Ground states of t-t′-J Model

for High-Tc superconductivity

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- Mott transition (Brinkman-Rice transition)

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

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

- Doped case

  Relation between Hubbard model and t-J model is clarified.

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

- ***t-J*** -like region

  Coexistence of AF and SC

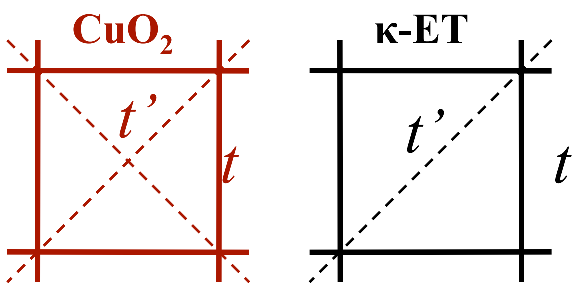
  Effects of t′: hole doped vs electron doped

  ($t' < 0$) ($t' > 0$)

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

t - t′ - J Model for high-Tc superconductivity

$$\mathcal{H} = -\sum_{(i,j)\sigma} P_{\mathrm{G}}\left(t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{h.c.}\right) P_{\mathrm{G}} + J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$



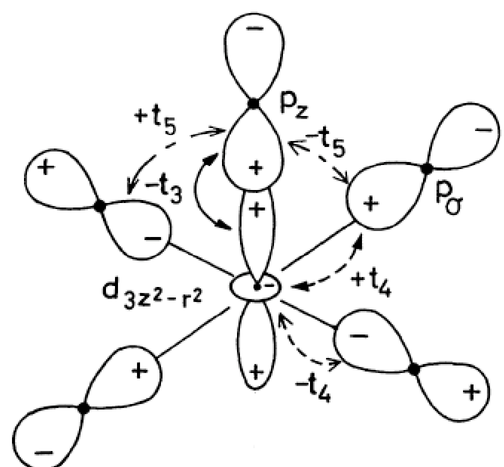
cf. **Spin-Liquid** state κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$

- Origin of next-nearest hopping, ***t′*** term

$t' < 0$ for hole-doped cuprates

$|t'|$ --- larger in BSCCO
smaller in LSCO

determining Tc



apical oxygens affect

Matsukawa-Fukuyama (1989, 1990)

Mott transition at half-filling

- "**Doped Mott insulator**" ----- What is Mott insulator?

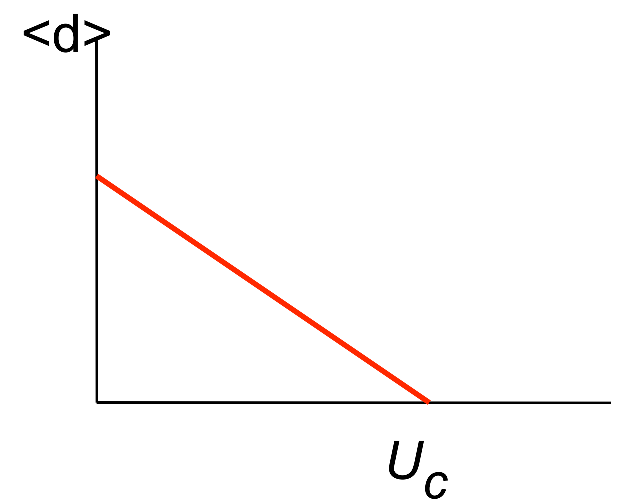
  t-J model → Heisenberg model ($\delta \to 0$)
  We need to study Hubbard model.

- Brinkman-Rice transition

  doublon number → 0 at U_c (second-order phase transition)

However this Brinkman-Rice transition
is not observed in VMC !

Yokoyama-Shiba, JPSJ (1987)



Mott transition at half-filling

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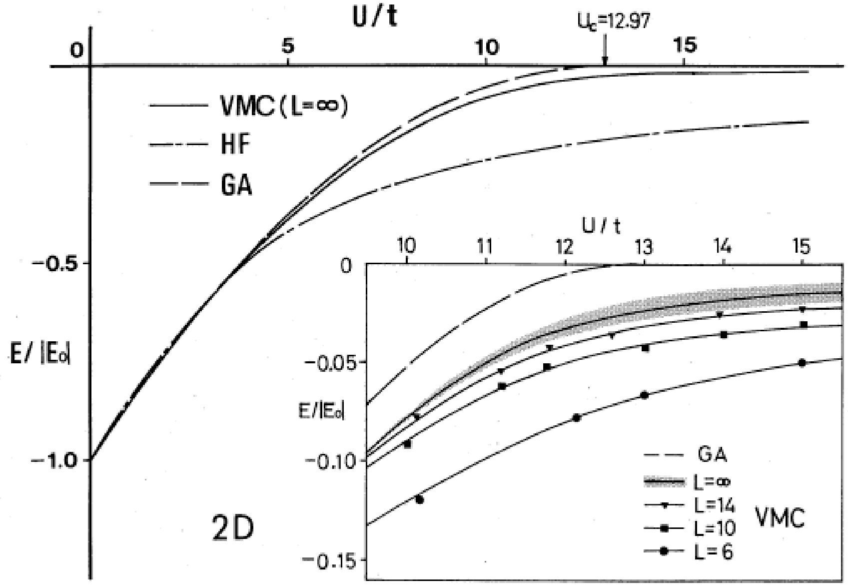

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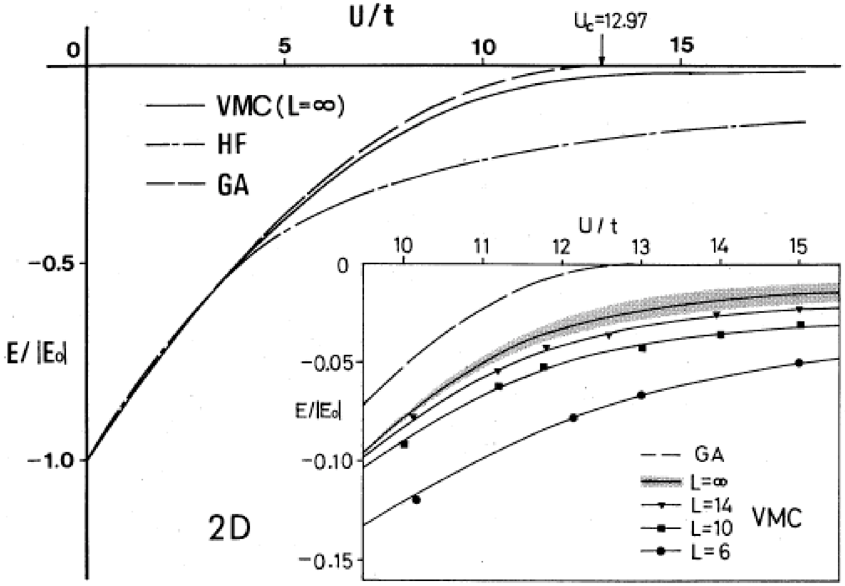


Yokoyama-Shiba, JPSJ (1987)

There is no phase transition.

We modify variational states.

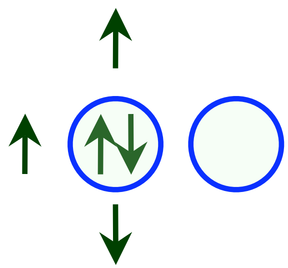
Mott transition as a first-order (a liquid-gas phase transition)

Variational wavefunction

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

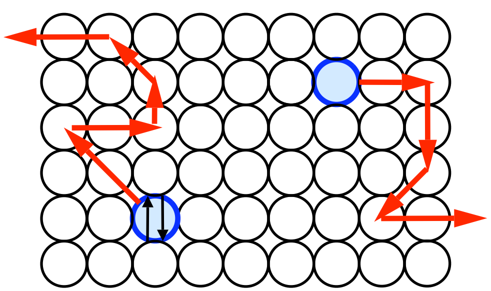
P_G determines the number of doublons

P_Q : ~~Nearest-neighbor doublon – holon correlation~~

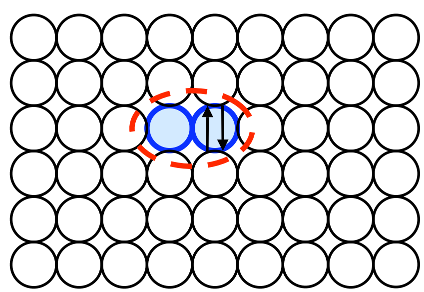


Doublon-holon bound states are favored in wave functions

free doublon & holon ⟷ bound state



conductive



insulating

Mott Transition

Correlation factors

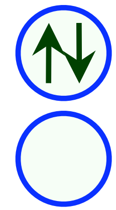
$$\mathcal{P}_G = \prod_i [1-(1-g)n_{i\uparrow}n_{i\downarrow}]$$ ← Usual Gutzwiller factor

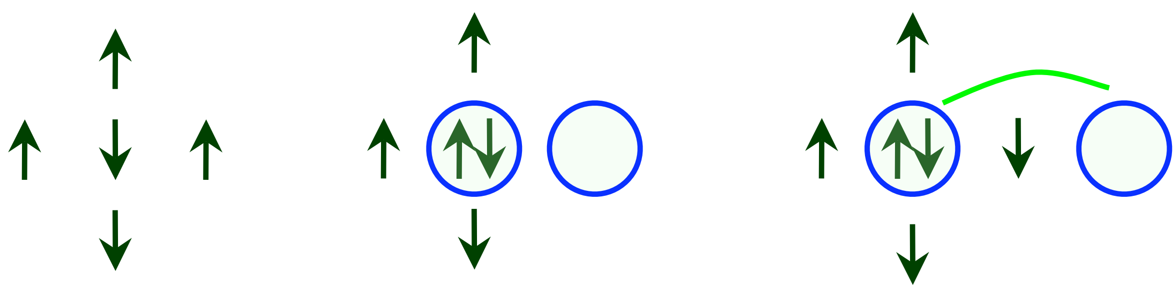
$$\mathcal{P}_Q = \prod_i (1-\mu Q_i^\tau)$$ ← nearest-neighbor doublon-holon correlation

$$Q_i^\tau = \prod_\tau [d_i(1-e_{i+\tau}) + e_i(1-d_{i+\tau})]$$

$d_j = n_{j\uparrow} n_{j\downarrow}$ doublon

$e_j = (1-n_{j\uparrow})(1-n_{j\downarrow})$ holon





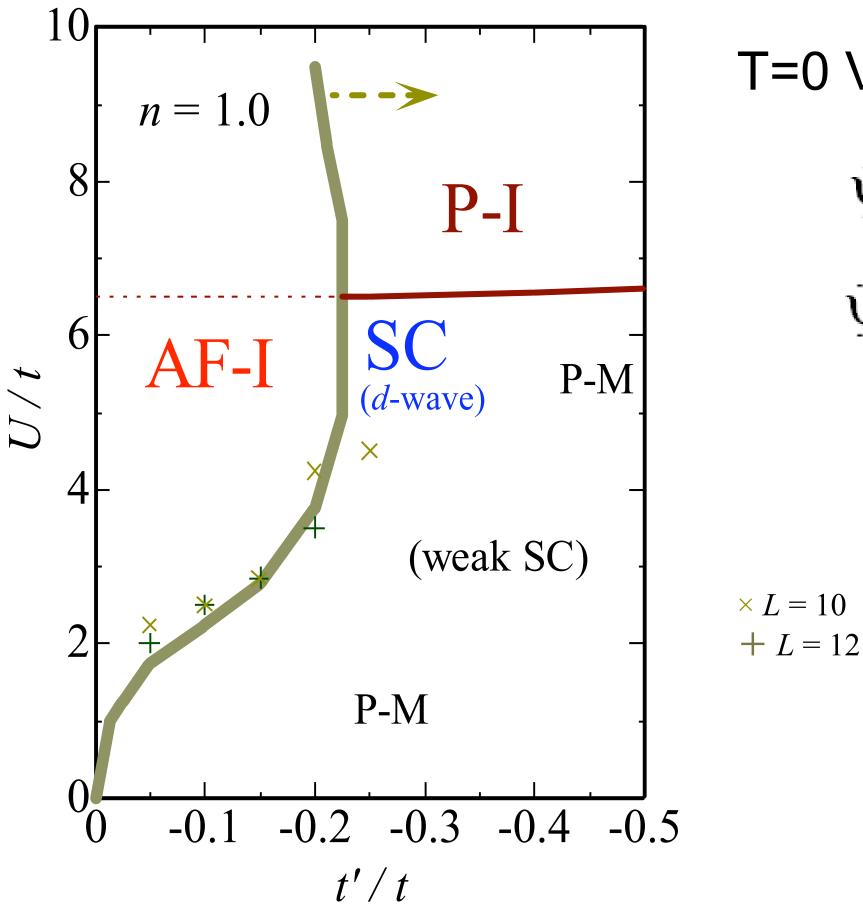
Factor: 1 | g (g<1: reduced) | g(1-μ) (reduced further)

⇨ Doublon-holon bound states are favored in wave functions (g, μ, Δ are variational parameters)

Obtained Phase diagram

half filling (δ=0)

t-t′-U Hubbard model



T=0 Variational Theory

$$\Psi_{SC} = \mathcal{P}_Q \mathcal{P}_G |\mathrm{BCS}(\Delta)\rangle$$

$$\Psi_{AF} = \mathcal{P}_Q \mathcal{P}_G |\mathrm{AF}(m)\rangle$$

Δ is finite !

