Crossover between BCS Superconductor and doped Mott ins.

Possible normal state in the two-dimensional Hubbard model

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Variational Monte Carlo（VMC) study (cf. BCS variational theory)

Yokoyama, et al, J. Phys. Soc. Japan **82**, 014707 (2013)

Crossover between BCS Superconductor and doped Mott ins.

Possible normal state in the two-dimensional Hubbard model

- Mott transition (Brinkman-Rice-like transition)

  t-t′-U Hubbard model at half-filling

  First order phase transition: doublon-holon bound state (RVB-Insulator)

- Superconductivity in the doped case

Weak coupling U<W	BCS-like
Strong coupling U>W	*t-J* like = doped Mott insulator

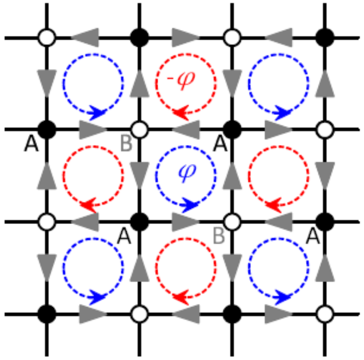
Relation between Hubbard model and t-J model

- Staggered flux state as a possible normal state

  Energy: d-wave < SF < projected FS

  Properties: gap in spin sector, Fermi arc…

(a)



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Hubbard model

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow} \qquad (U \geq 0)$$

A typical model for strongly correlated electron systems

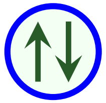
In Hubbard model, we expect a metal-insulator transition at a critical value of *U*c when n=1.

Insulator in large *U / t* –region (*t-J* like)
Metal in small *U / t* -region

Mott transition as a first-order phase transition (similar to gas-liquid)

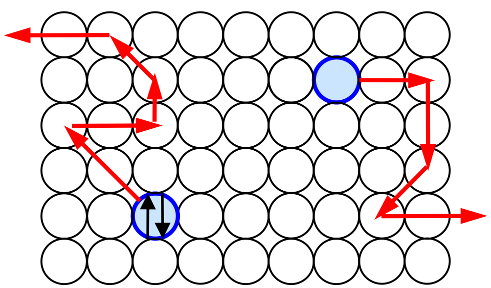
Variational wave function at T=0

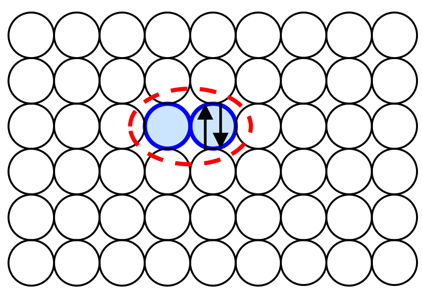
$$\Psi_{\rm SC} = \mathcal{P}_Q \mathcal{P}_{\rm G} \big| {\rm BCS}(\Delta) \rangle$$

P_G : projection operator controlling doublon number 

P_Q : projection operator controlling
the correlation between doublons and holons is **Essential**

free doublon & holon ↔ **bound state**





Mott Transition

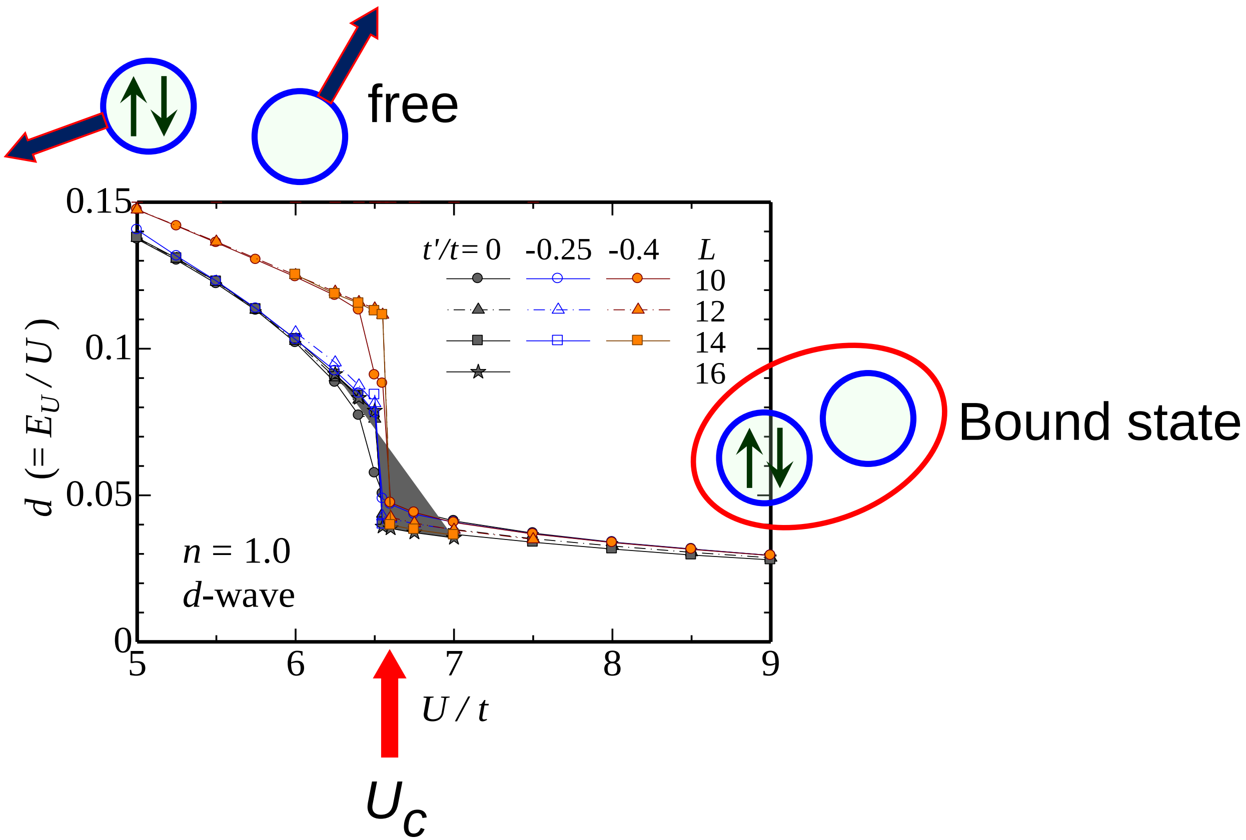
conductive

insulating

Mott transition as a first-order transition

- Density of doublons

“order parameter” in Mott trantision
(similar to gas-liquid transition)

