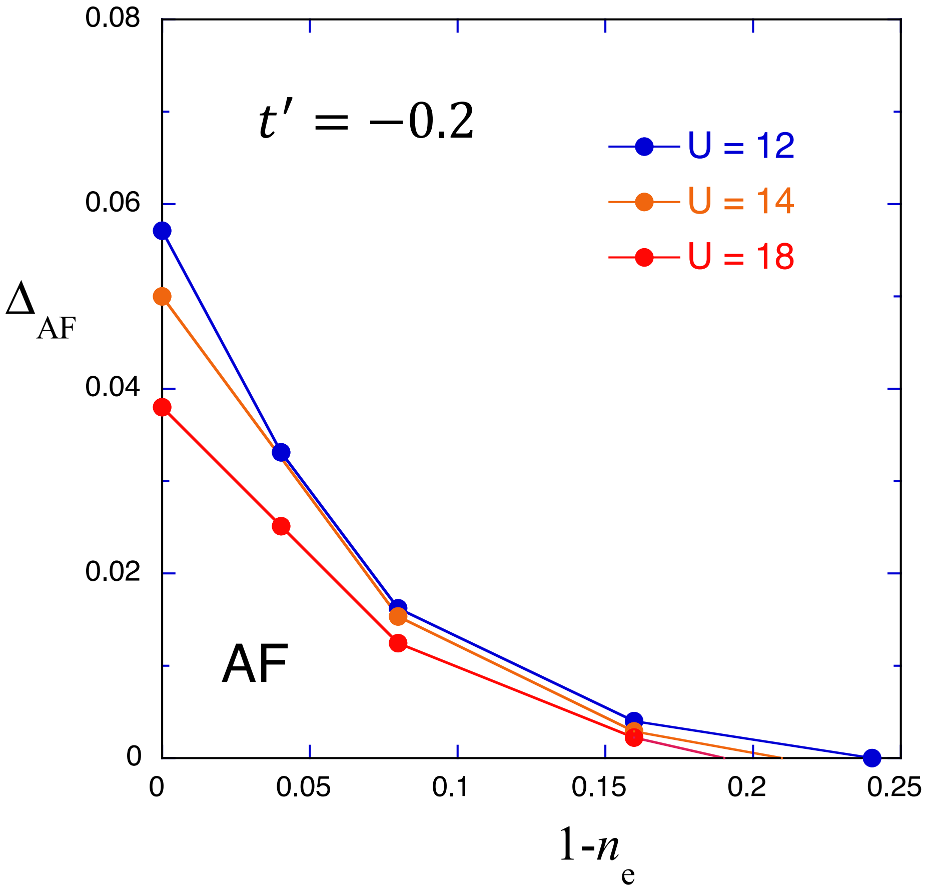
t' and AF order

AF order parameter as a function of the hole density x

Δ_{AF} vs $x = 1 - n_e$

AF area is large for $t' = -0.2$.