Qualitatively same as Imada's group

Yokoyama, Ogata, Tanaka, J. Phys. Soc. Japan **75**, 114706 (2006)

Obtained Phase diagram

half filling (δ=0)

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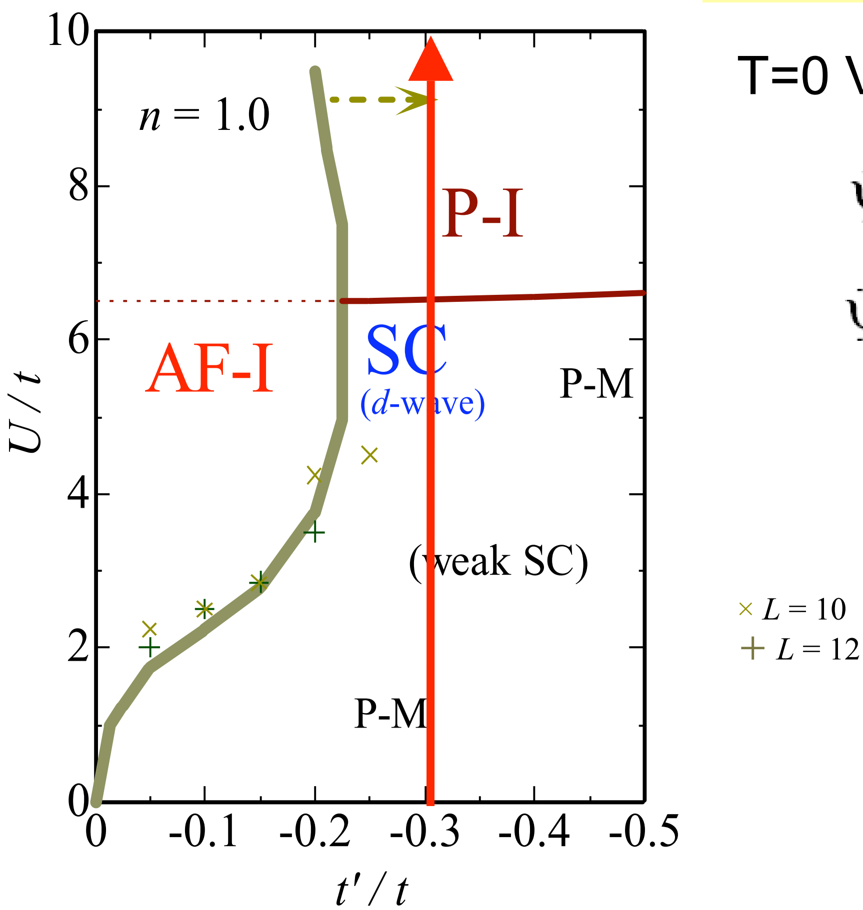

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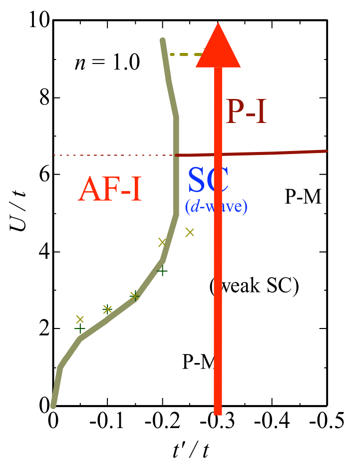
First-order Mott transition

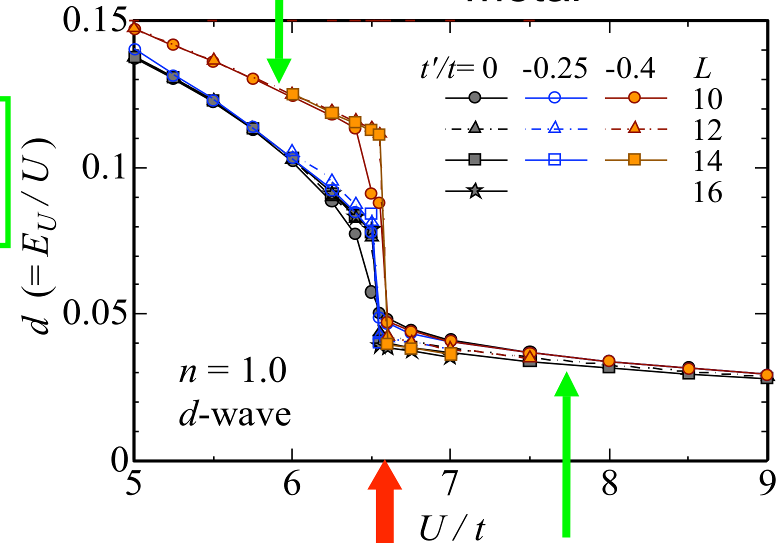
half filling (δ=0)

- Doublon density

order parameter of Mott transition
(similar to gas-liquid transition)

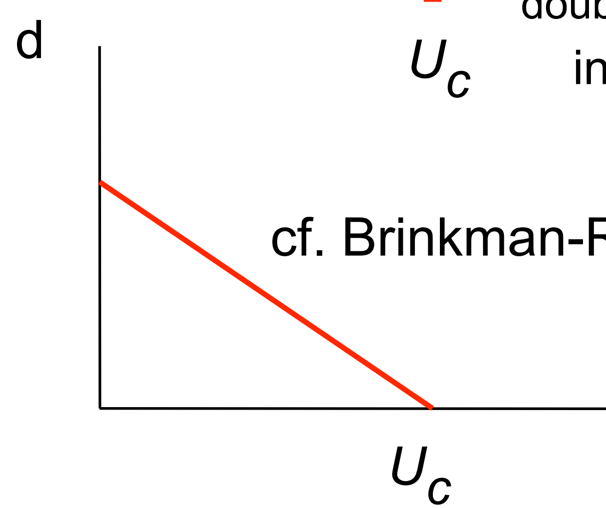


free doublons and holons
metal



U_c

doublon-holon bound state
insulator



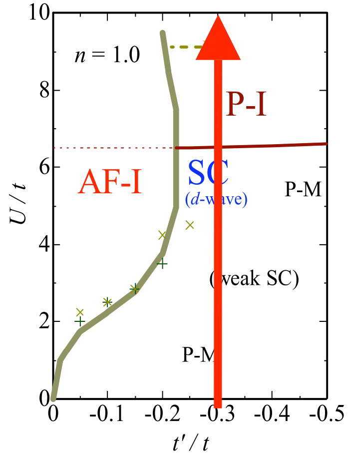
cf. Brinkman-Rice

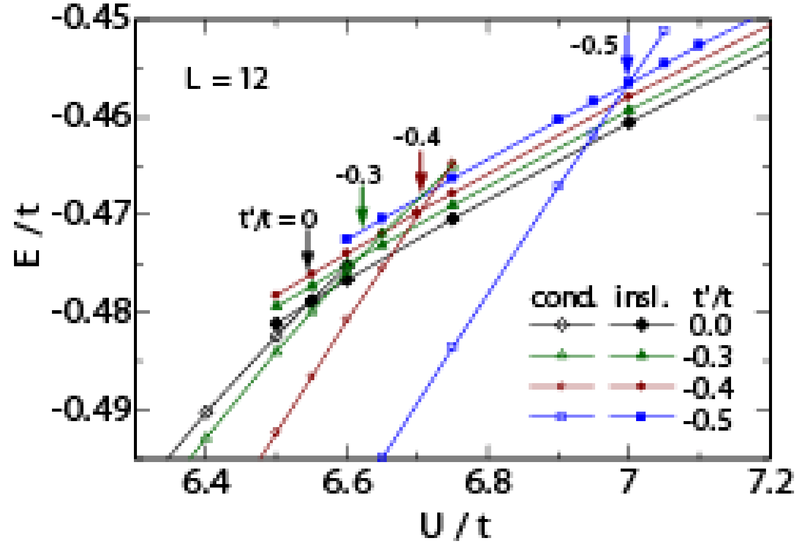
First-order Mott transition

half filling (δ=0)

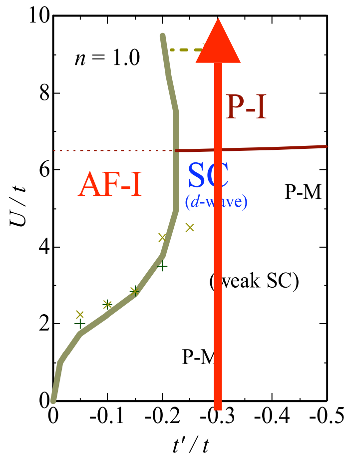
- Energy crossing

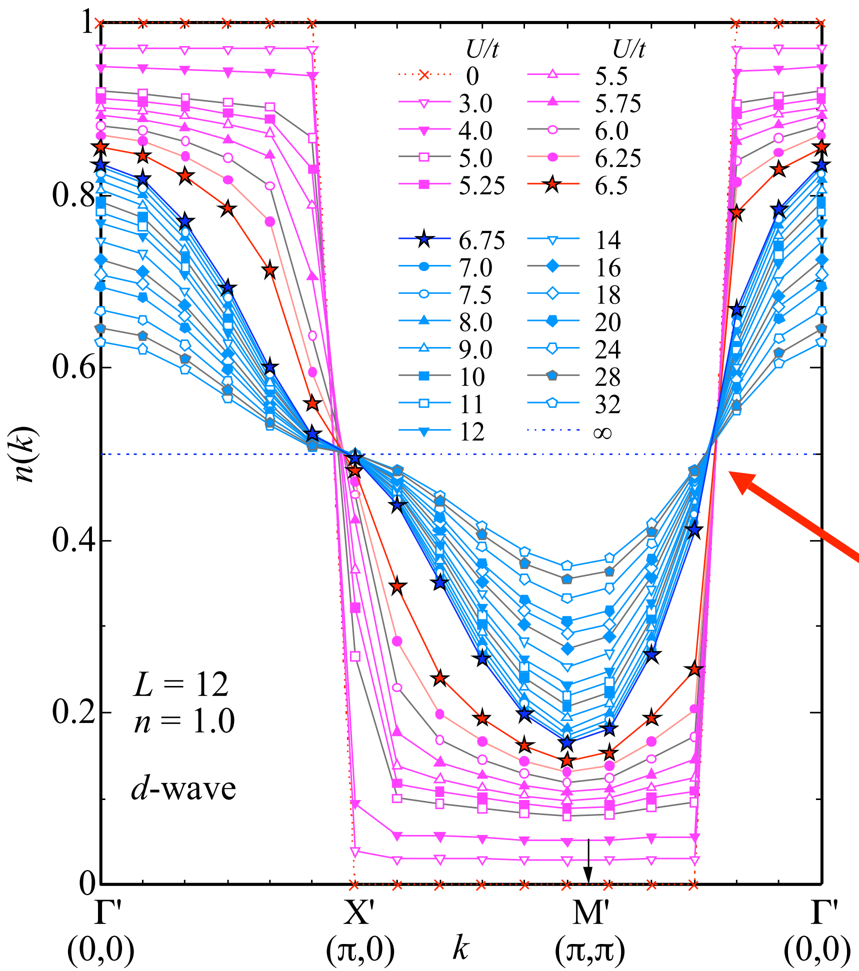
First-order Mott transition
(similar to gas-liquid transition)





Momentum distribution function





metal

insulator

nodal point
(π / 2, π / 2)

$U < U_c$: Fermi surface (metallic)

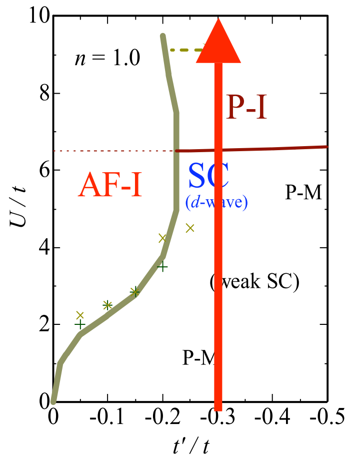
$U > U_c$: no Fermi surface (insulator)

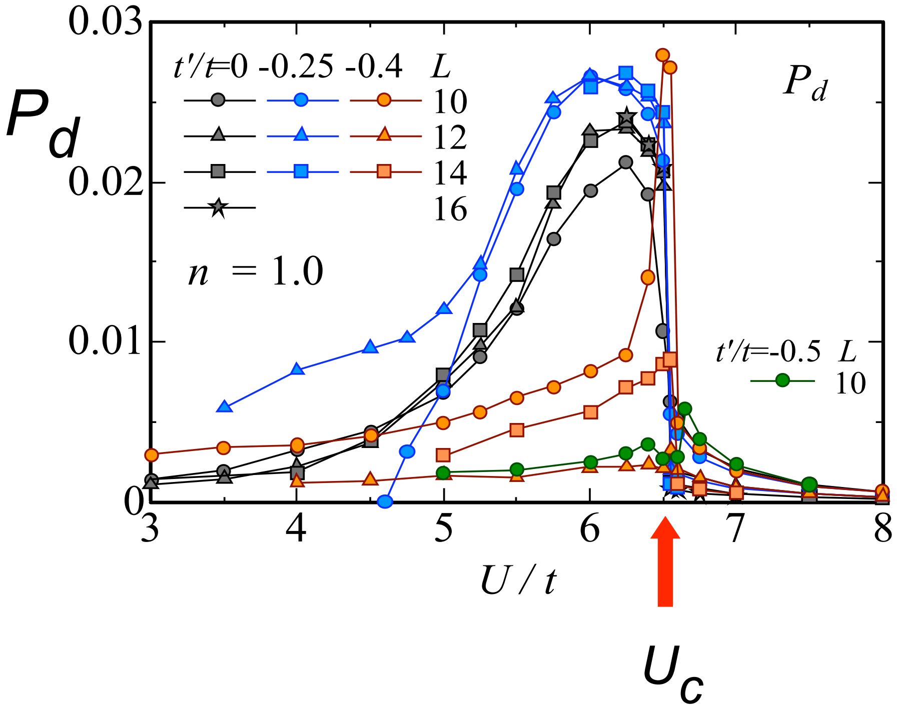
d-wave to RVB insulator

half filling (δ=0)

- d-wave pair correlation function

$$P_d(\boldsymbol{r}) = \frac{1}{N}\sum_i \sum_{\tau,\tau'} (-1)^{\tau+\tau'} \langle \Delta_\tau^\dagger(\boldsymbol{r}_i)\Delta_{\tau'}(\boldsymbol{r}_i+\boldsymbol{r})\rangle$$