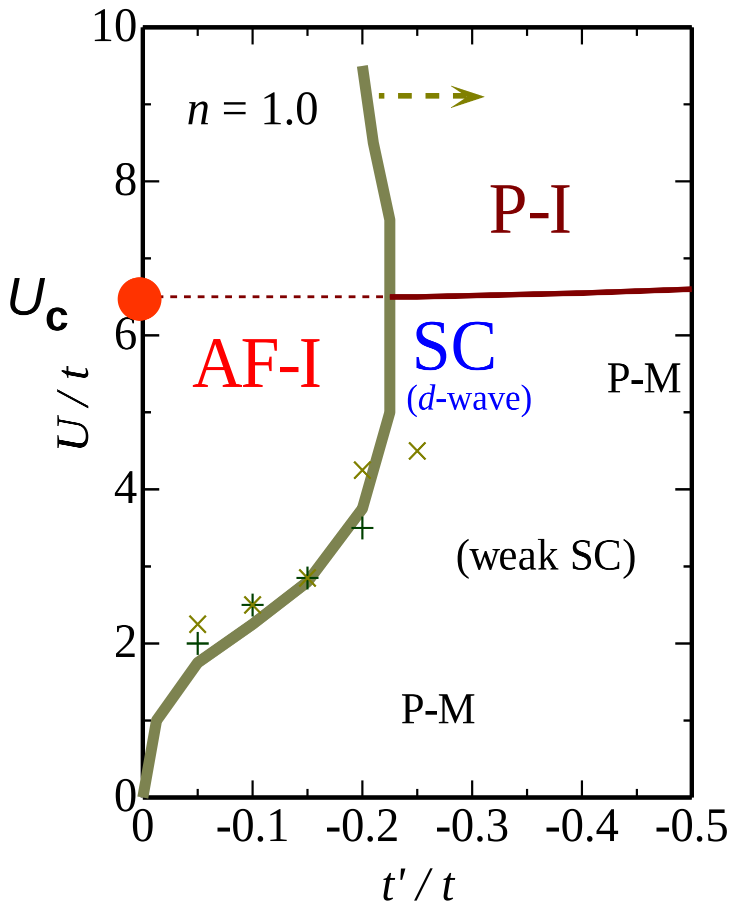


Phase diagram

half filling (δ=0)

T=0 Variational Theory

t-t′-U **Hubbard model**



Yokoyama, Ogata et al, J. Phys. Soc. Japan **75**, 114706 (2006)
J. Phys. Soc. Japan **82**, 014707 (2013)

Phase diagram

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T=0 Variational Theory

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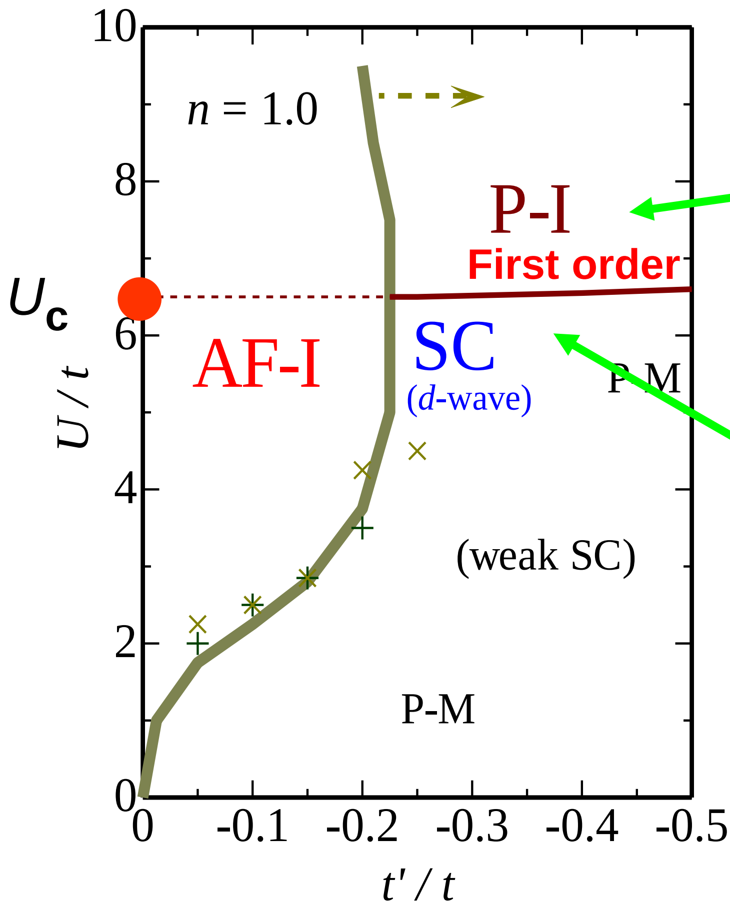

doublon-holon bound states
= RVB insulator
= Mott insulator

$$\Psi_{\rm SC} = \mathcal{P}_Q \mathcal{P}_{\rm G} \left| {\rm BCS}(\Delta) \right\rangle$$

(=RVB state)

free doublons and holons

Yokoyama, Ogata et al, J. Phys. Soc. Japan **75**, 114706 (2006)
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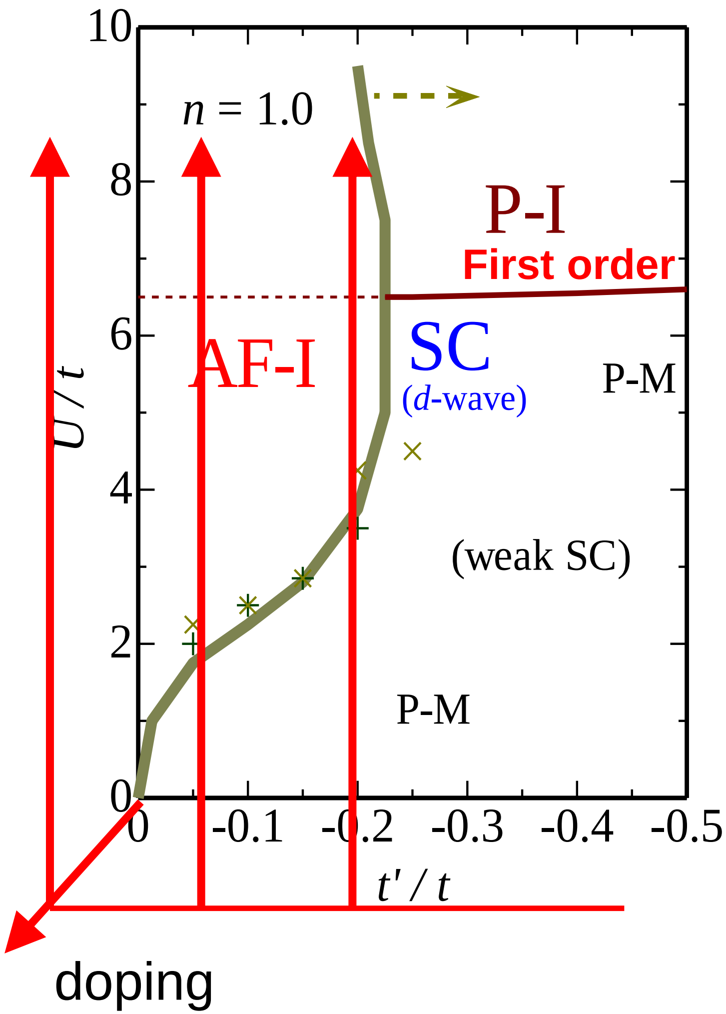
Phase diagram

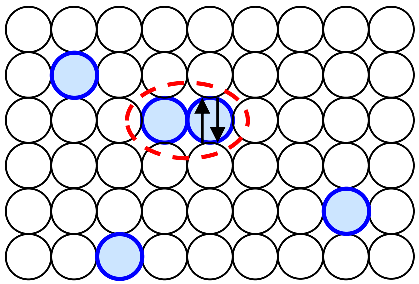
half filling (δ=0)

T=0 Variational Theory

***t-t′-U* Hubbard model**



High-Tc will appear when holes are doped in such a Mott insulator.