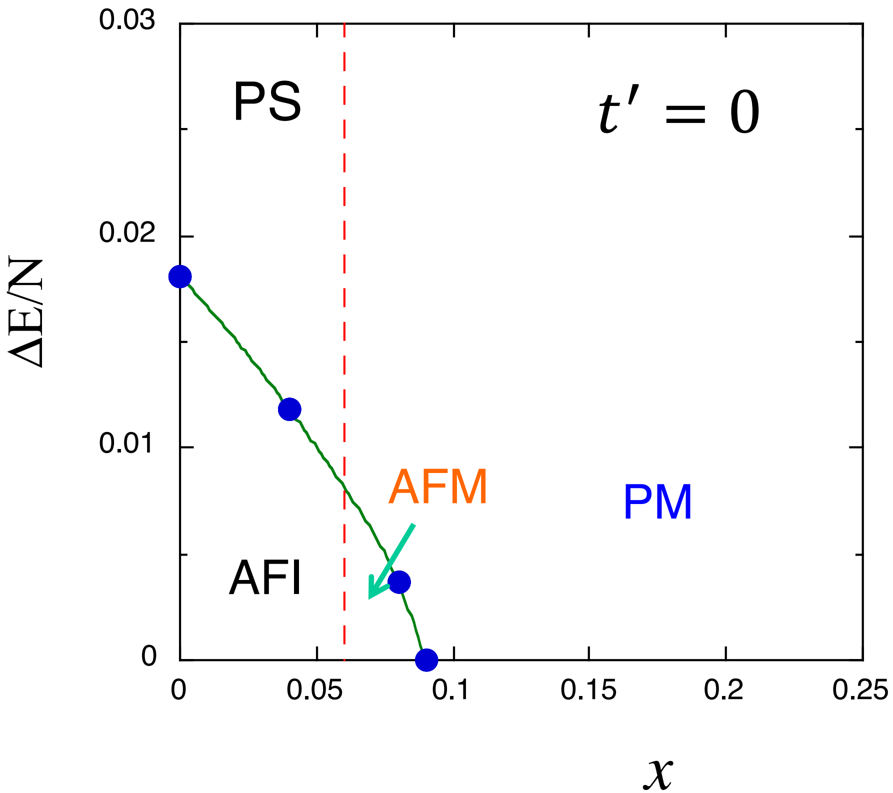


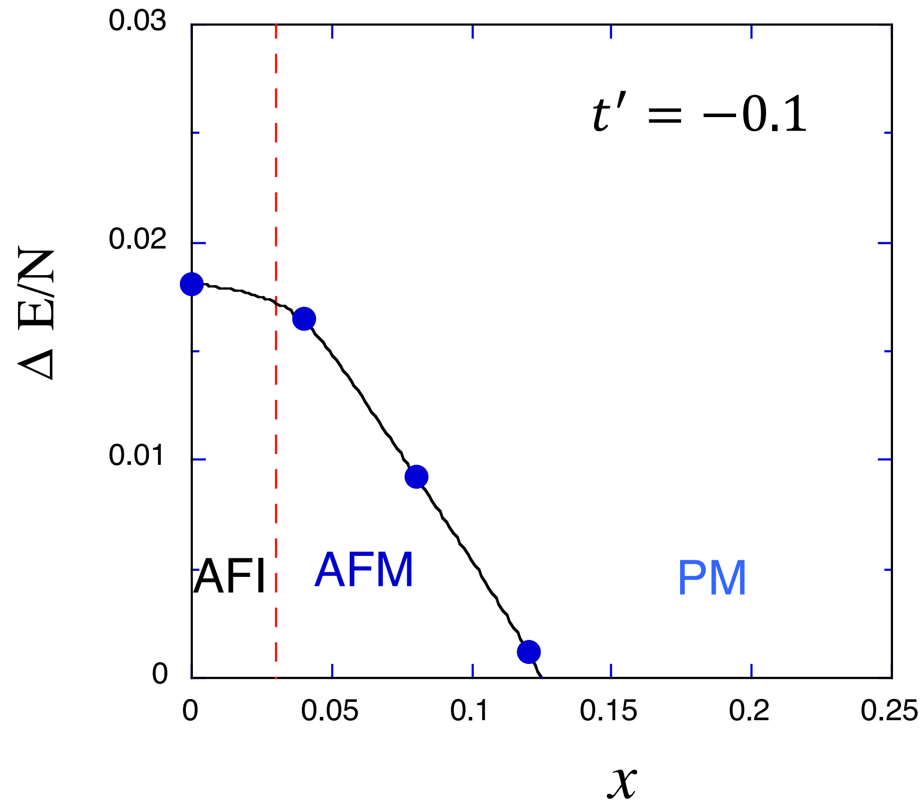


AF and Phase Separation

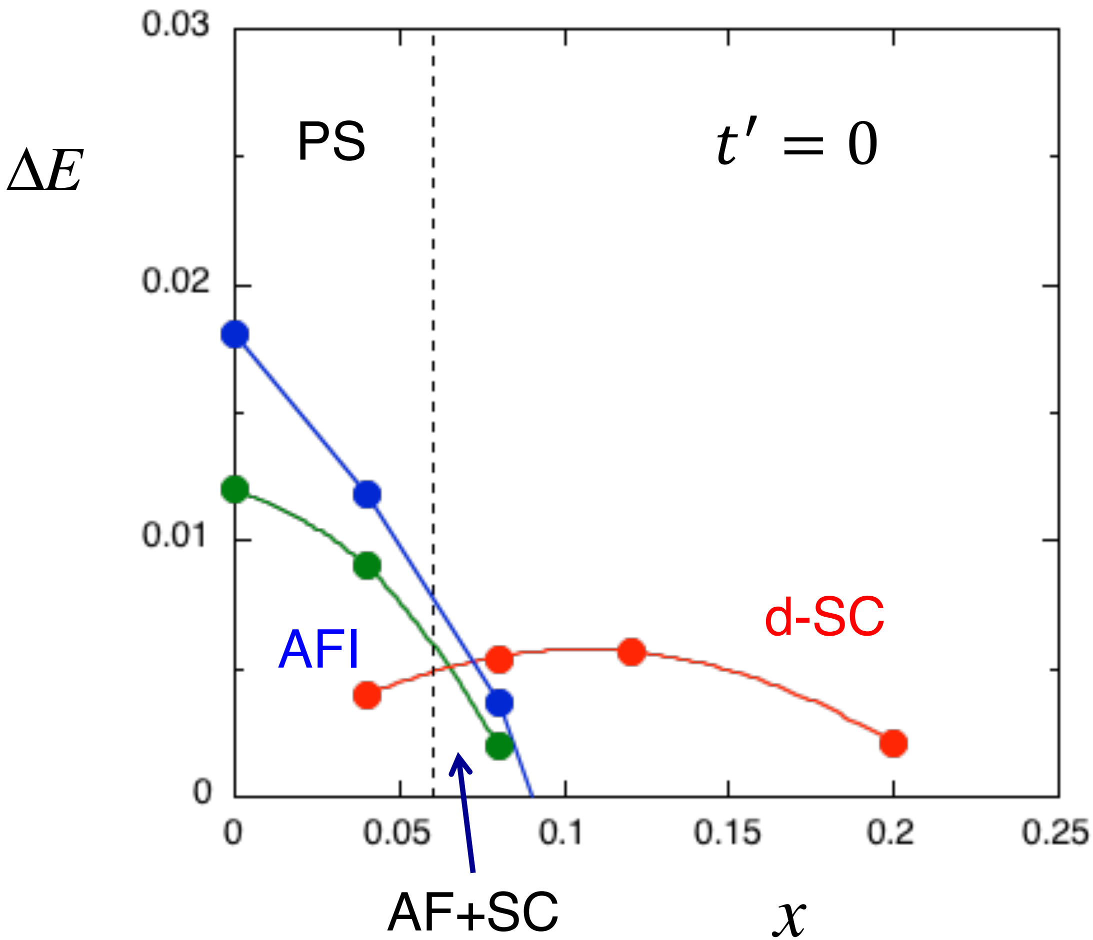
Phase separation in the AF region

PS region decreases due to t'.





Phase Diagram



$t' = 0$ is most favourable for SC

Blue line: $\psi^{(2)}$

Green line: $\psi^{(4)}$

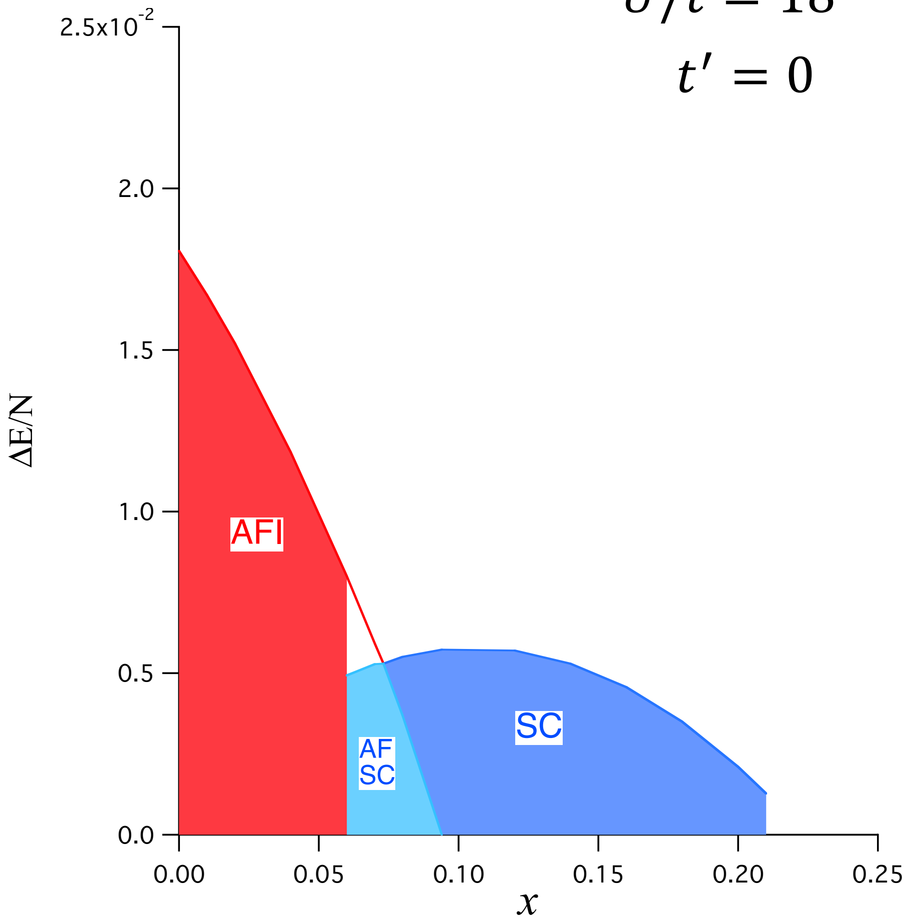
JPSJ 88, 054702 (2019)