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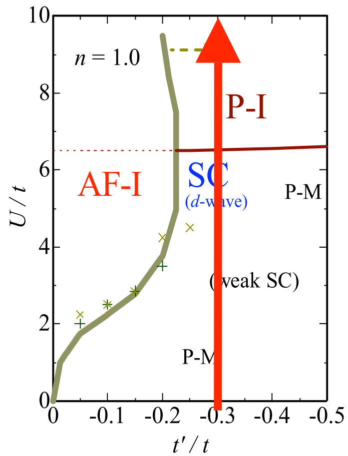
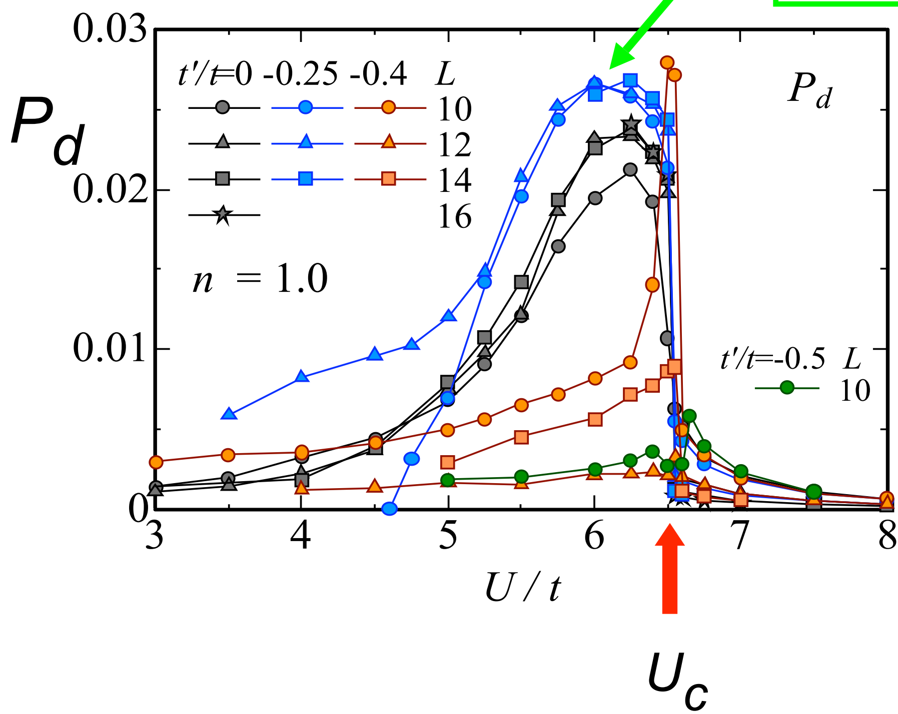
d-wave is enhanced at

$U / t < 6.5$

$t' / t \sim -0.25$





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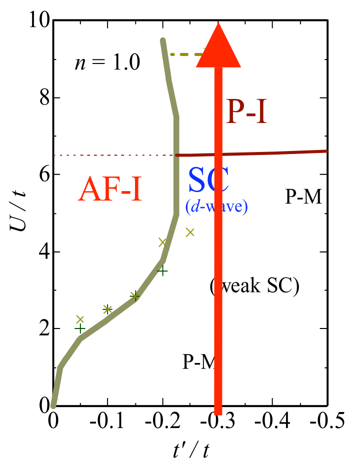

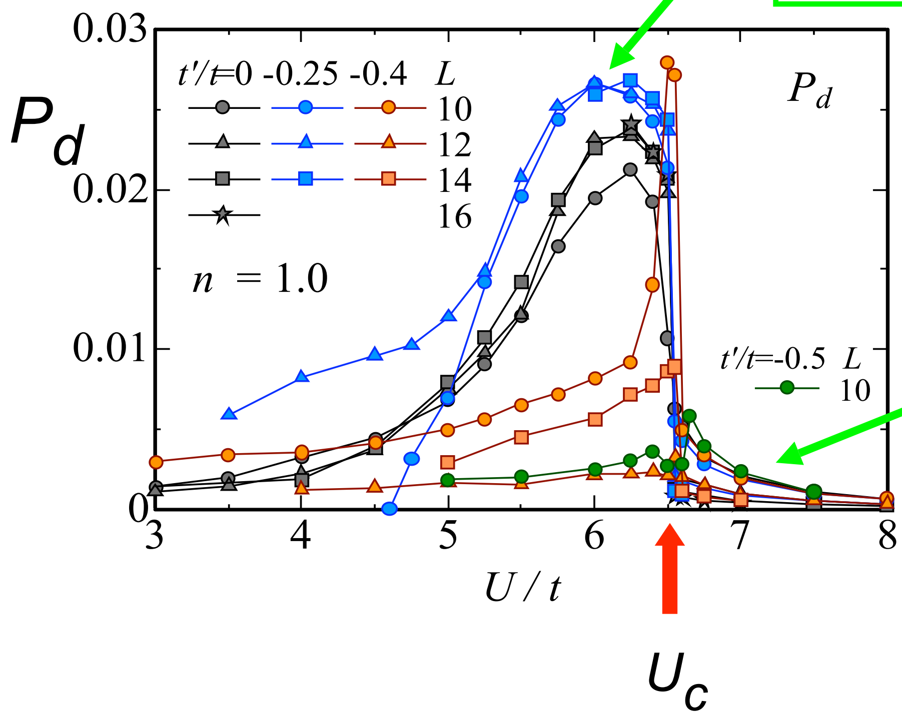

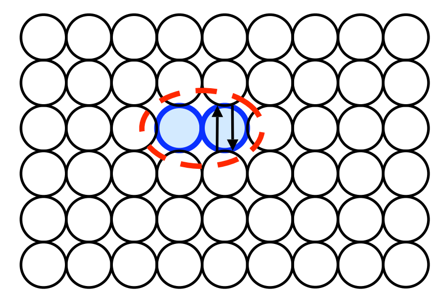

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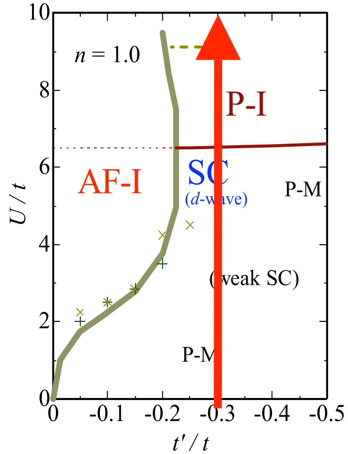

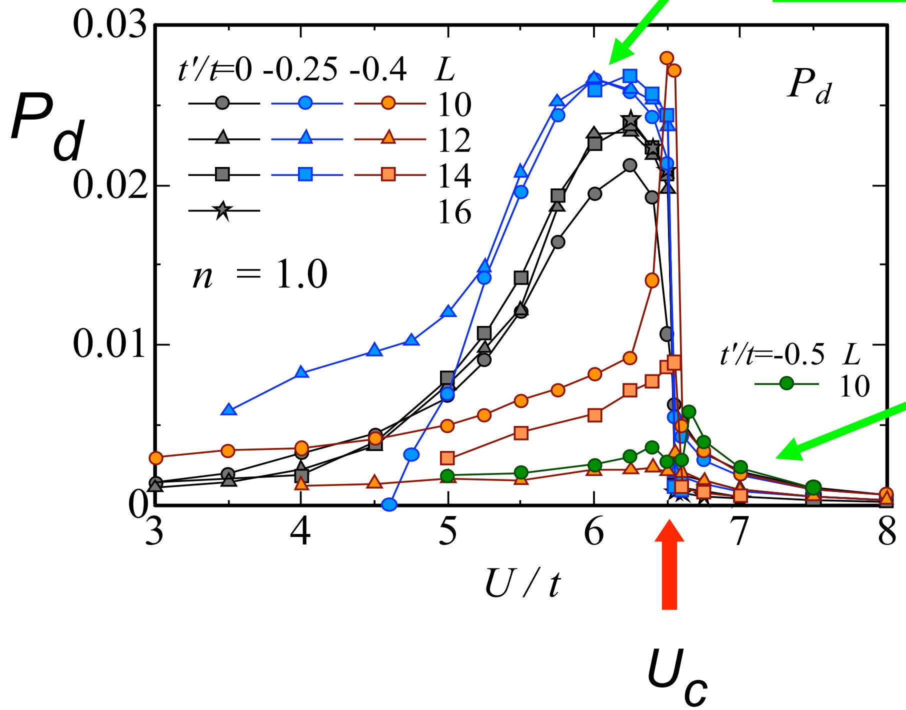

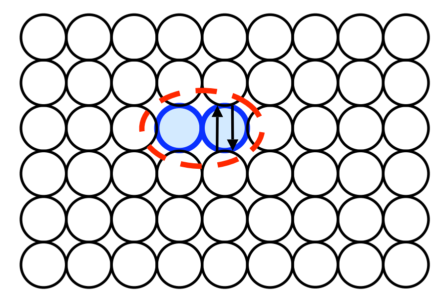

doublon-holon exist, but

form virtual states to induce J

d-wave to RVB insulator

half filling (δ=0)

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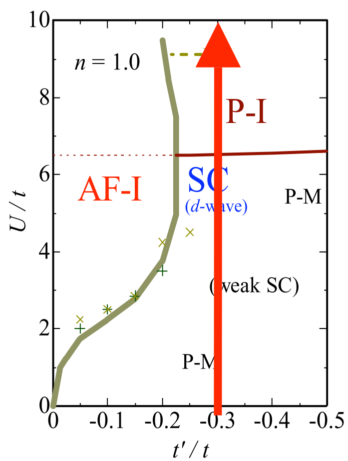

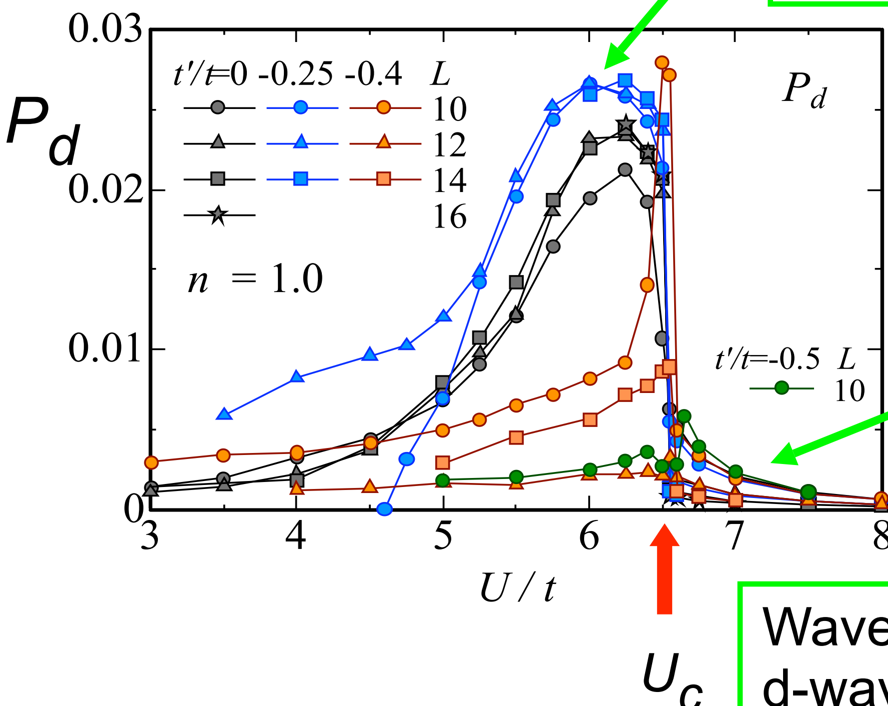

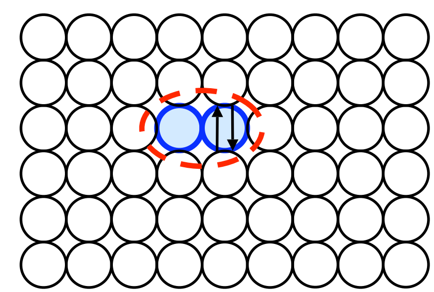

Wave function has d-wave order parameter, but P_d vanishes.

doublon-holon exist, but
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d-wave to RVB insulator

half filling (δ=0)

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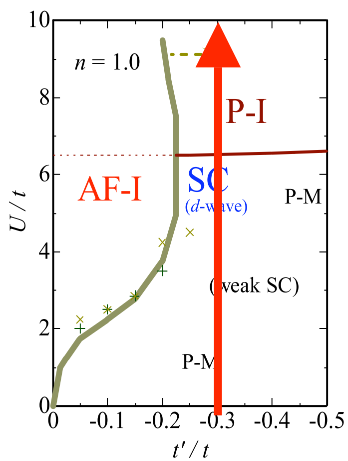
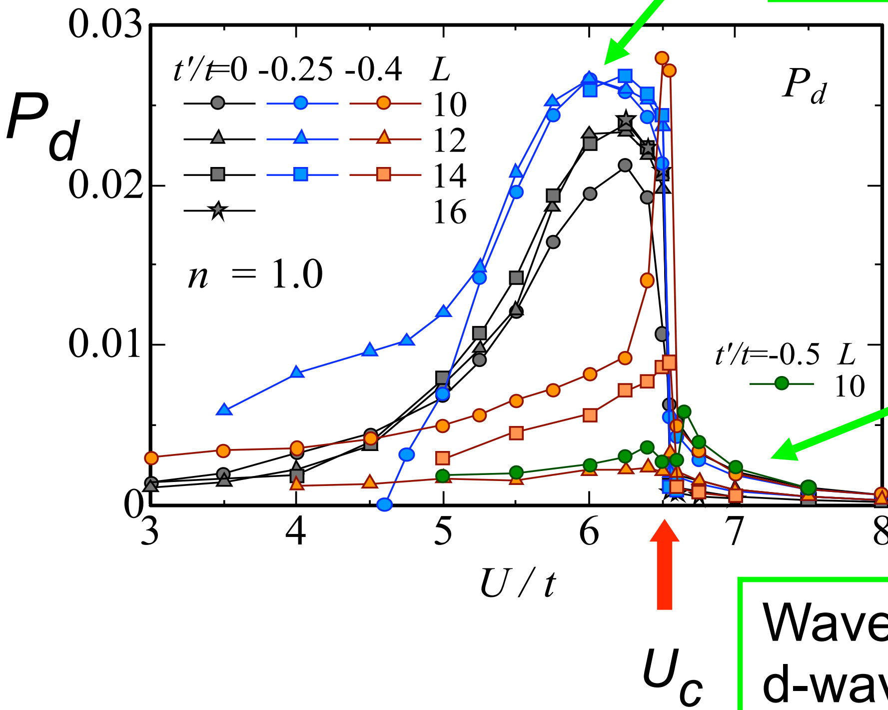
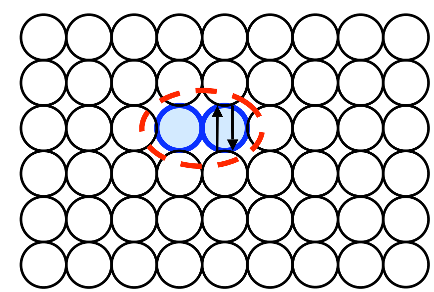






Wave function has d-wave order parameter, but P_d vanishes.