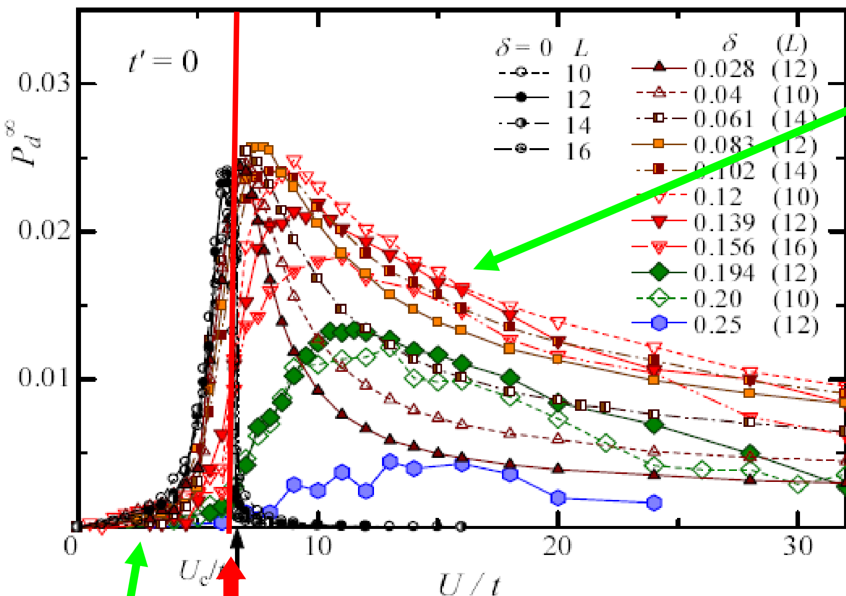
We need phase diagram at n<1

Yokoyama, et al, J. Phys. Soc. Japan **82**, 014707 (2013)

Finite doping（n < 1）

Crossover (not phase transition), but physical picture is different !

Correlation function for d-wave superconductivity

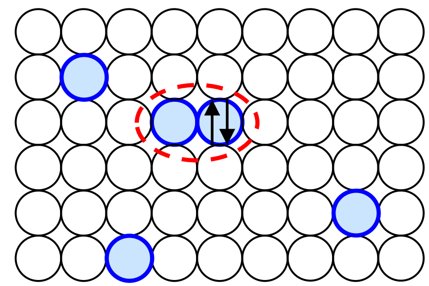


$U_{\text{crossover}}$

- Small U ($U < U_{\mathbf{co}}$)
  weak correlation:
  weak superconductivity

- Large U ($U > U_{\mathbf{co}}$)

bound state + free holons



“Doped Mott insulator”