Phase Diagram

Phase diagram

2D Hubbard model

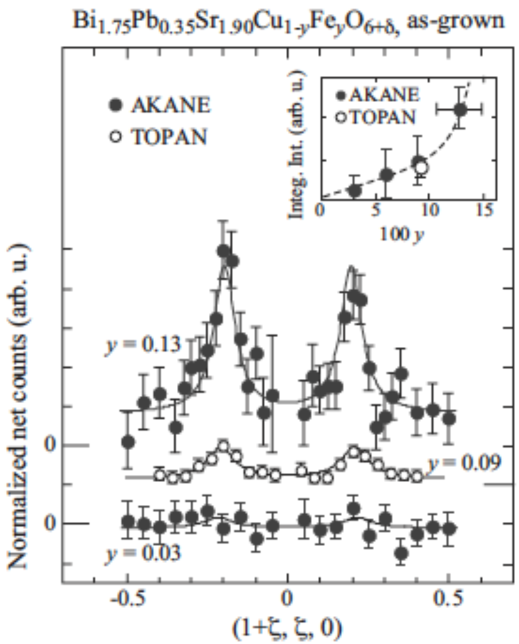
$$U/t = 18$$
$$t' = 0$$

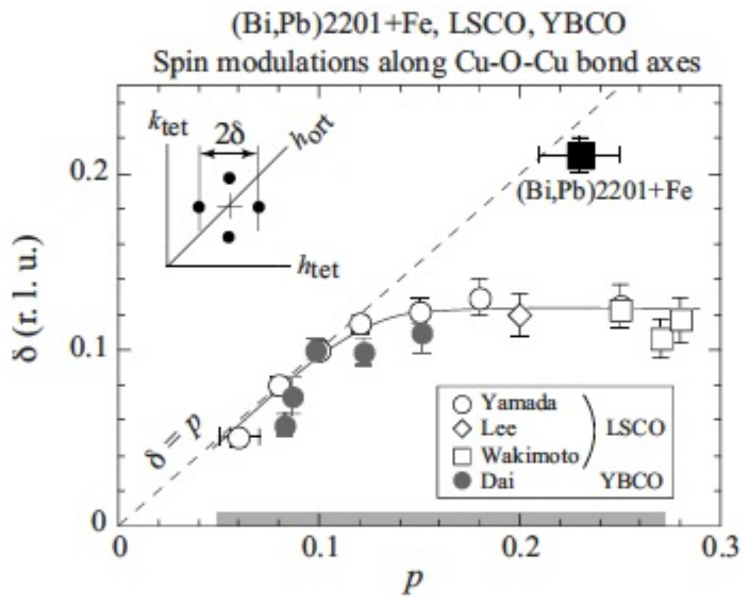


$x < 0.06$	Insulator
$0.06 < x < 0.09$	AF+SC
$0.09 < x$	d-SC

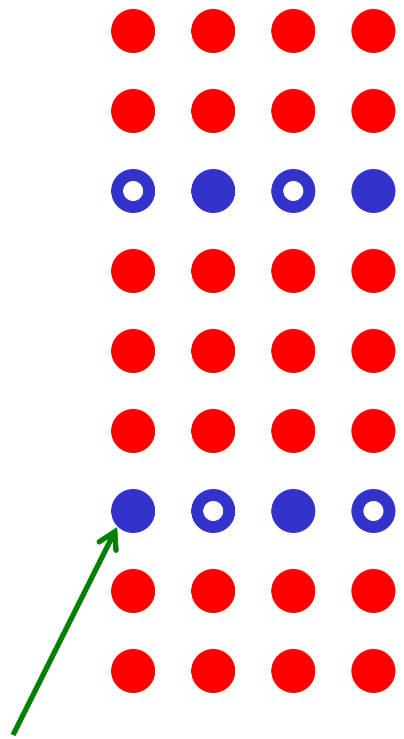
Stripes in Cuprates

Neutron scattering experiment in Cuprates





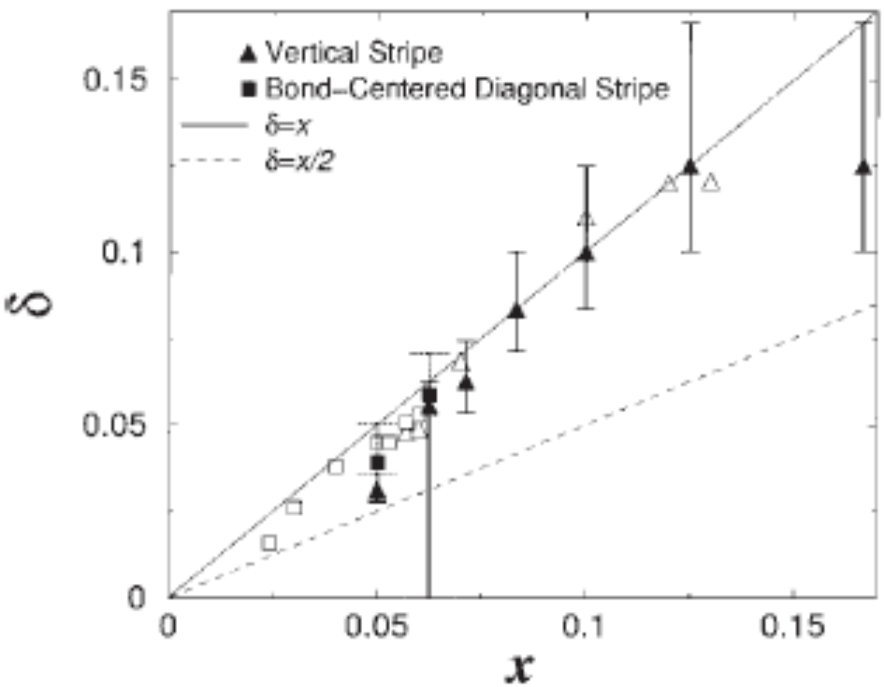
H. Hiraka et al.: PRB 81, 144501 (2010)



One-dimensional electrons
with 1/4-filling

⇒ Possible stripe state in a two-dimensional t-t'-U Hubbard model

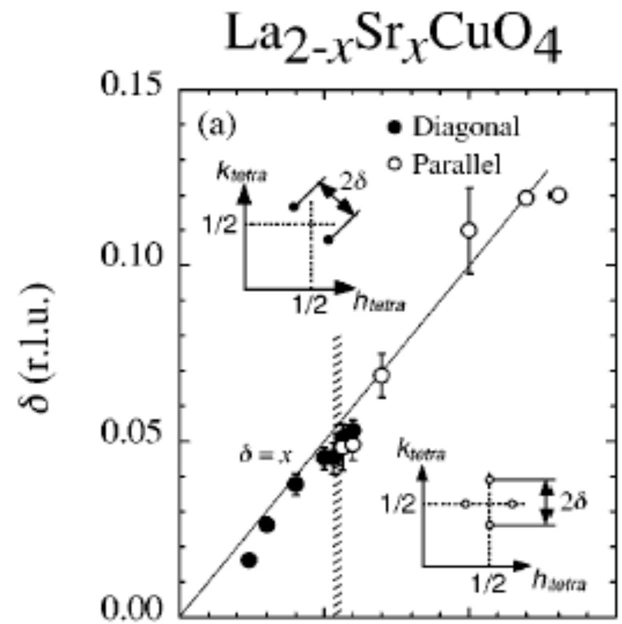
Incommensurability and Stripes



U = 8.0 t’= –0.2

Gutzwiller function

Miyazaki et al, JPSJ 71, 1643 (2004)



Neutron scattering

Incommensurability δ can be explained by the Hubbard model.