"RVB insulator"

doublon-holon exist, but

form virtual states to induce J

RVB insulator (Anderson 1987)

Projected BCS state
= RVB insulator

$$
\begin{aligned}
P_G|\Phi_{\mathrm{SC}}\rangle &= P_G \prod_{\boldsymbol{k}} \left[u_{\boldsymbol{k}} + v_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\uparrow} c^{\dagger}_{-\boldsymbol{k}\downarrow}\right] |0\rangle \\
&= P_G (\prod_{\boldsymbol{k}} u_{\boldsymbol{k}}) \prod_{\boldsymbol{k}} \left[1 + \frac{v_{\boldsymbol{k}}}{u_{\boldsymbol{k}}} c^{\dagger}_{\boldsymbol{k}\uparrow} c^{\dagger}_{-\boldsymbol{k}\downarrow}\right] |0\rangle \\
&= P_G (\prod_{\boldsymbol{k}} u_{\boldsymbol{k}}) \prod_{\boldsymbol{k}} \exp\left(\frac{v_{\boldsymbol{k}}}{u_{\boldsymbol{k}}} c^{\dagger}_{\boldsymbol{k}\uparrow} c^{\dagger}_{-\boldsymbol{k}\downarrow}\right) |0\rangle \\
&= P_G (\prod_{\boldsymbol{k}} u_{\boldsymbol{k}}) \exp\left(\sum_{\boldsymbol{k}} a_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\uparrow} c^{\dagger}_{-\boldsymbol{k}\downarrow}\right) |0\rangle \\
&= P_G (\prod_{\boldsymbol{k}} u_{\boldsymbol{k}}) \exp\left(\sum_{i,j} a_{i,j} c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow}\right) |0\rangle,
\end{aligned}
$$

$$
P_N P_G |\Phi_{\mathrm{SC}}\rangle = \frac{1}{(N/2)!} (\prod_{\boldsymbol{k}} u_{\boldsymbol{k}}) P_G \left(\sum_{i,j} a_{i,j} c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow}\right)^{\frac{N}{2}} |0\rangle
$$

$$
a_{i,j} = \frac{1}{N} \sum_{\boldsymbol{k}} a_{\boldsymbol{k}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)},
$$

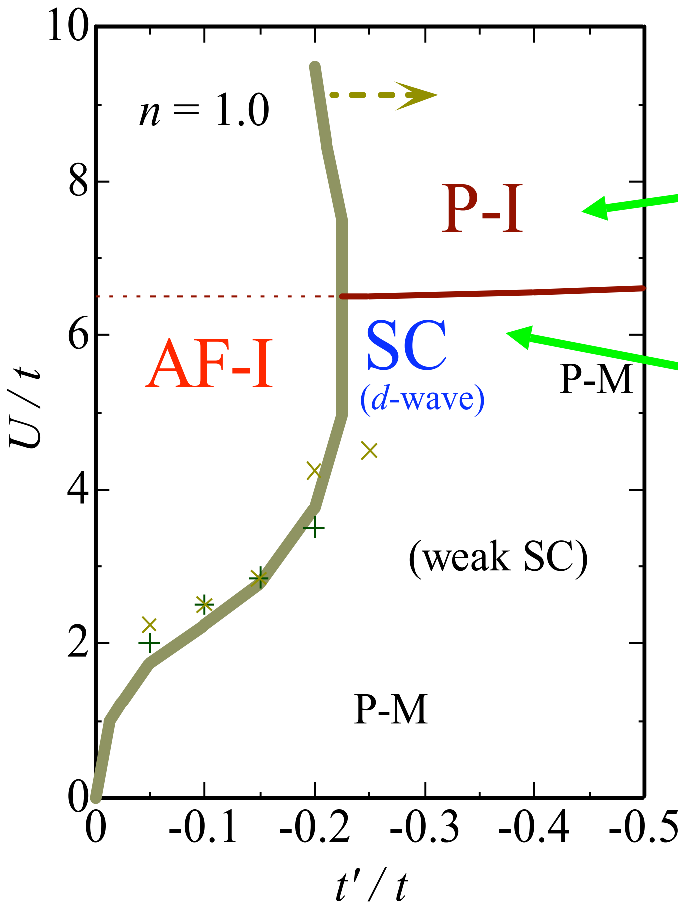
$$
a_{\boldsymbol{k}} = \frac{v_{\boldsymbol{k}}}{u_{\boldsymbol{k}}} = \frac{\Delta_{\boldsymbol{k}}}{\varepsilon^{(0)}_{\boldsymbol{k}} - \mu + \sqrt{(\varepsilon^{(0)}_{\boldsymbol{k}} - \mu)^2 + |\Delta_{\boldsymbol{k}}|^2}}.
$$

Phase diagram

half filling (δ=0)

T=0 Variational Theory

t-t′-U Hubbard model



doublon-holon bound states
= RVB insulator

free doublons and holons
= d-wave SC

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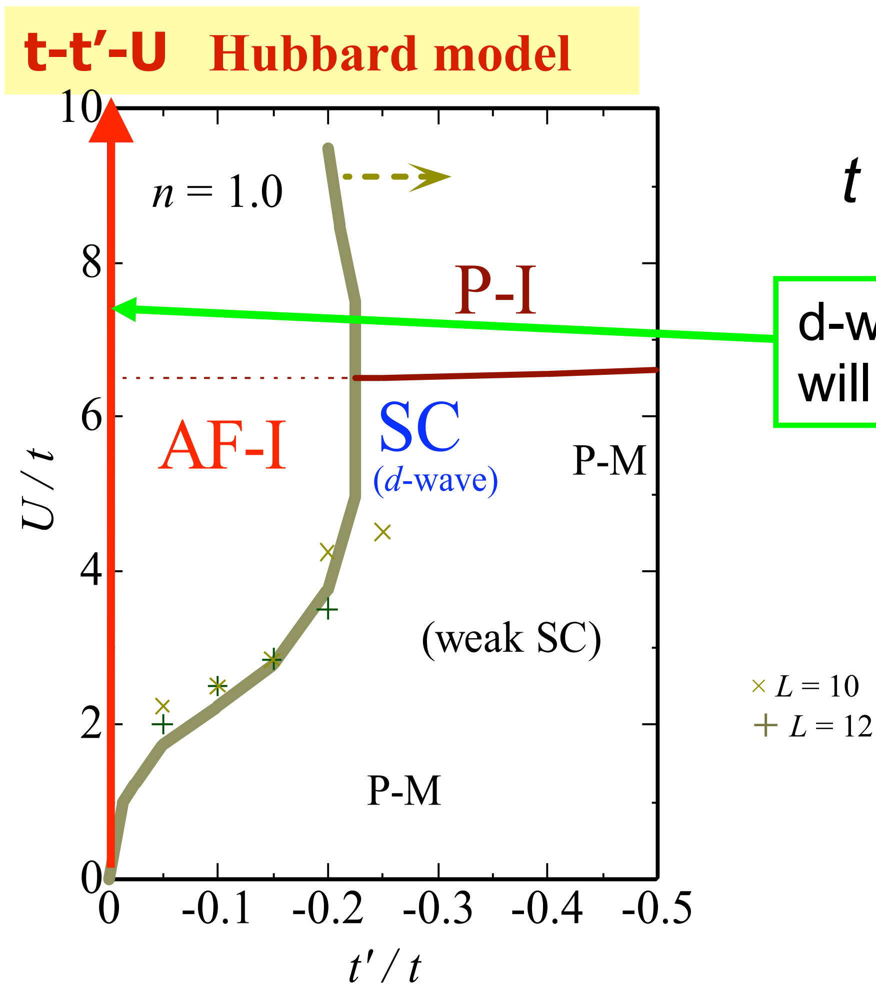
half filling (δ=0)



t'= 0 case ----

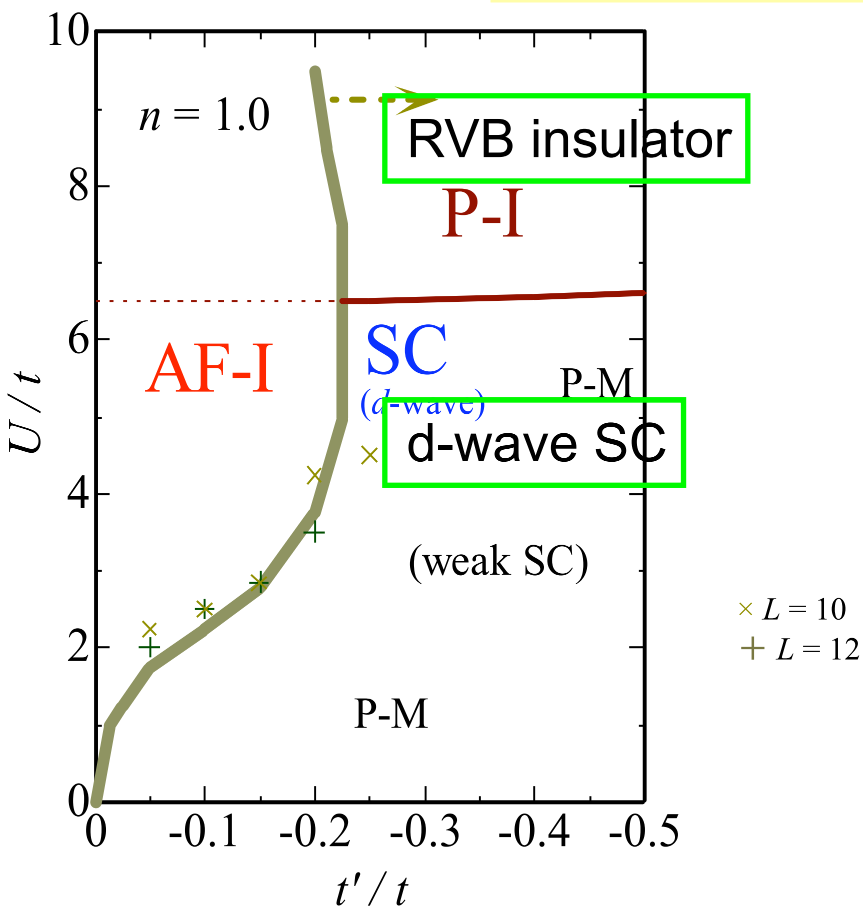
d-wave RVB (insulator) + AF LRO will be the best variational state.

Hsu, Giamarchi-Lhuillier, Himeda-Ogata

II. Doped Case

less-than-half filling

t-t′-U Hubbard model



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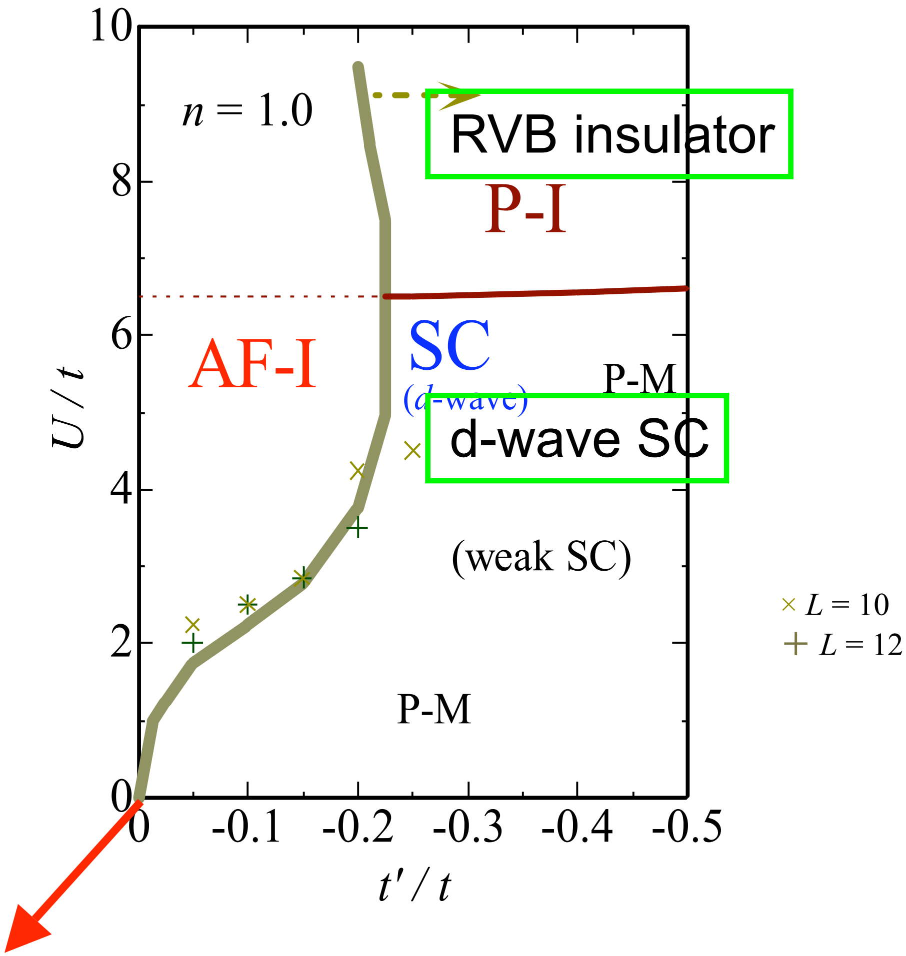