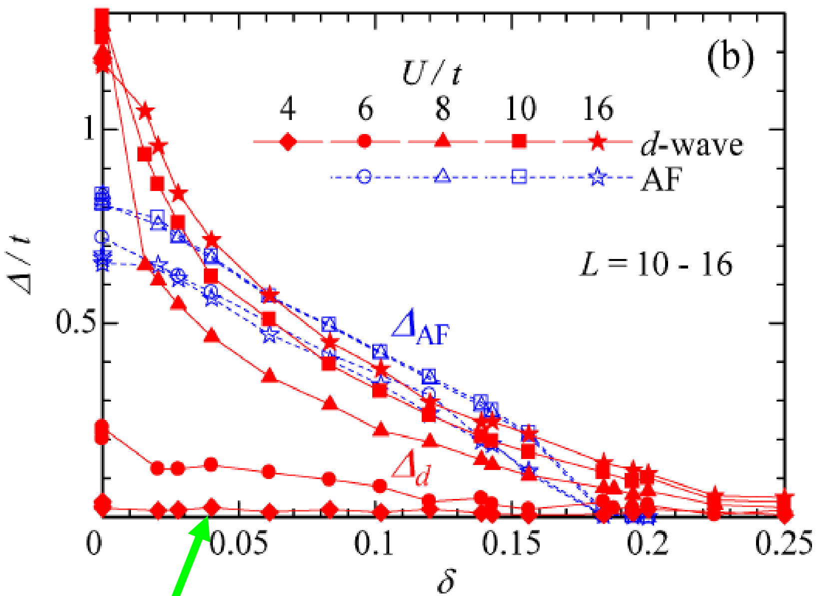
＝ High-Tc

doublon-holon bound state
= n.n. doublon-holon
= virtual process inducing J-term

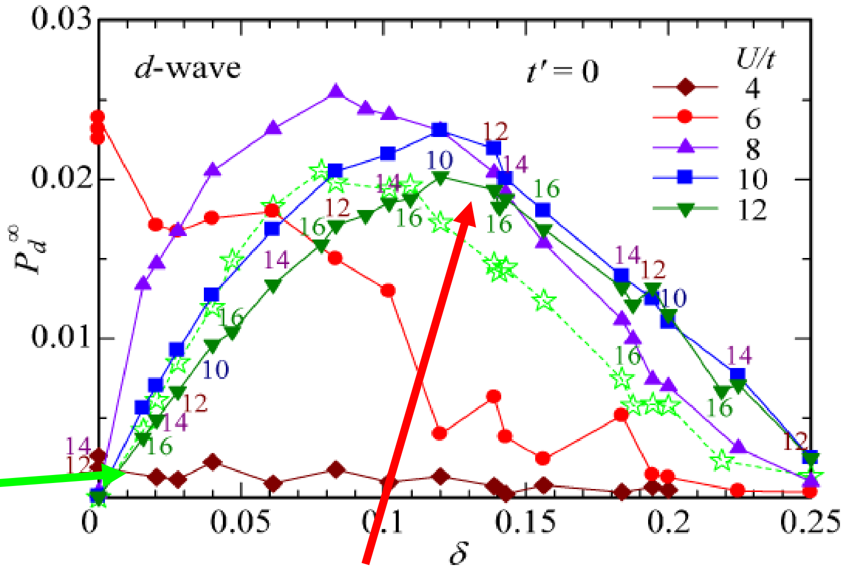
⇨ t-J region

Doping dependence

Variation parameter Δ ----- excitation gap near (π,0) & singlet formation



Superconducting correlation function



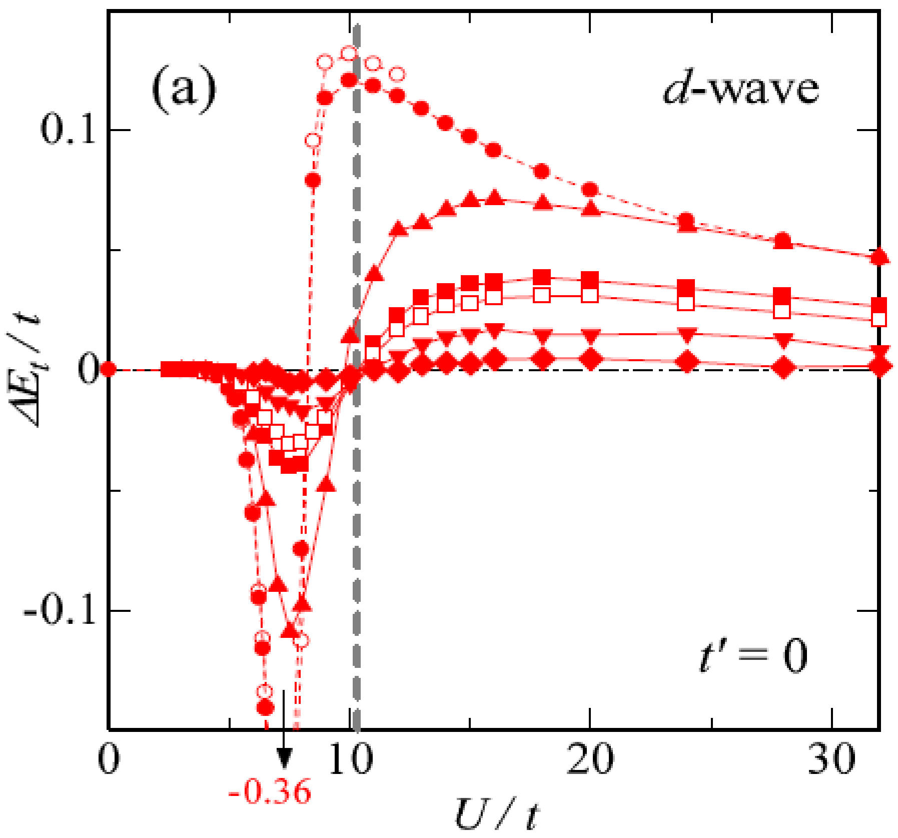
- Small U ($U < U_{co}$)
weak correlation:
weak superconductivity

- Large U ($U > U_{co}$) doped Mott

$$\Delta_{SC} = \frac{2\delta}{1+\delta}\Delta$$

T_c

Kinetic energy gain !



Kinetic energy gain in the Large *U* region (*t*-*J* region)

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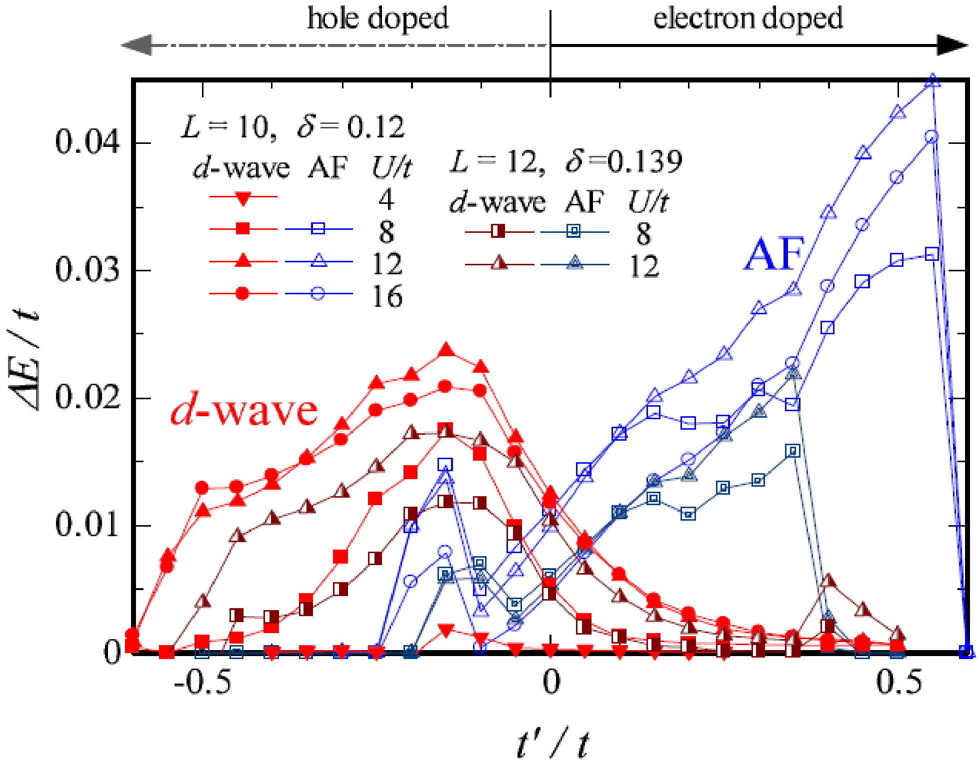
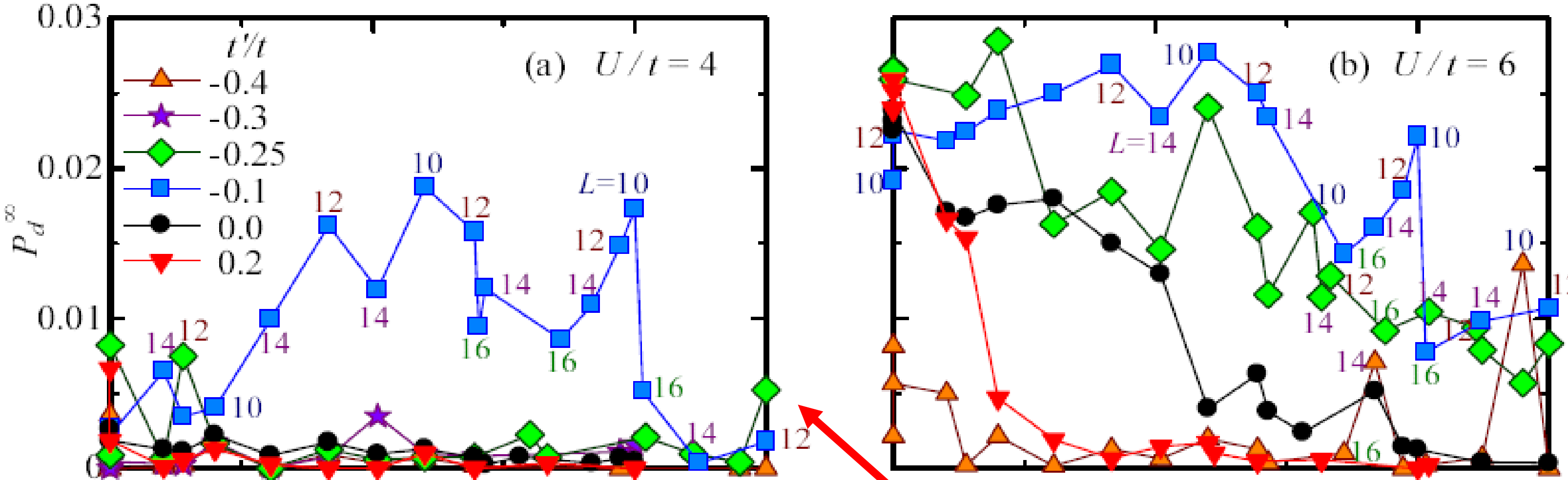
t ′ -dependence

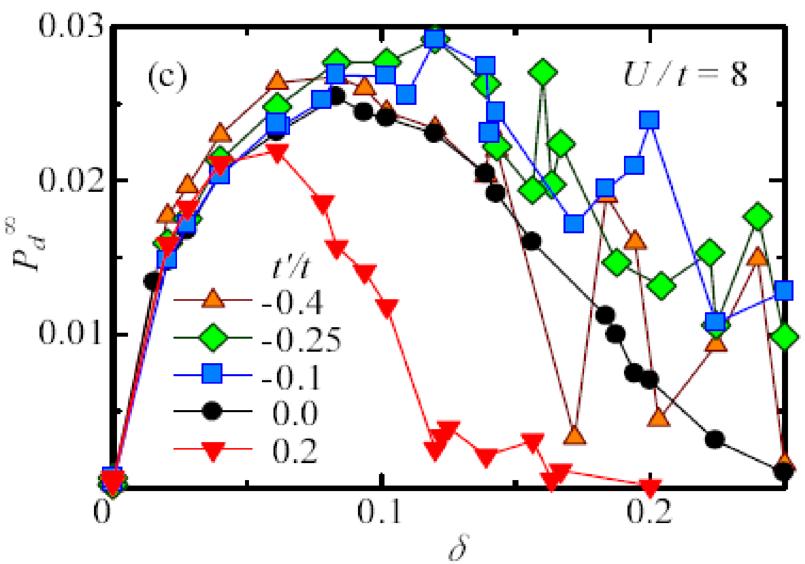


t-t′-U **Hubbard model**

Doping-dependence of d-wave correlation function

T_c





- Small U ($U < U_{co}$)
  weak correlation:
  weak superconductivity

$t' = -0.1$

Special case where van Hove singulari
is located at the Fermi energy.