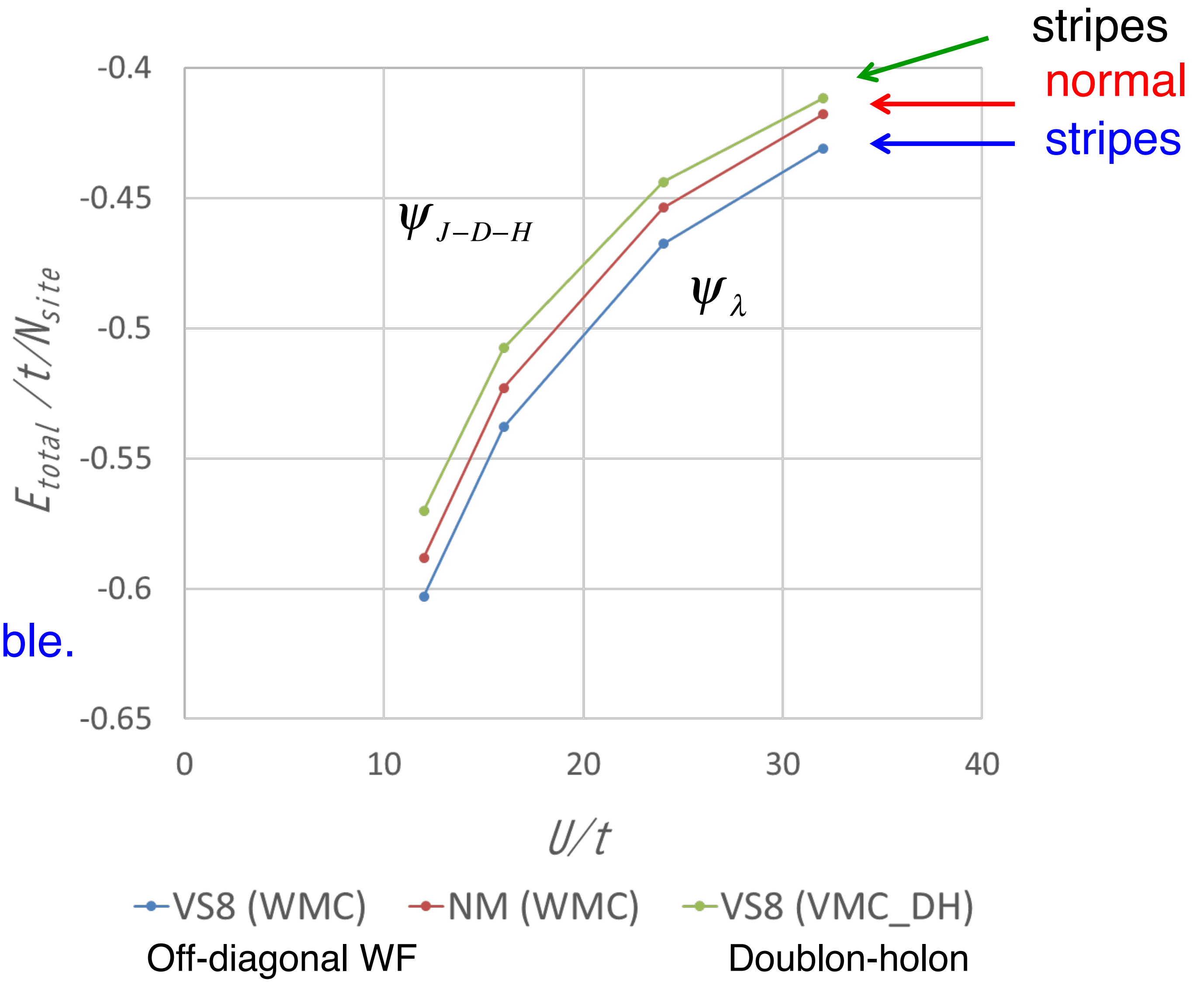
Stripes of Improved wave function

16×16

$x = 0.125$

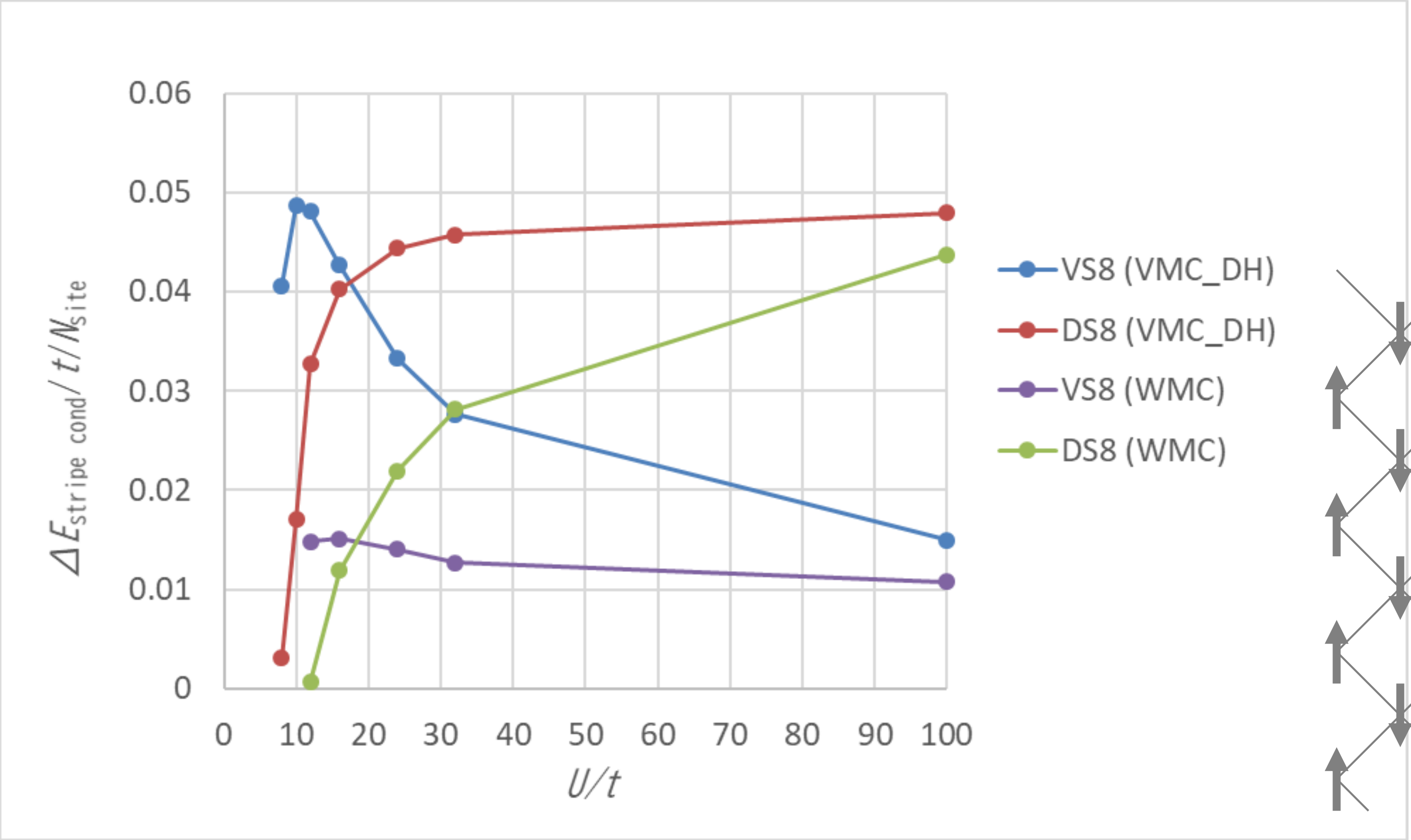
$t' = -0.30$

Striped state is stable.