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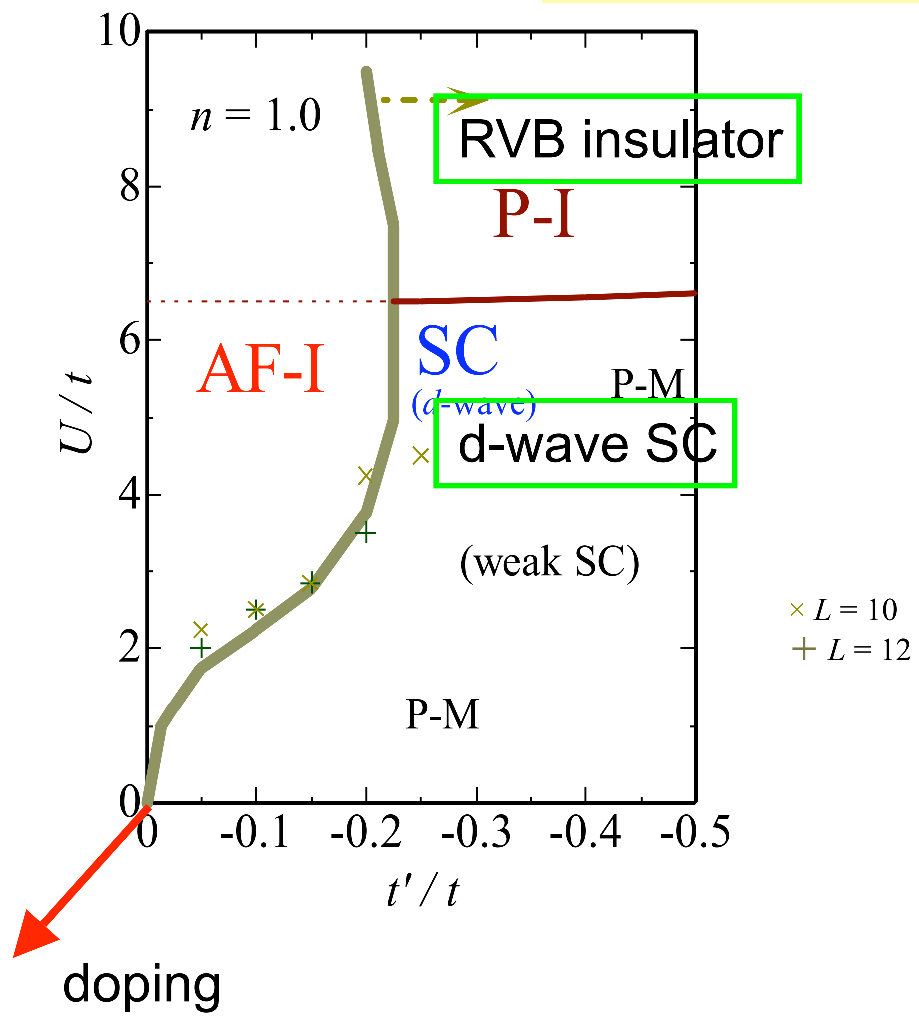

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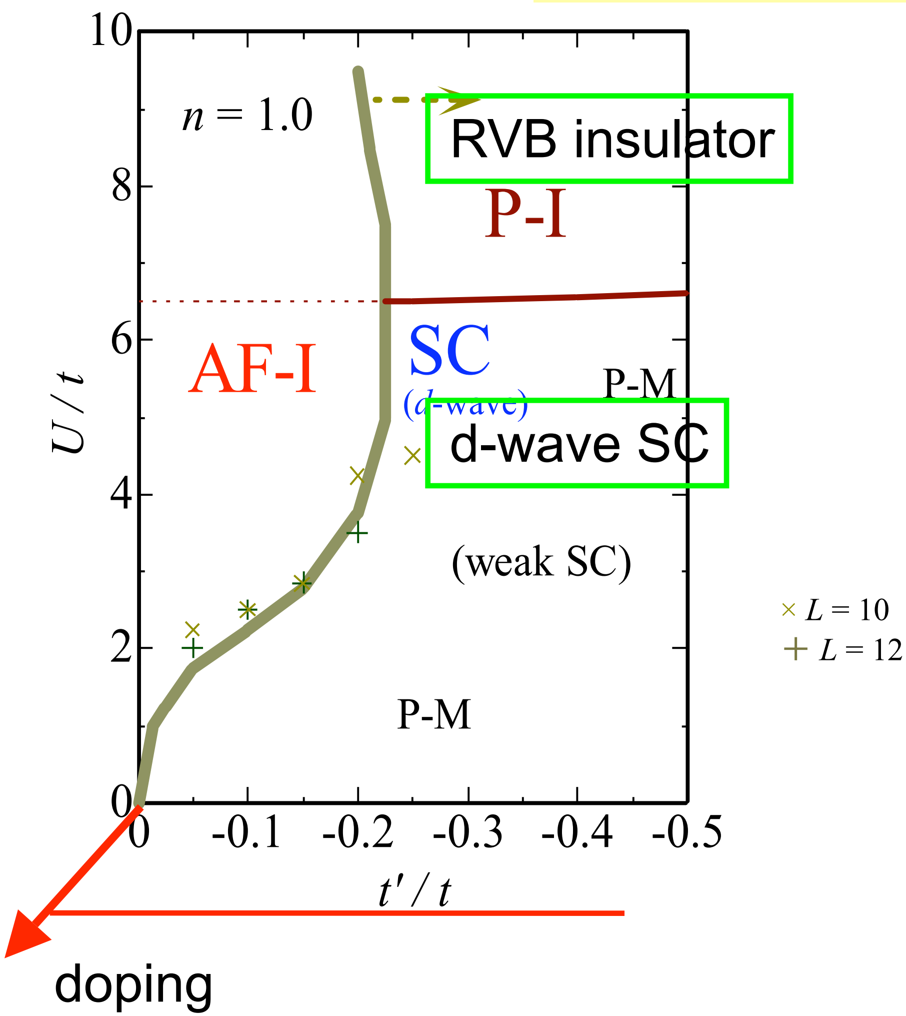

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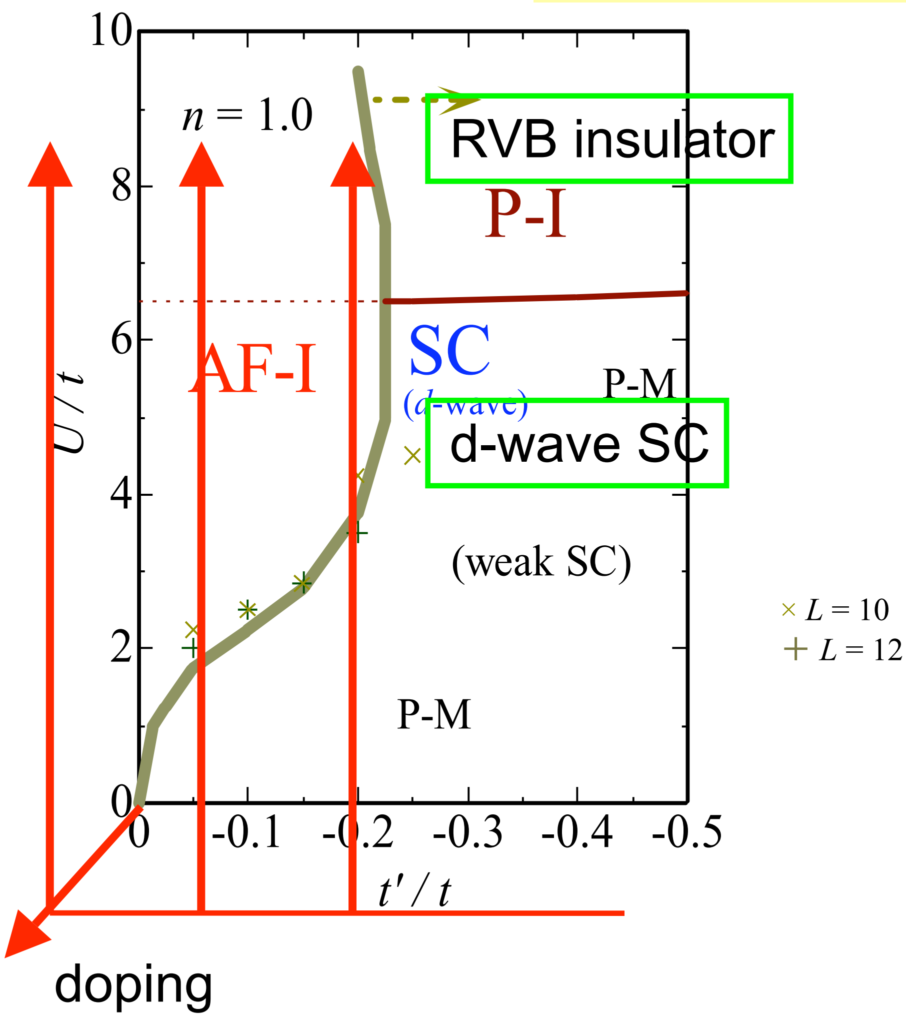
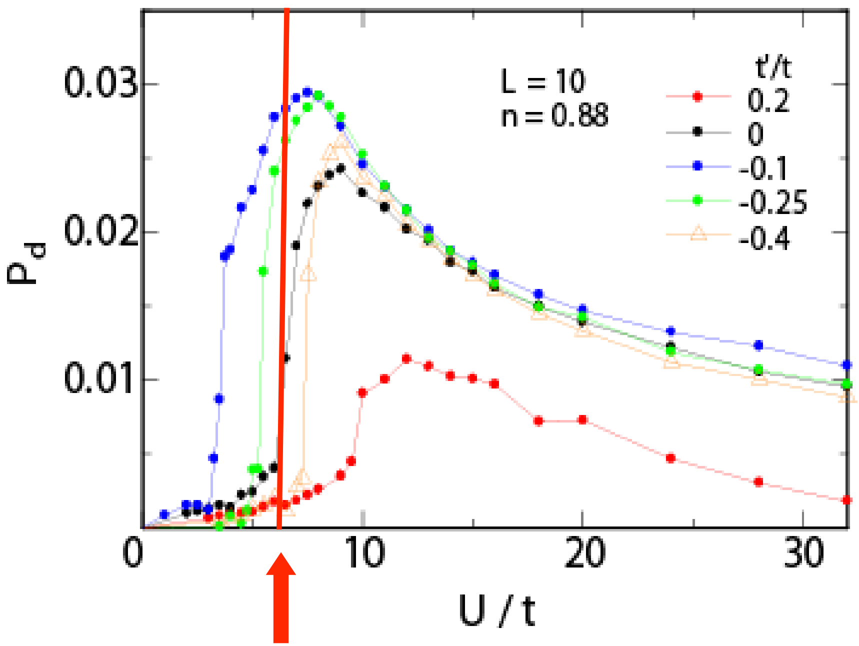


Doped Case

d-wave pair correlation function



$U_{crossover}$

Crossover, but features are very different.

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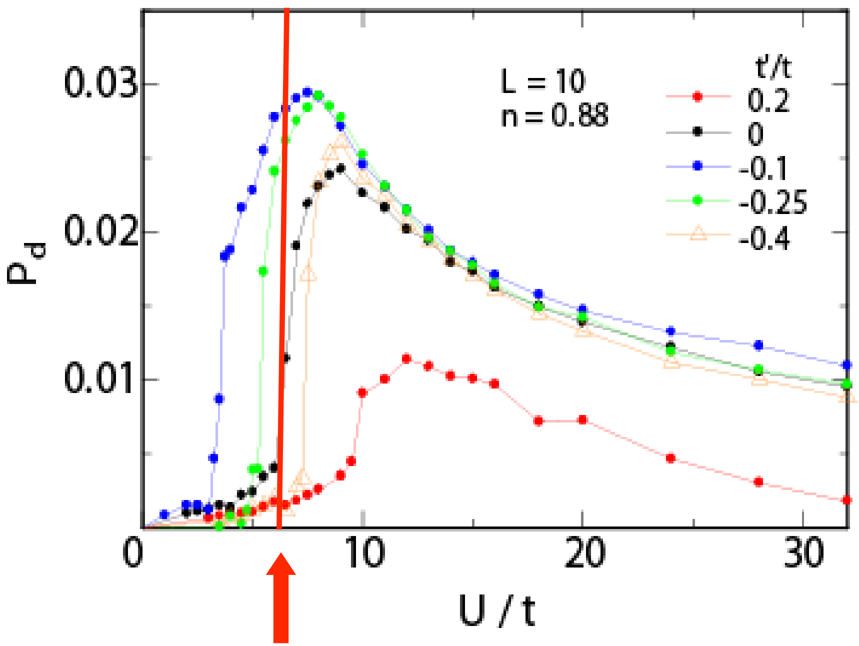

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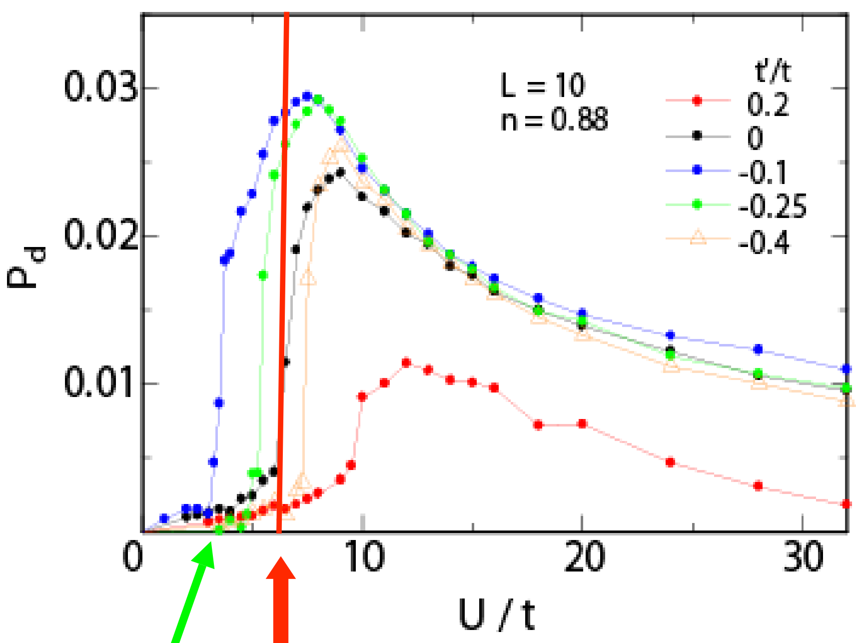