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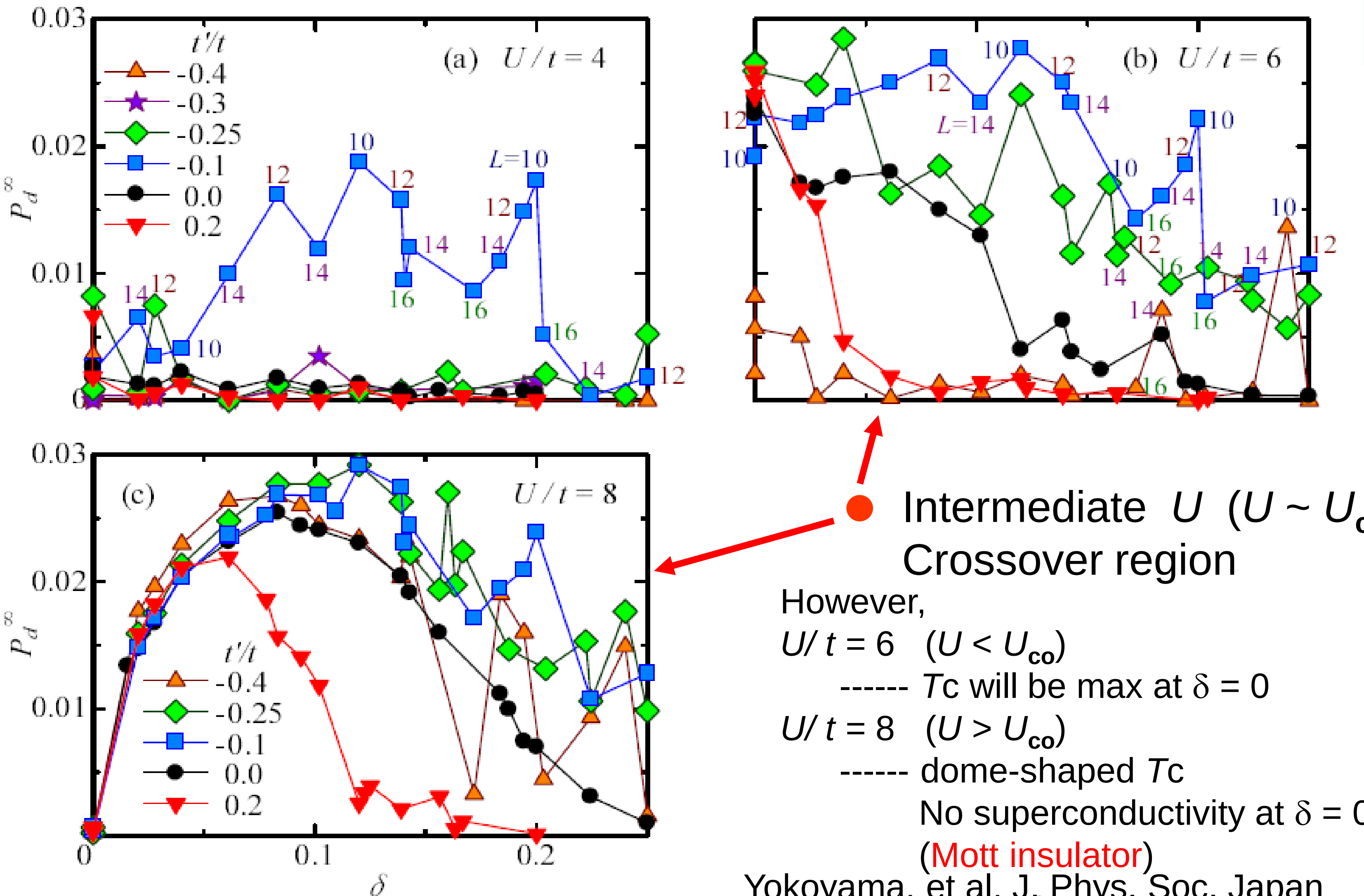
Doping-dependence of d-wave correlation function

T_c



- Intermediate U ($U \sim U_{co}$)
  Crossover region

However,

$U/t = 6$ ($U < U_{co}$)

------ Tc will be max at $\delta = 0$

$U/t = 8$ ($U > U_{co}$)

------ dome-shaped Tc

No superconductivity at $\delta = 0$

(Mott insulator)

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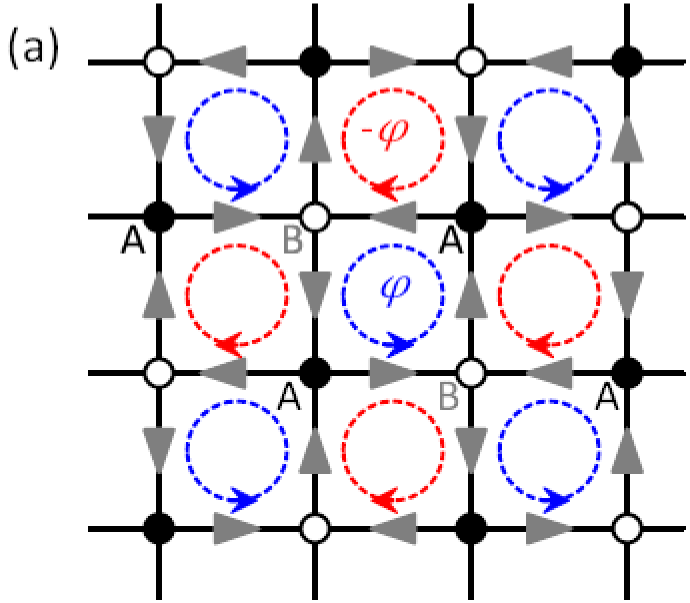
Staggered Flux state（possible anomalous metallic state）

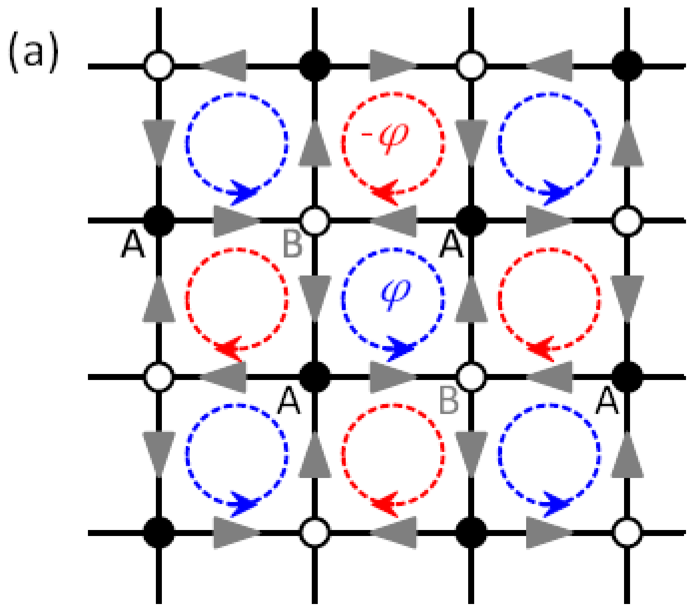


This is not the lowest variational state.
But lower than the projected FS.