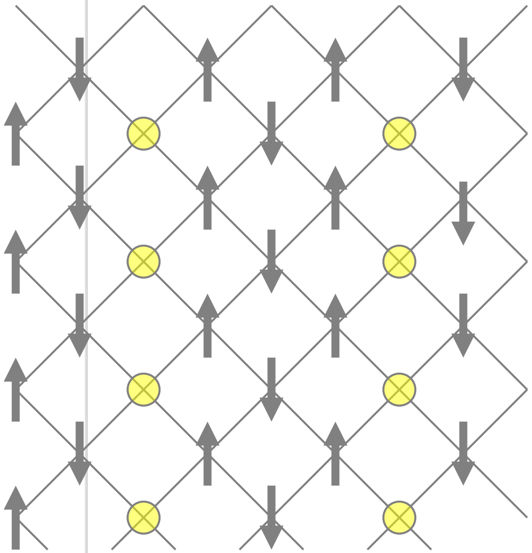


Vertical and Diagonal stripes

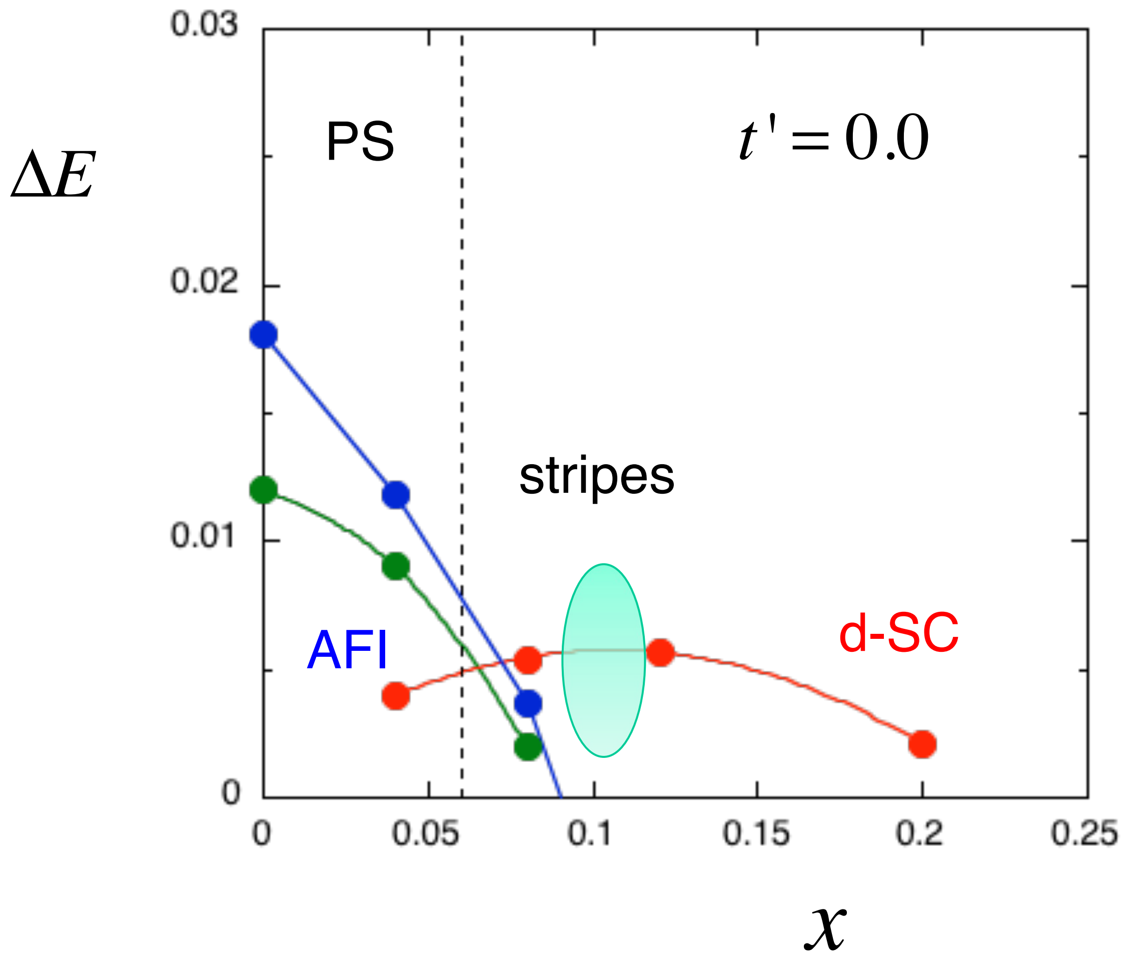
Diagonal striped state is stable for large U.