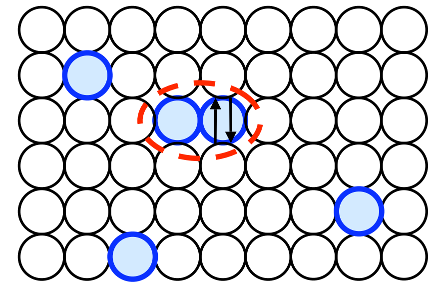
$U_{crossover}$

- Small U ($U < U_{co}$)
  weak-coupling region, consistent with QMC

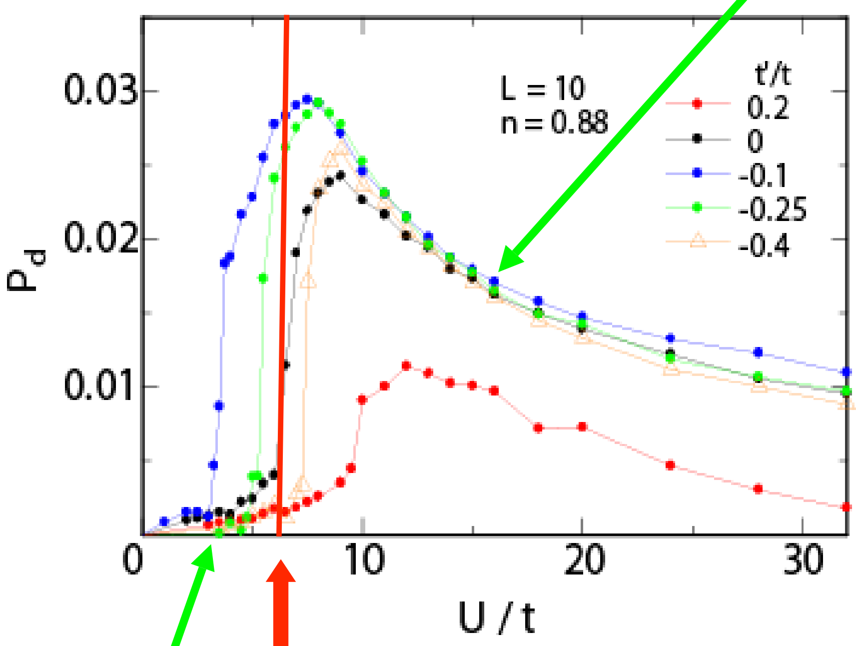
Crossover, but features are very different.

Doped Case

- Large U $(U > U_{co})$
  bound state + free holons



d-wave pair correlation function



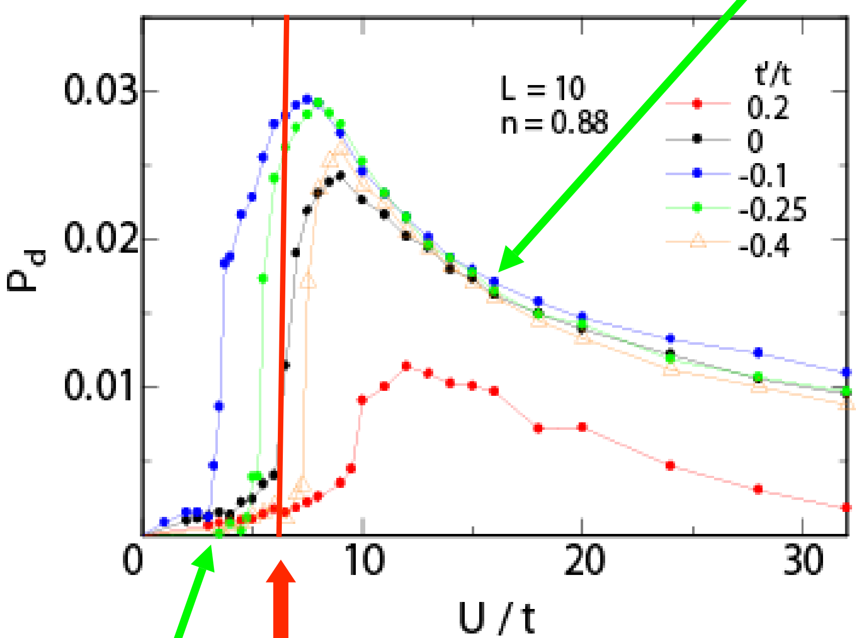
$U_{crossover}$

- Small U $(U < U_{co})$
  weak-coupling region, consistent with QMC

Crossover, but features are very different.

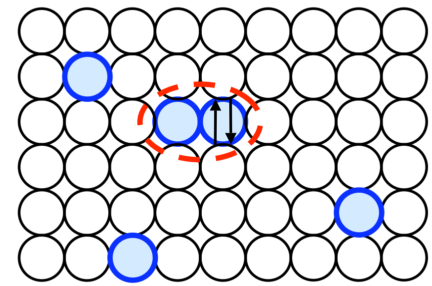
Doped Case

d-wave pair correlation function



$U_{crossover}$

- Large U $(U > U_{co})$
  bound state + free holons



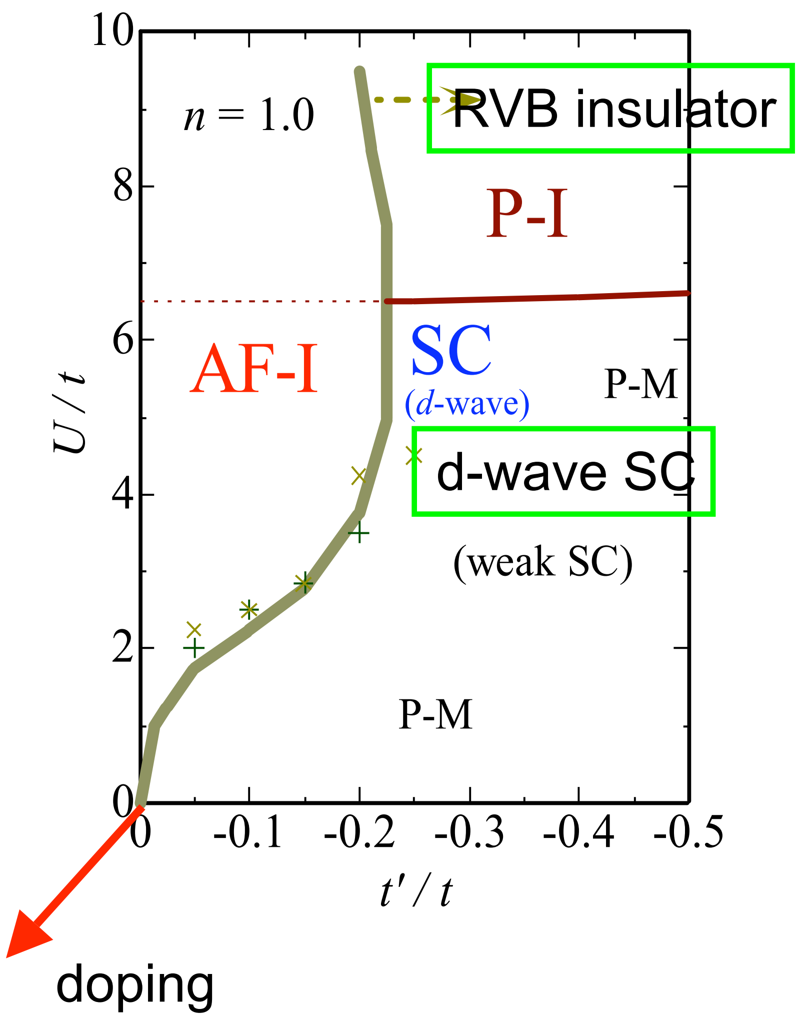
"Doped Mott insulator"

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

⇒ *t*-*J* region

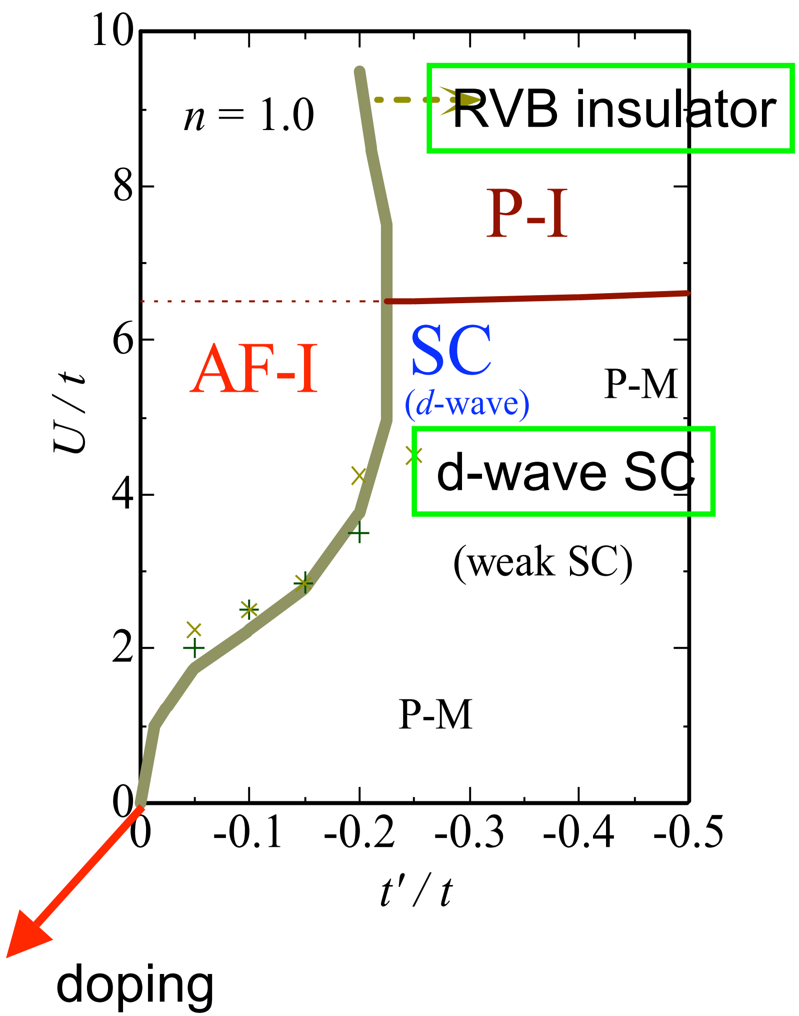
- Small U $(U < U_{co})$
  weak-coupling region, consistent with QMC

t* - *t′* - *J Model



10
8
6
4
2
0
0
-0.1
-0.2
-0.3
-0.4
-0.5
U / t
t′ / t
n = 1.0
RVB insulator
P-I
AF-I
SC
(d-wave)
P-M
d-wave SC
(weak SC)
P-M
doping

t - t′ - J Model

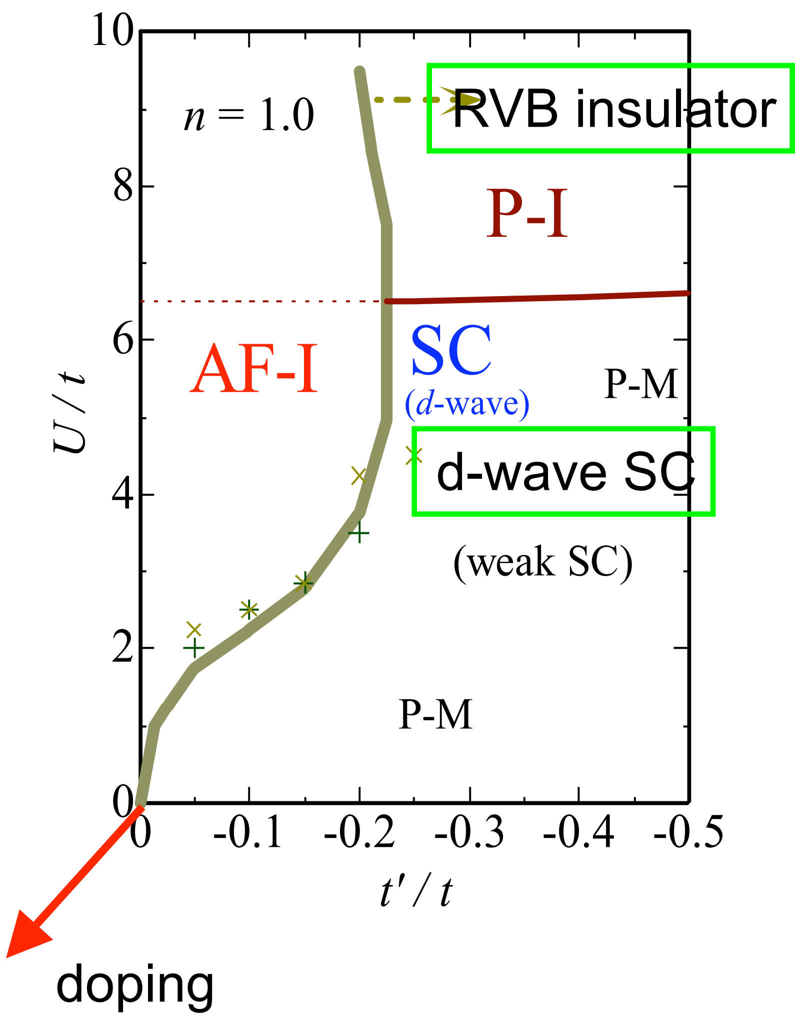


In the large U ($U > U_{co}$) region, we study

$t - t'$ - J model by fixing $J / t = 0.3$.