A candidate of
"Symmetry-broken" normal state

$$\Phi_{SF}$$

Staggered Flux state (possible anomalous metallic state)



For the t-J model, flux state was discussed.
(mainly for the condensation energy)

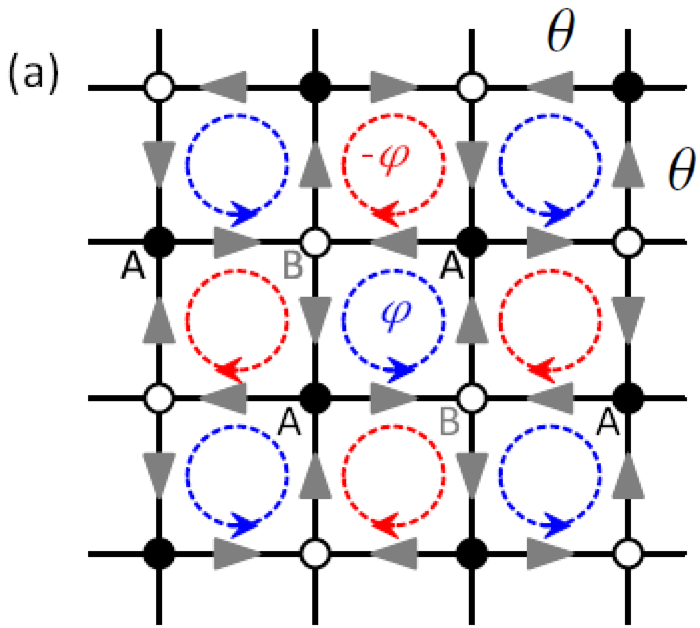
Ivanov and Lee: PRB **68** (2003) 132501.

For the Hubbard model, flux state was not stabilized.
Also what is the property of this state?

$$\mathcal{P}_Q \mathcal{P}_G \ \Phi_{SF}$$

⇨ We find that another Projection operator which introduces "configuration-dependent phase factor" is important.

Staggered Flux state (possible anomalous metallic state)



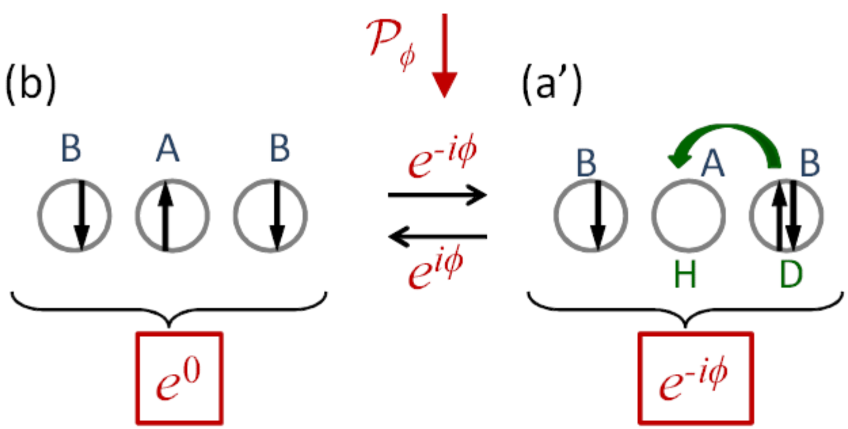
$$\mathcal{P}_Q \mathcal{P}_\mathrm{G} \ \Phi_\mathrm{SF}$$

This state is not stabilized
In the Hubbard model.

$$\boxed{\mathcal{P}_\phi(\phi)} \mathcal{P}_Q \mathcal{P}_\mathrm{G} \ \Phi_\mathrm{SF}$$

----- stabilized !

$$\mathcal{P}_\phi = \exp\left[i\phi \sum_{\lambda=1}^{2} (-1)^{\lambda+1} \sum_j d_{\lambda,j} \times \left(h_{\lambda,j+\mathbf{x}} + h_{\lambda,j-\mathbf{x}} - h_{\lambda,j+\mathbf{y}} - h_{\lambda,j-\mathbf{y}} \right) \right],$$

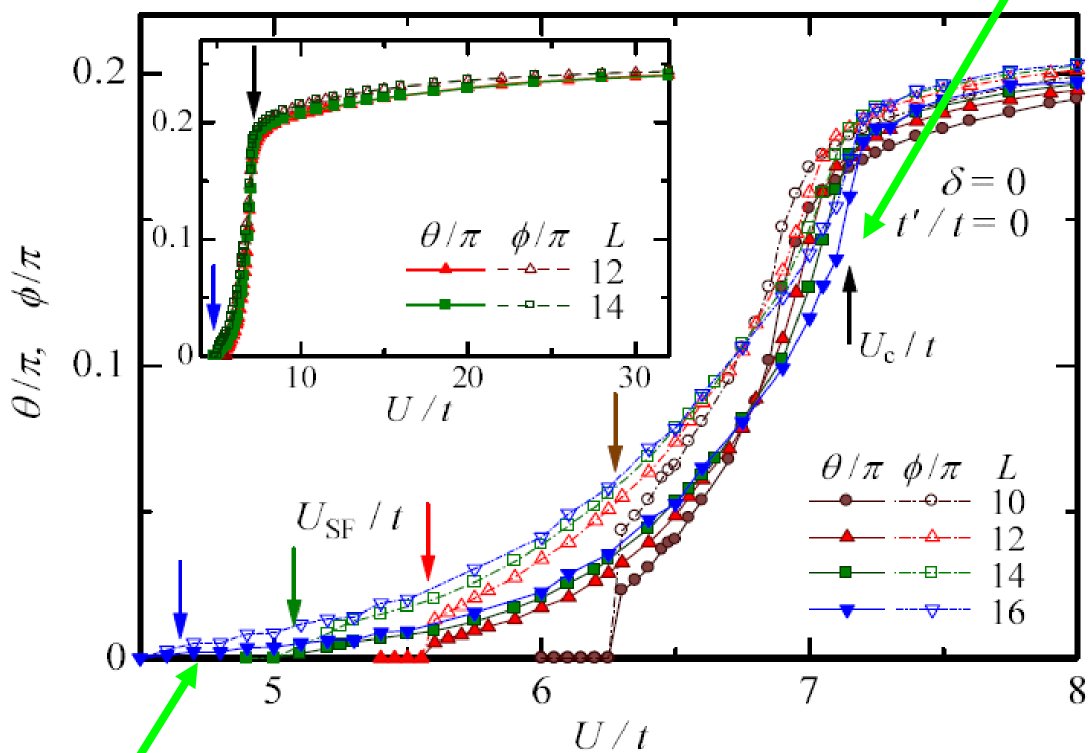


This phase factor appears
in the D-H creation processes.