Diagonal stripes



Stripes in the phase diagram



Blue line $\psi^{(2)}$

Green line $\psi^{(4)}$

Kinetic energy driven SC

Kinetic energy driven superconductivity

Pairing interaction + Kinetic energy effect

→ High temperature superconductivity

Possibility of kinetic-energy driven high-T_c
in the large-U region

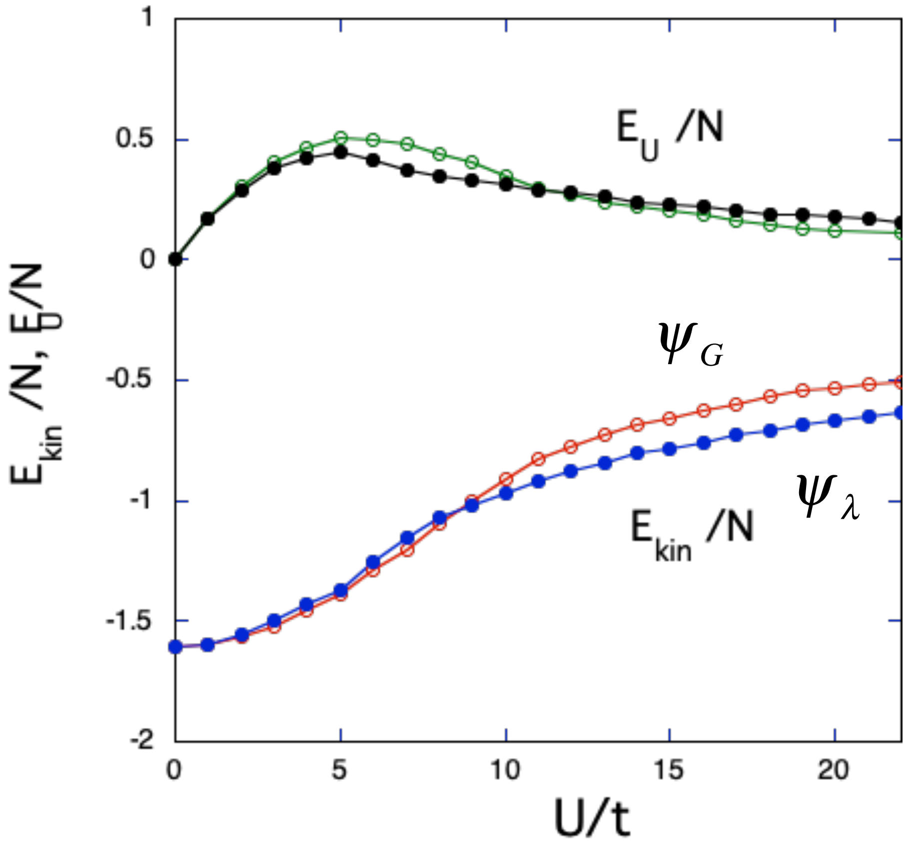
T_c is enhanced by the kinetic-energy effect.

Kinetic energy and U

$$E = E_{kin} + E_U$$

E_{kin} : Kinetic energy

E_U : Potential energy



There is a large kinetic Energy gain in the improved function ψ_λ.

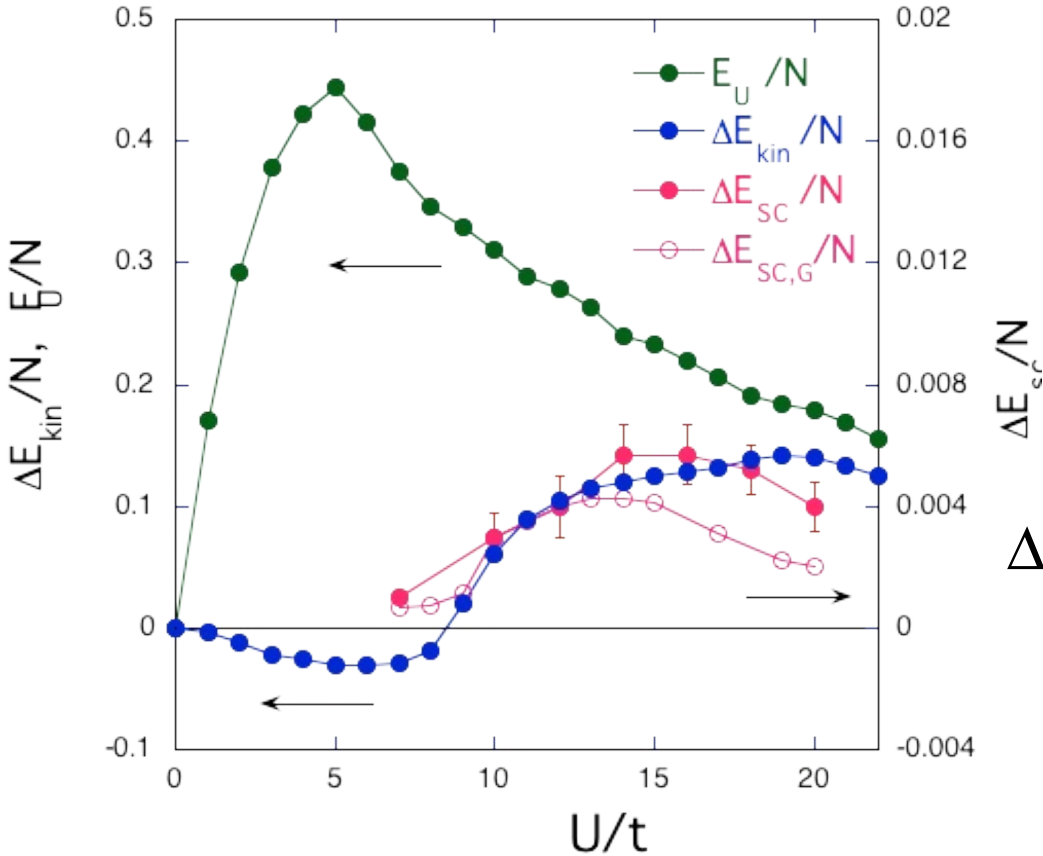
Kinetic energy and Condensation energy

Kinetic energy difference = $\Delta E_{kin} = E_{kin}(\lambda = 0) - E_{kin}(\lambda = \lambda_{opt})$

$$= E_{kin}(\psi_G) - E_{kin}(\psi_\lambda)$$

ΔE_{kin} and ΔE_{SC} show similar behaviors.