$J / t = 0.3$ corresponds to $U / t = 13$

t - t' - J Model



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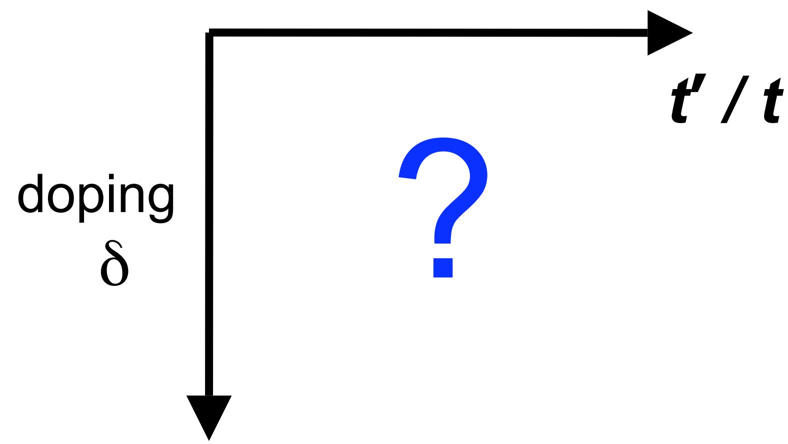

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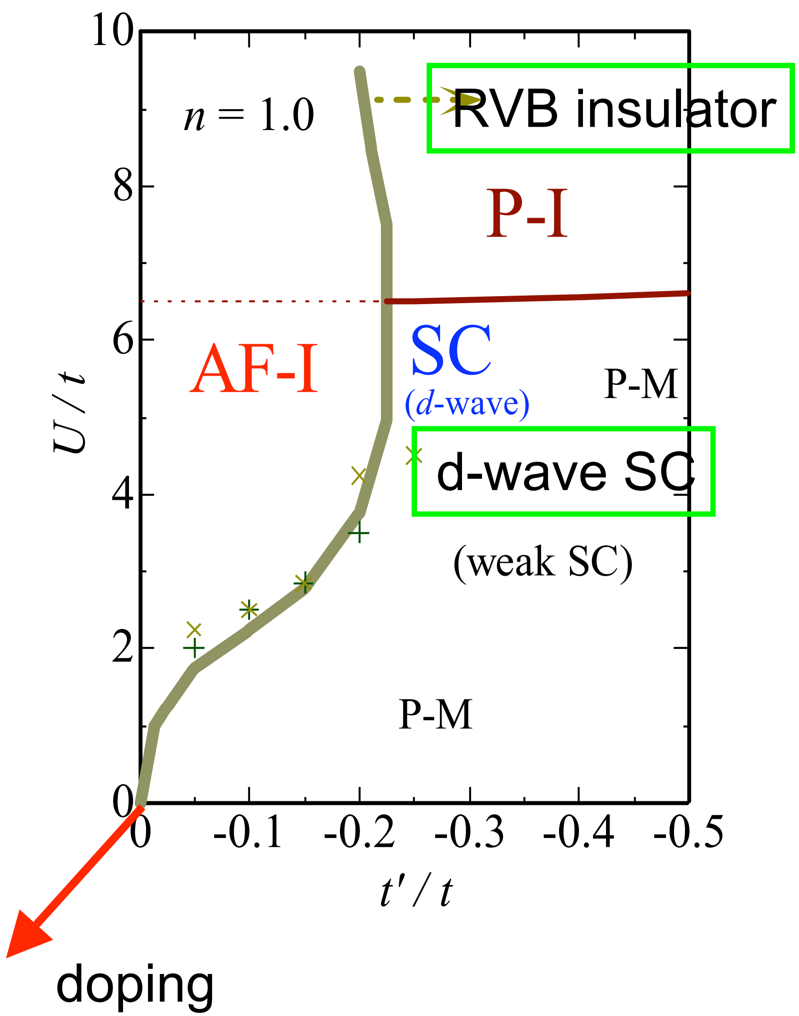

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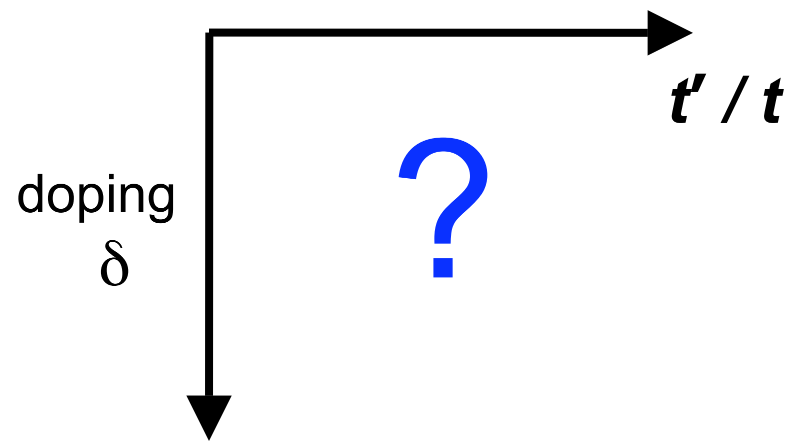
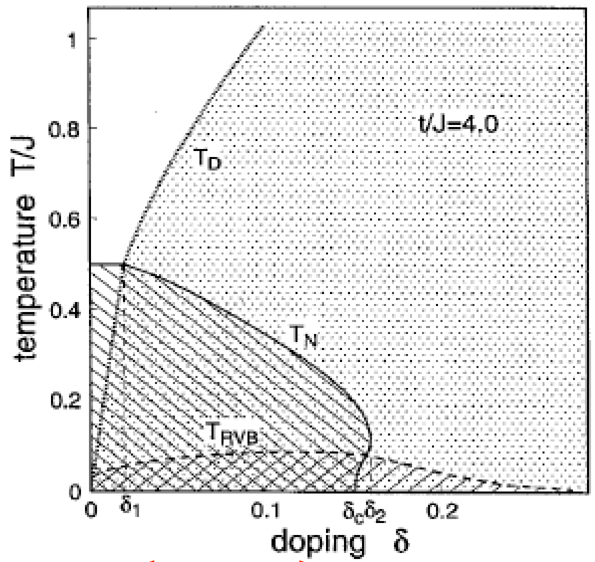


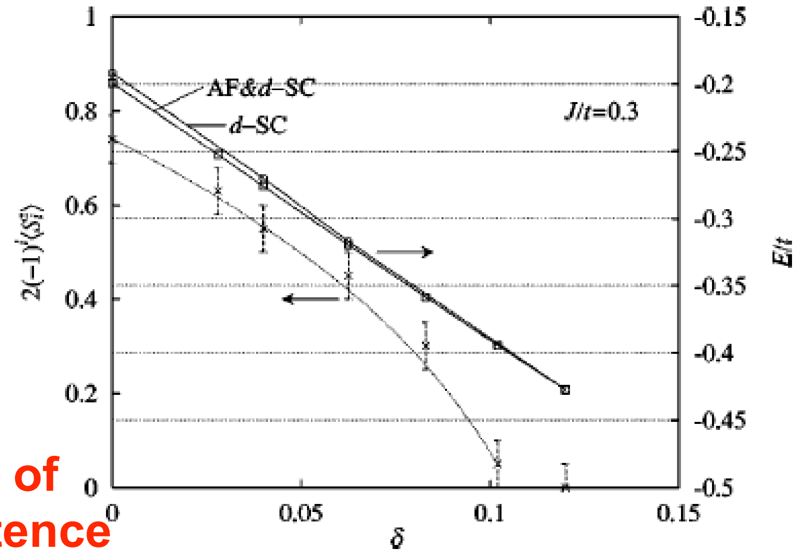
- Coexistence of AF and d-wave
- Effects of t'

AF and SC coexist in *t* -*J* model

t′ = 0



Region of coexistence



Inaba *et al.*, Physica C (1996)

(slave boson mean-field)

Himeda-Ogata, PRB 60 (1999)

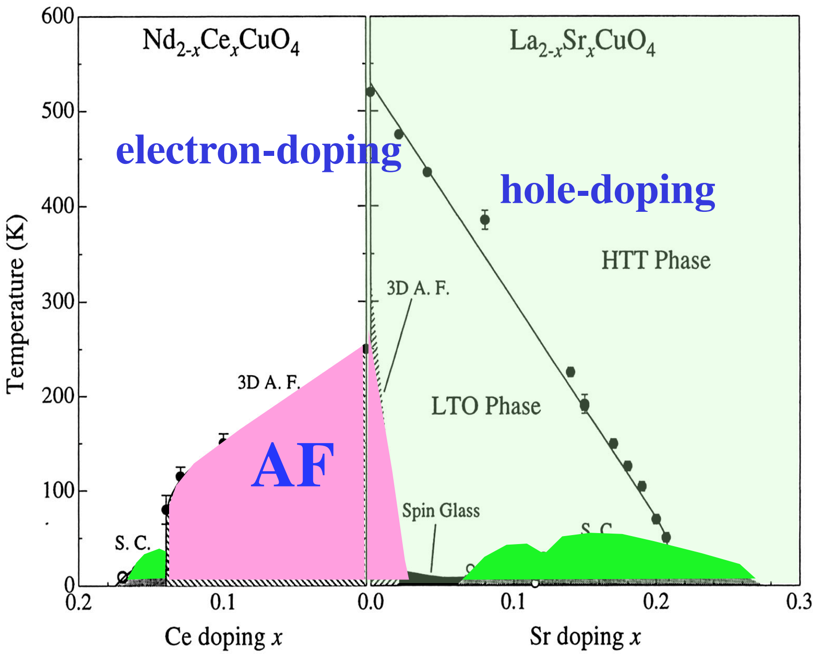
(variational Monte Carlo *T*=0)

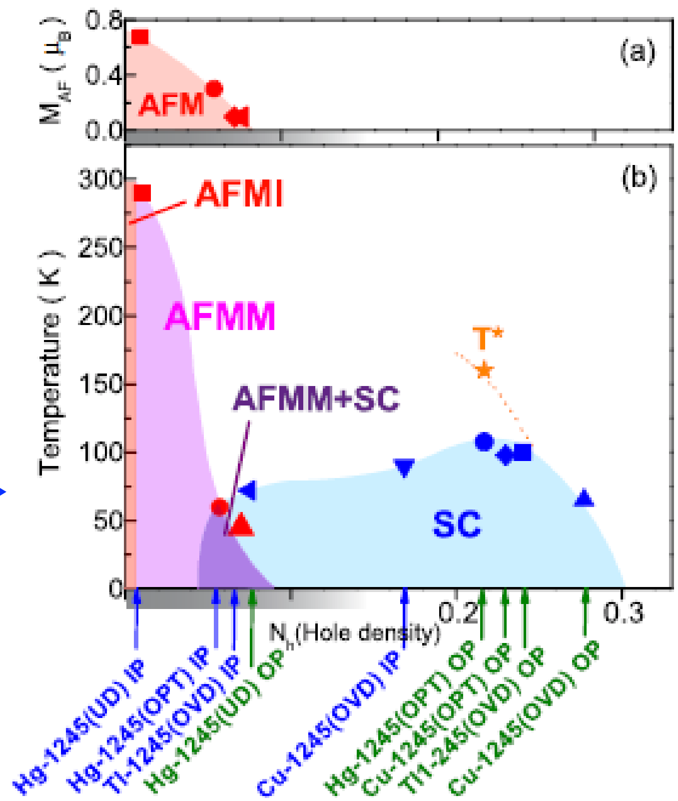
The best variational state for 0< δ < 0.1

$$P_G|\Psi_{SC-AF}(\Delta_{var}, \Delta_{AF}, \mu)\rangle$$

Coexistence in the Bulk

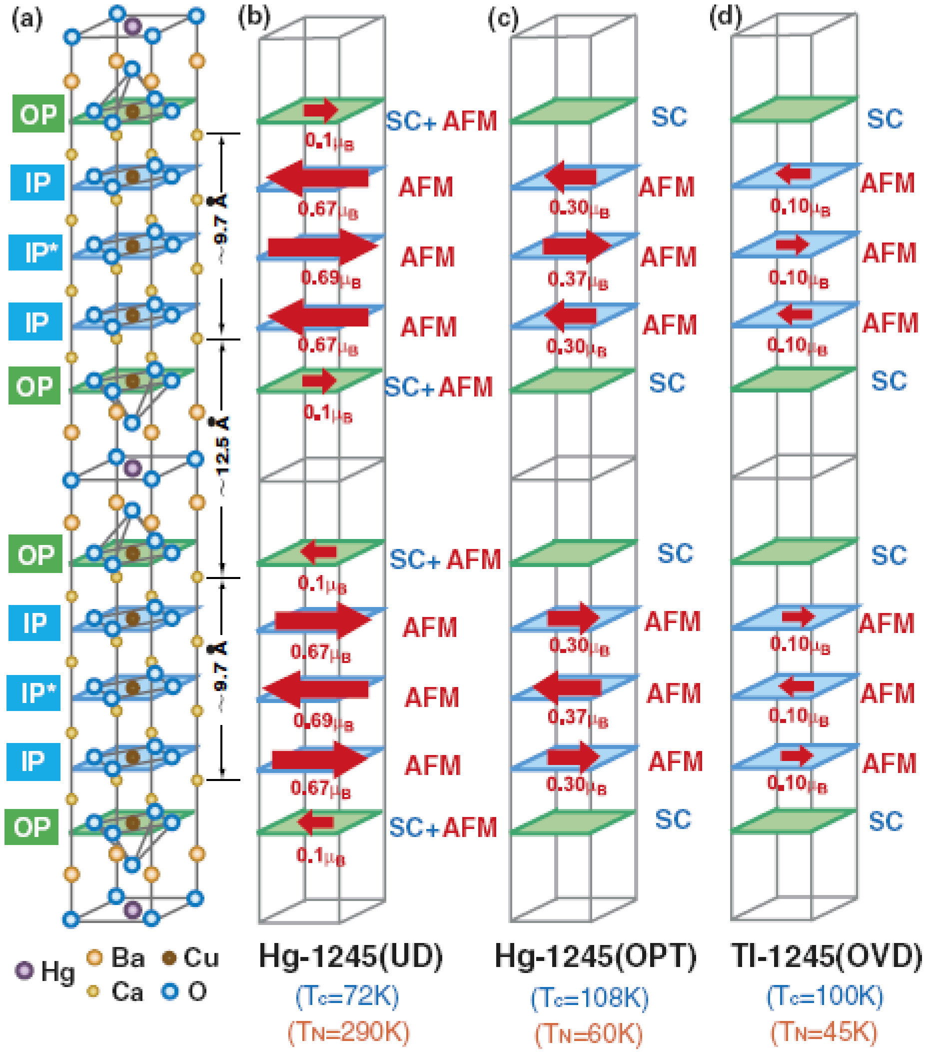
Experimental phase diagram

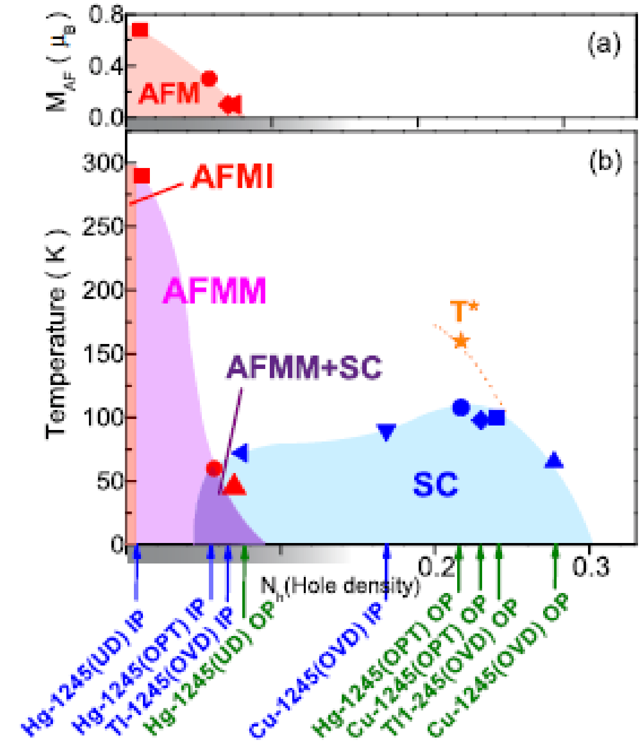




In clean systems, AF and SC coexist !