1. Half-filling ($t'/t = 0$)

Staggered Flux

Mott transition



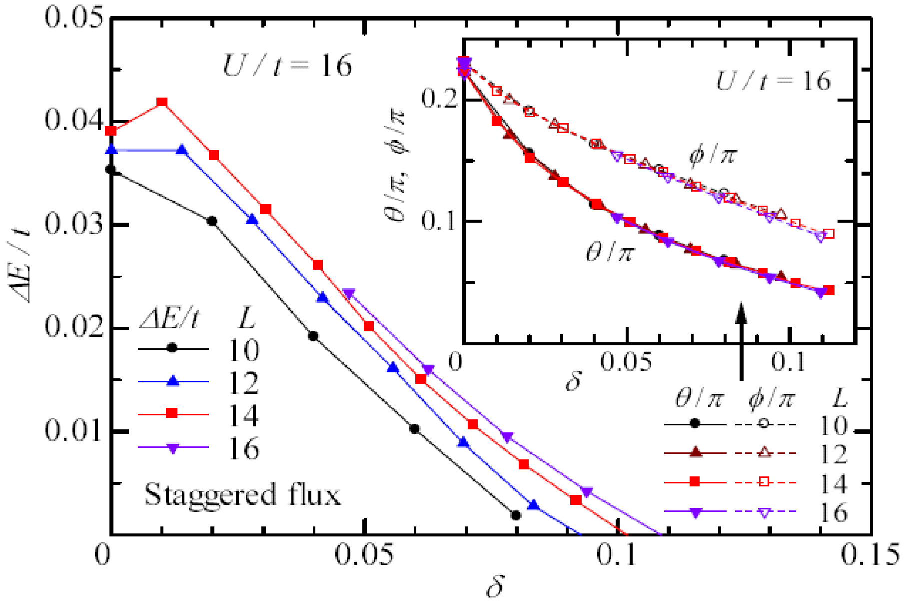
θ is nearly equal to ϕ but staggered current flows.

Phase transition from projected FS → staggered flux (SF)

2. Doping case ($t'/t = 0$)

Staggered Flux

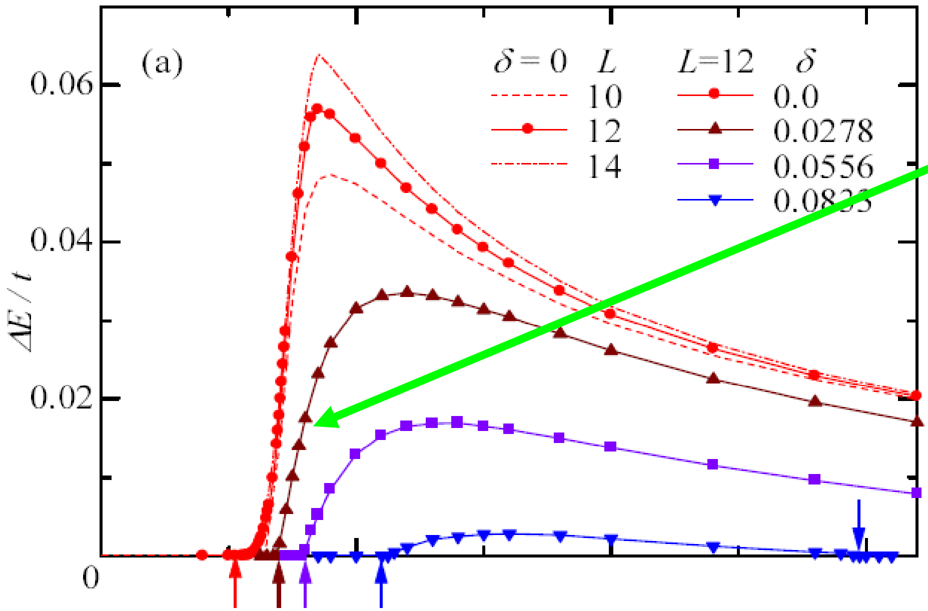
Phase diagram: SF state is a candidate for under-doped region.



ϕ is larger than θ

2. Doping case (*t'*/ *t* = 0)

Staggered Flux



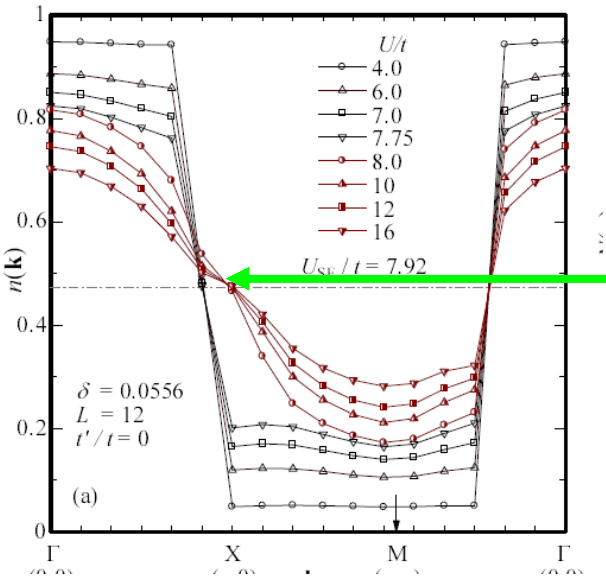
There is a sharp crossover near the Mott transition at δ=0

Very close to d-wave SC.

But the variational enegies are d-wave SC < SF < projected FS

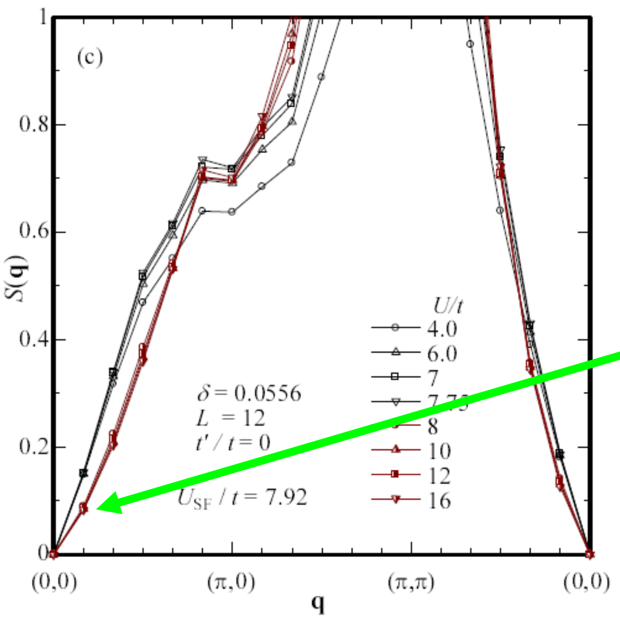
2. Doping case ($t'/\ t = 0$)

Staggered Flux



Momentum distribution function:
close to d-wave SC (Fermi arc-like)