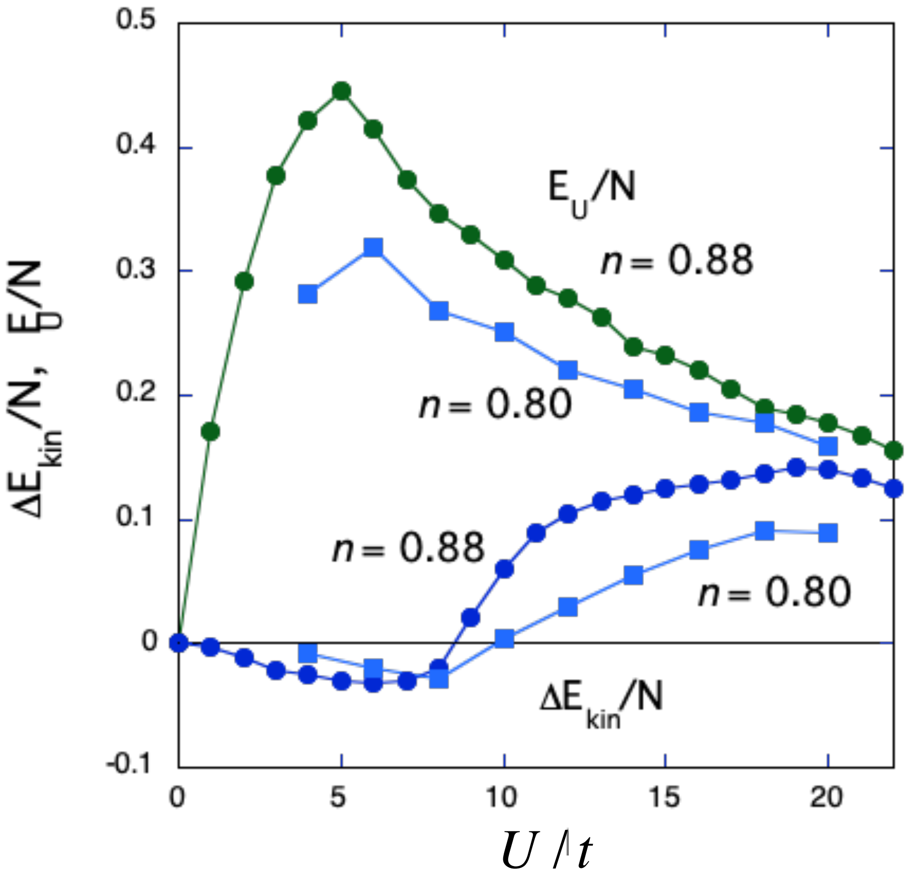
Possibility of kinetic-energy enhancement of superconductivity



$\Delta E_{kin} > 0$

Kinetic energy and doping rate

Doping dependence of kinetic energy effect ΔE_{kin}

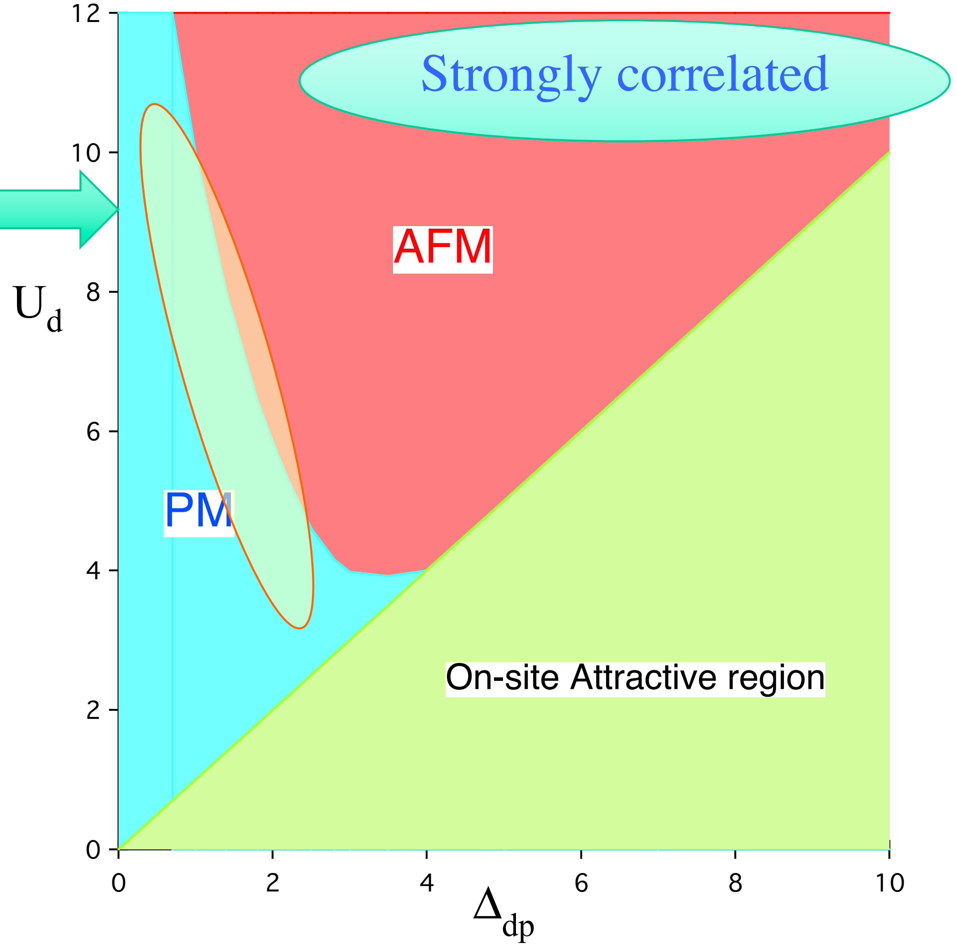


ΔE_{kin} is small in the overdoped region

Ref.
Phys. Lett. A
403, 127382 (2021)