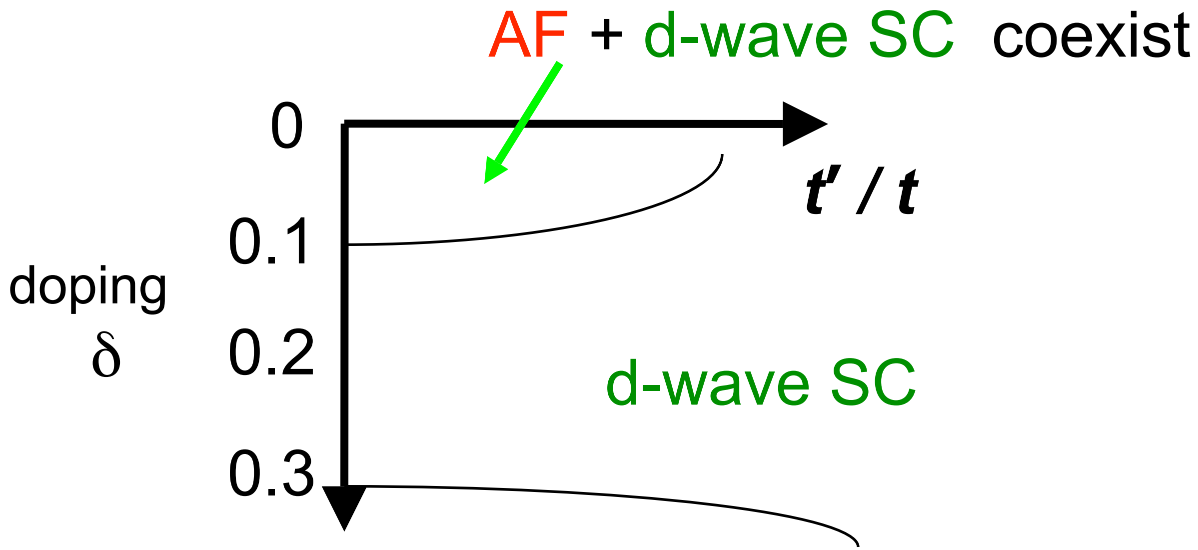
H. Mukuda *et al*, PRL 96, 087001 (2006)



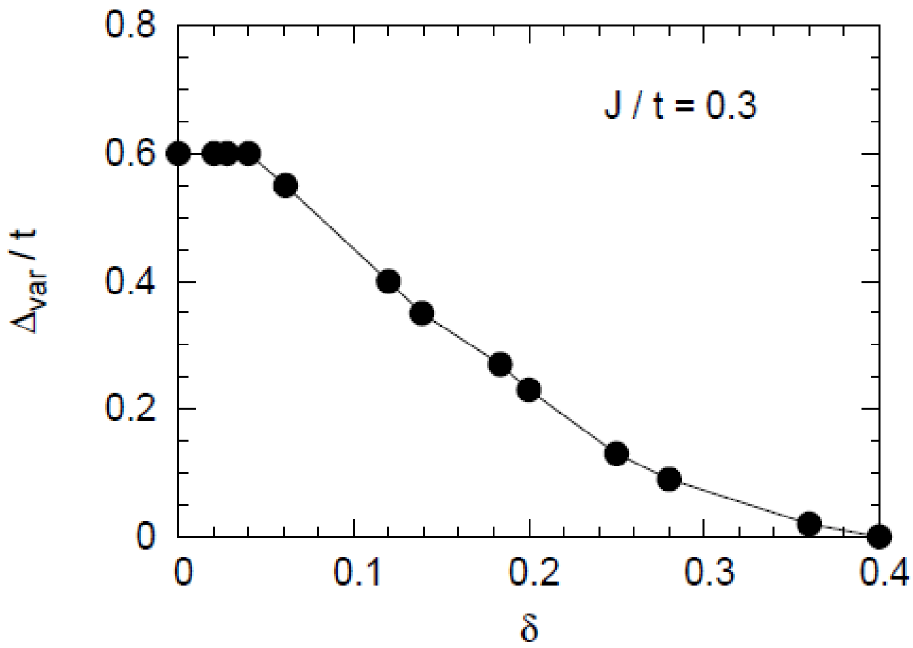


H. Mukuda *et al*, PRL 96, 087001 (2006)

Obtained phase diagram in t - t'-J model



RVB order parameter in variational wave functions



This will be related to Pseudo-Gap .

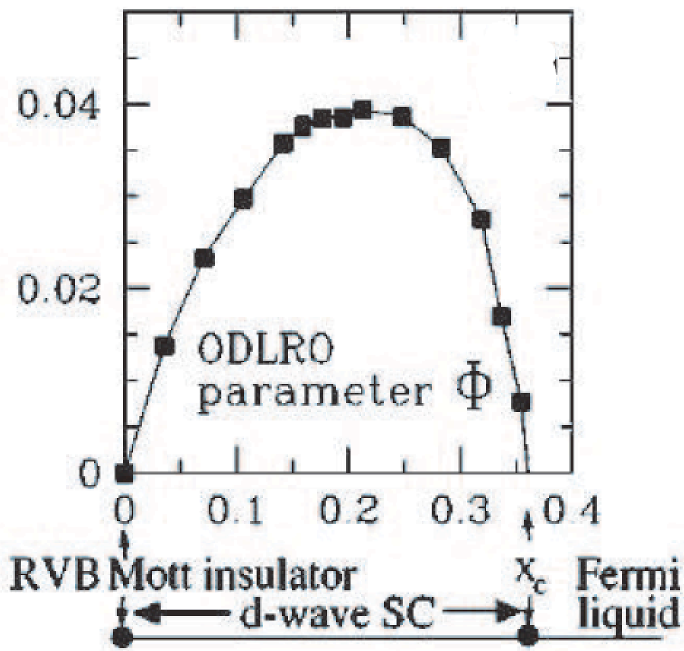
Excitated states will have gap proportional to Δ_{var}

$$|\Psi^{+}_{\boldsymbol{k}\uparrow}\rangle = P_G \gamma^{\dagger}_{\boldsymbol{k}} |\Phi_{\text{SC}}\rangle = P_G c^{\dagger}_{\boldsymbol{k}\uparrow} |\Phi_{\text{SC}}\rangle$$

$$\gamma^{\dagger}_{\boldsymbol{k}} = u_{\boldsymbol{k}} c^{\dagger}_{\boldsymbol{k}\uparrow} - v_{\boldsymbol{k}} c_{-\boldsymbol{k}\downarrow}$$

Expectation value of SC order parameter

$$\langle \mathcal{O} \rangle \equiv \frac{\langle \psi | \mathcal{O} | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle \psi_0 | P_G \mathcal{O} P_G | \psi_0 \rangle}{\langle \psi_0 | P_G P_G | \psi_0 \rangle}$$

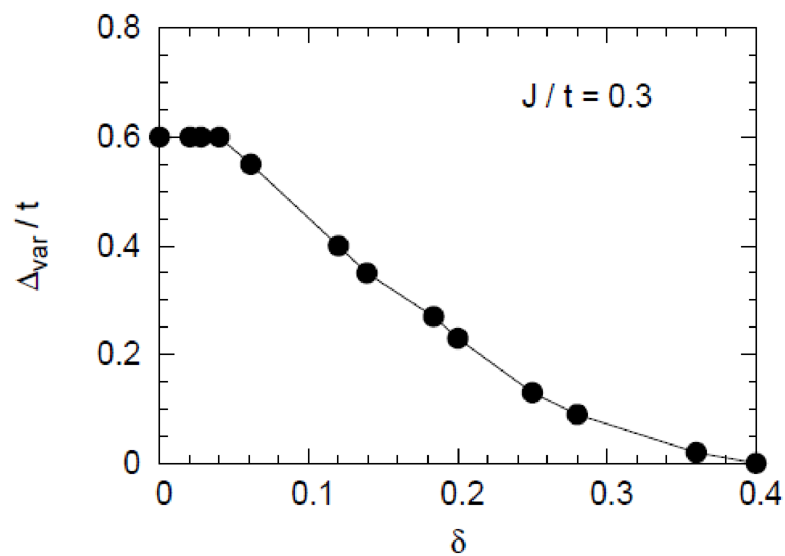


Paramekanti et al.

Δ_{exp} is different from Δ_{var}

Δ_{exp} will be related to Tc .

Δ_{var} will be related to Pseudo Gap .



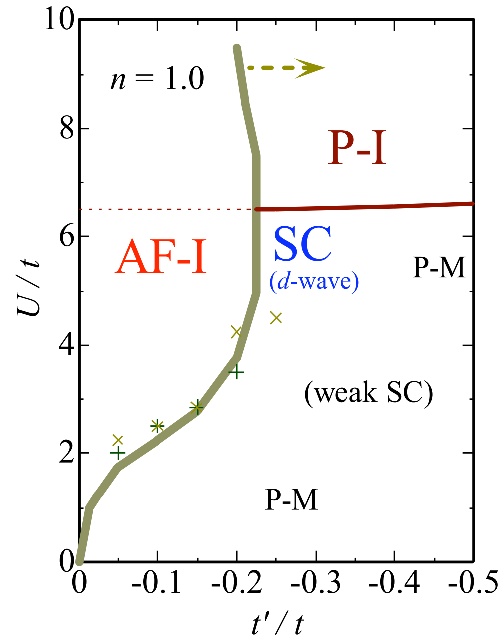
Conclusions

- Modified variational state doublon-holon bound state is important.
- Mott transition

- Doped case

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

  doublon-holon bound state + free holons



t-J -like region

Coexistence of AF and SC ------- cf. Mukuda

Effects of t ′ : hole doped vs electron doped

(t′ < 0) (t′ > 0)

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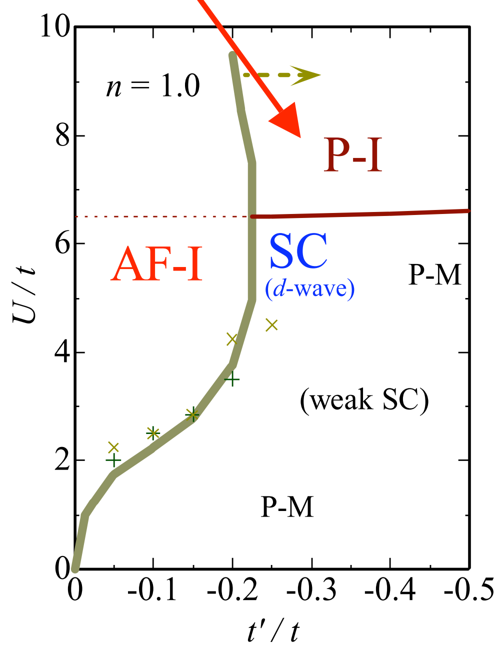

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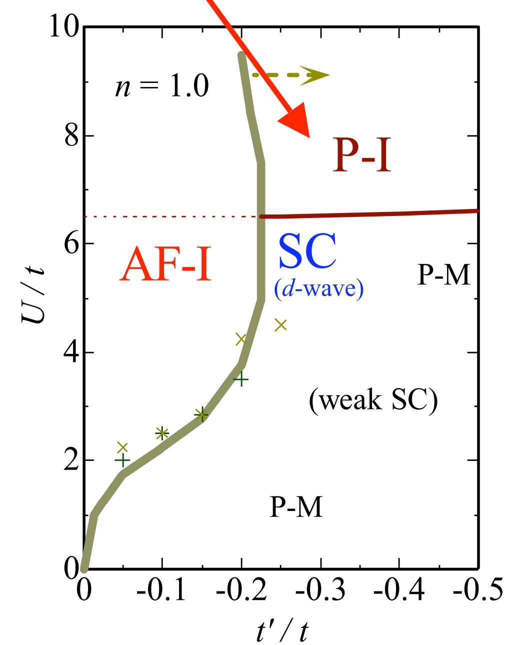

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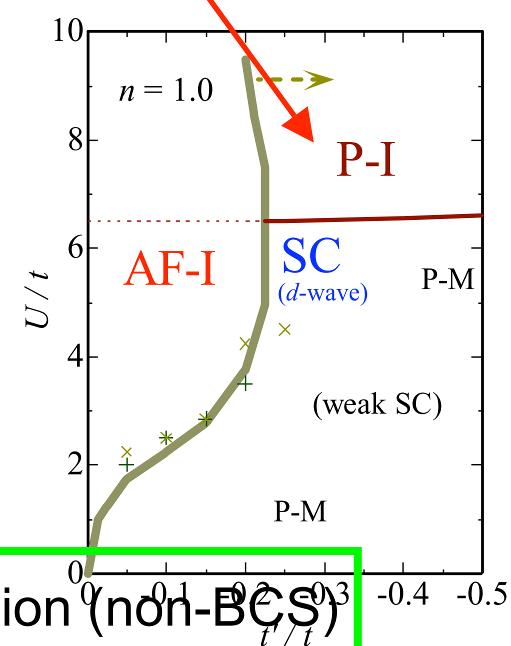

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● small U (BCS-like) (weak-coupling region)

● large U (non-BCS) (t-J region)

doublon-holon bound state + free holons

High-T_C cuprates belong to the strong-coupling region (non-BCS)

t-J -like region

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