No Fermi surface near $(0,\pi)$

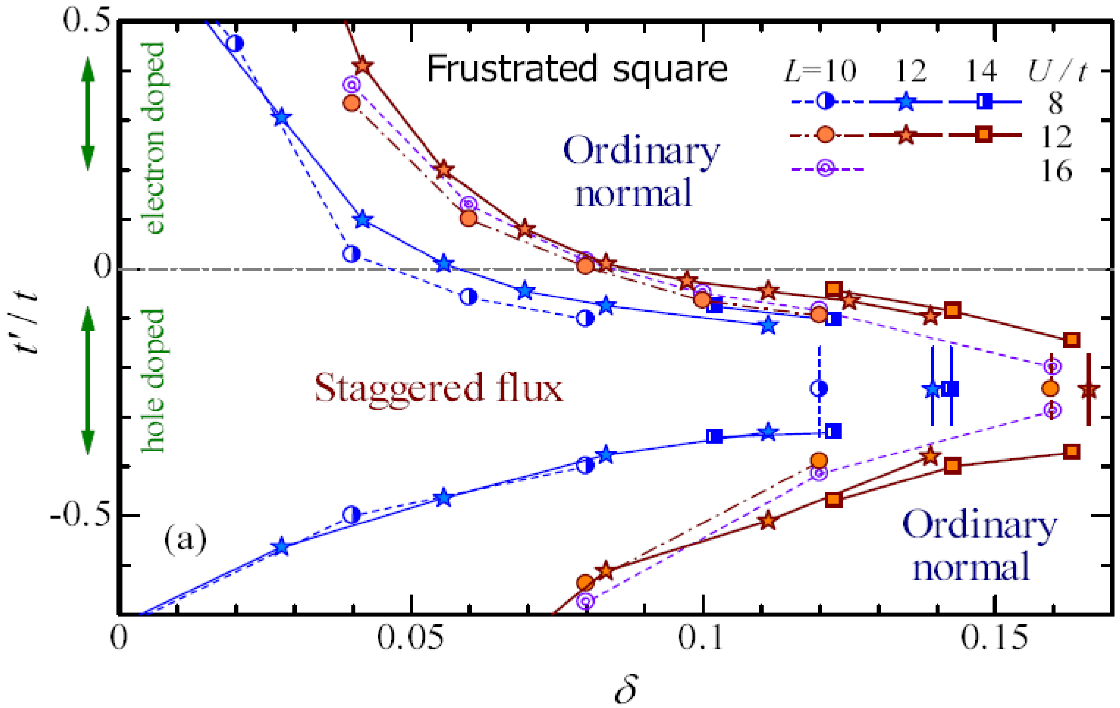


Spin correlation function: S(q)
q^2 near q=0 in the SF state.

Gap-like behavior in the spin sector !
~ pseudo-gap

3. Doping case (finite *t'/ t*)

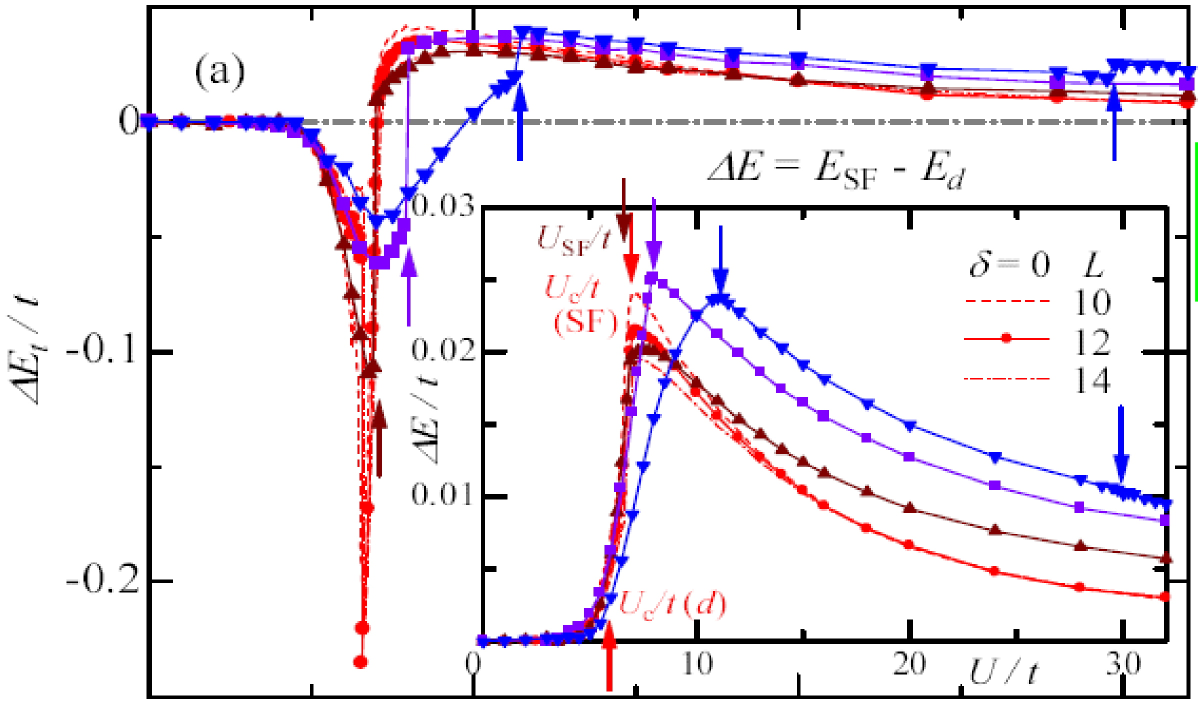
Staggered Flux



SF state is favorable for *t'/ t* < 0 (hole-doped case)

4. Kinetic energy gain

Staggered Flux



Kinetic energy gain in the Large *U* region (*t*-*J* region)

Kinetic energy
d-wave SC < SF < projected FS

Conclusions

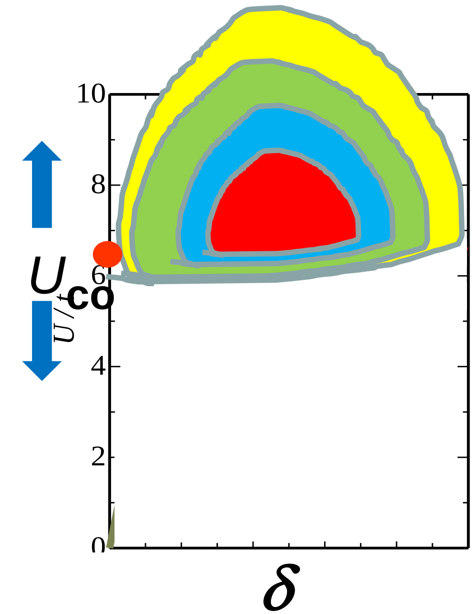
Yokoyama, Ogata et al, J. Phys. Soc. Japan **75**, 114706 (2006)
J. Phys. Soc. Japan **82**, 014707 (2013)

- Modified variational state   doublon-holon bound state is important

  - small *U* (BCS-like) (weak-coupling region)
  - large *U* (non-BCS) (*t-J* region)

  "Doped Mott insulator"

  doublon-holon bound state + free holons



- Flux state as a possible anomalous metallic state

  Energy: d-wave SC < SF < projected FS

  Gap-like behavior in the spin sector !
  ~ pseudo-gap

  Fermi arc
  Kinetic energy gain

  Staggered flux state is a typical sym. breaking state in strongly correlated region.