Phase diagram of d-p model

High-T_c region



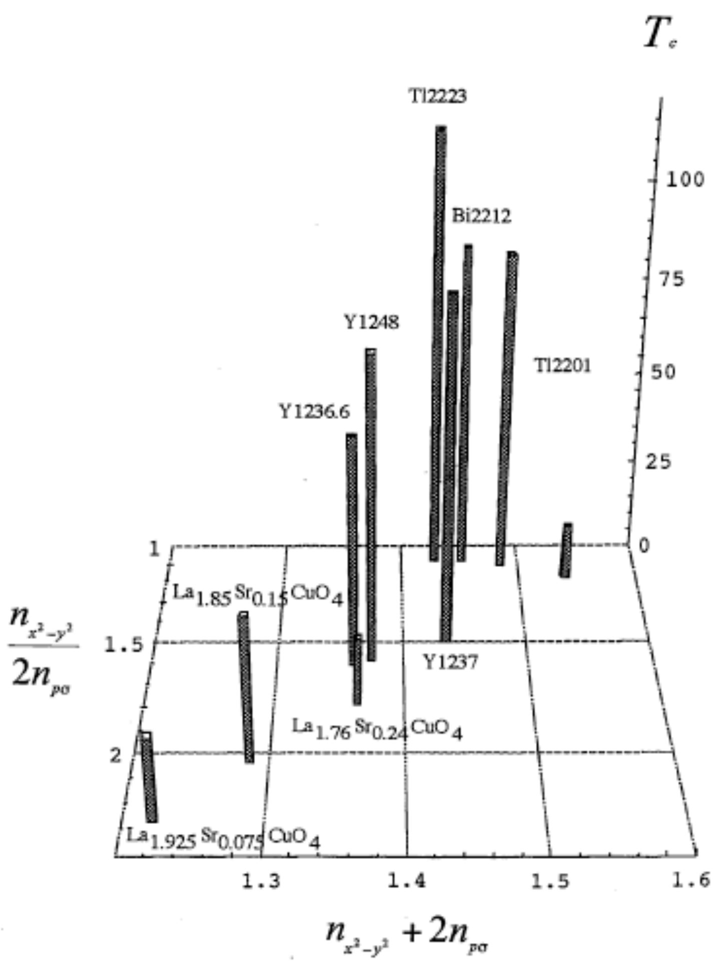
$t_d' = 0$

$x = n_h \simeq 0.18$

Level difference $\varepsilon_p - \varepsilon_d$

Level difference and Tc

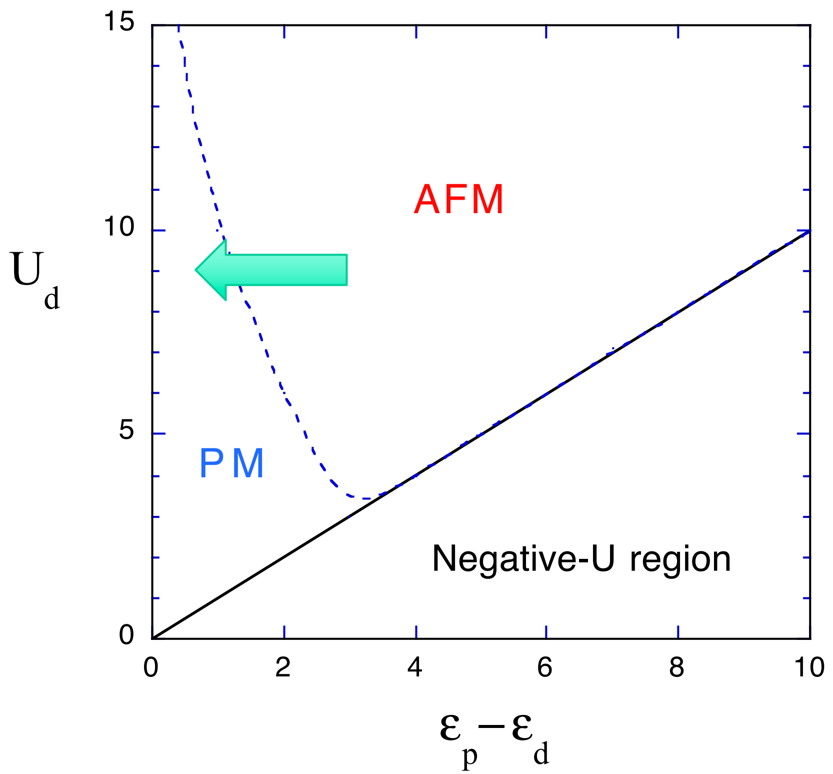
Higher T_c for larger hole density



Zheng et al. JPSJ 64, 2524 (1995)

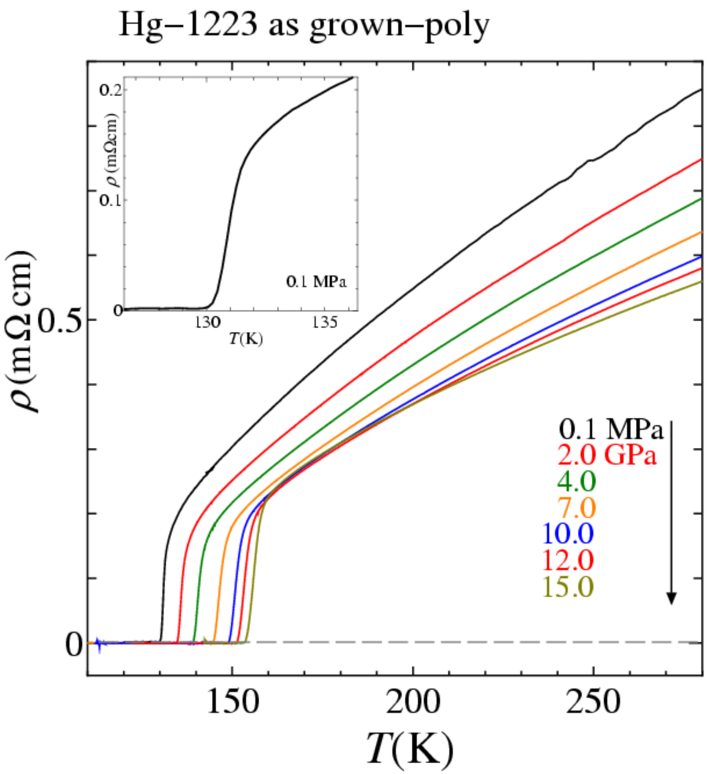
T_c increases as

$\varepsilon_p - \varepsilon_d$ decreases



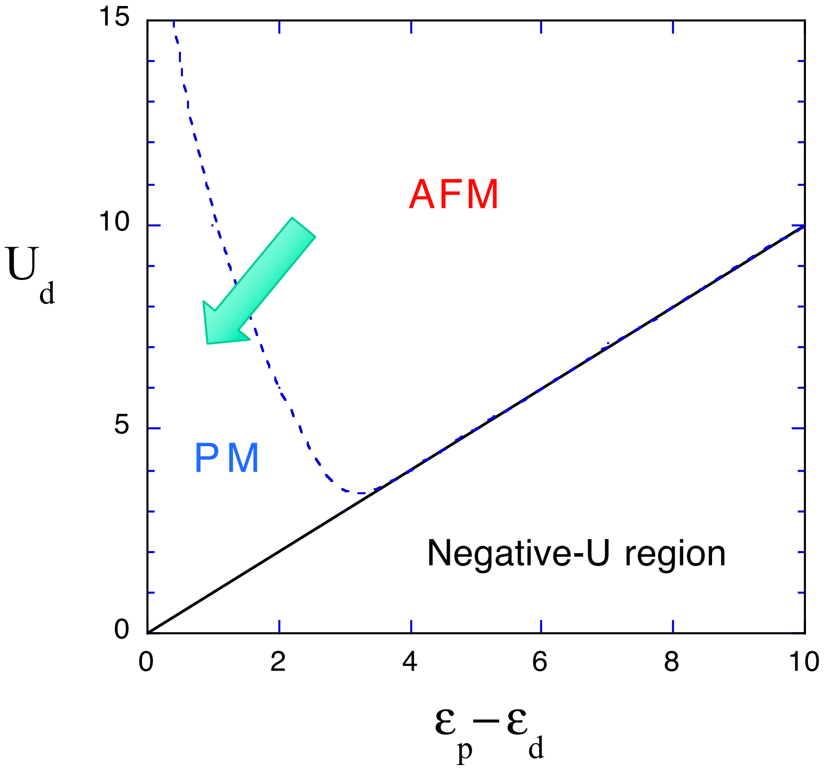
Pressure effect and Tc

Zero Resistivity
T_c = 153 K under pressure
(Takeshita et al. JPSJ)



$HgBa_2Ca_2Cu_3O_{8+\delta}$

Pressure dependence



Summary

Phase diagram of cuprate superconductors

1. There occurs a crossover in a hole-doped system.
2. AF magnetic correlation is controlled by *U* and *t'*.
3. Phase separation exists near half-filling.
4. Stability of striped state
5. Kinetic-energy enhancing of Tc.