Hidden Fermionic excitation at the origin of Mott insulator, pseudogap and high-temperature superconductivity

RIKEN Center for Emergent Matter Science

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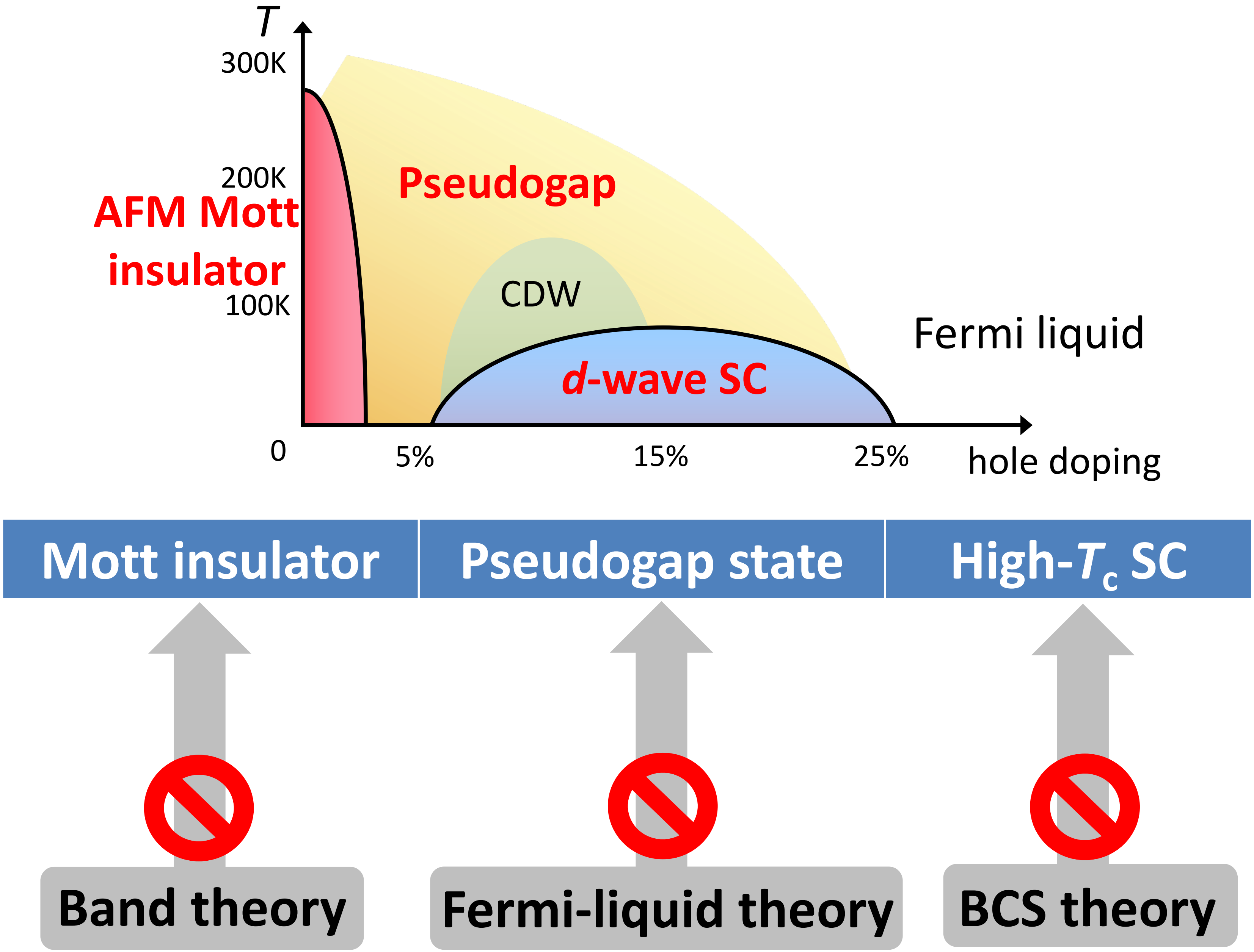
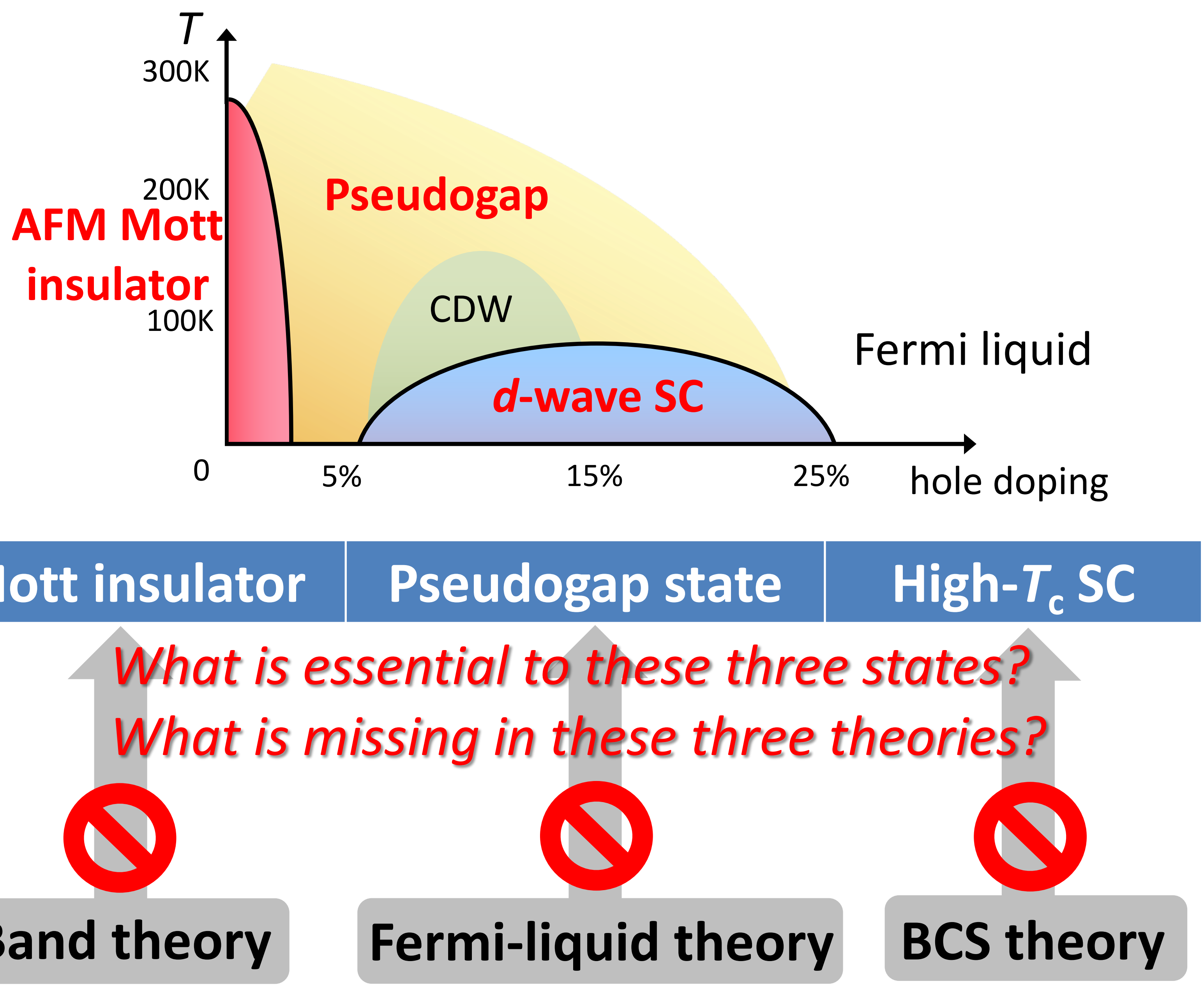
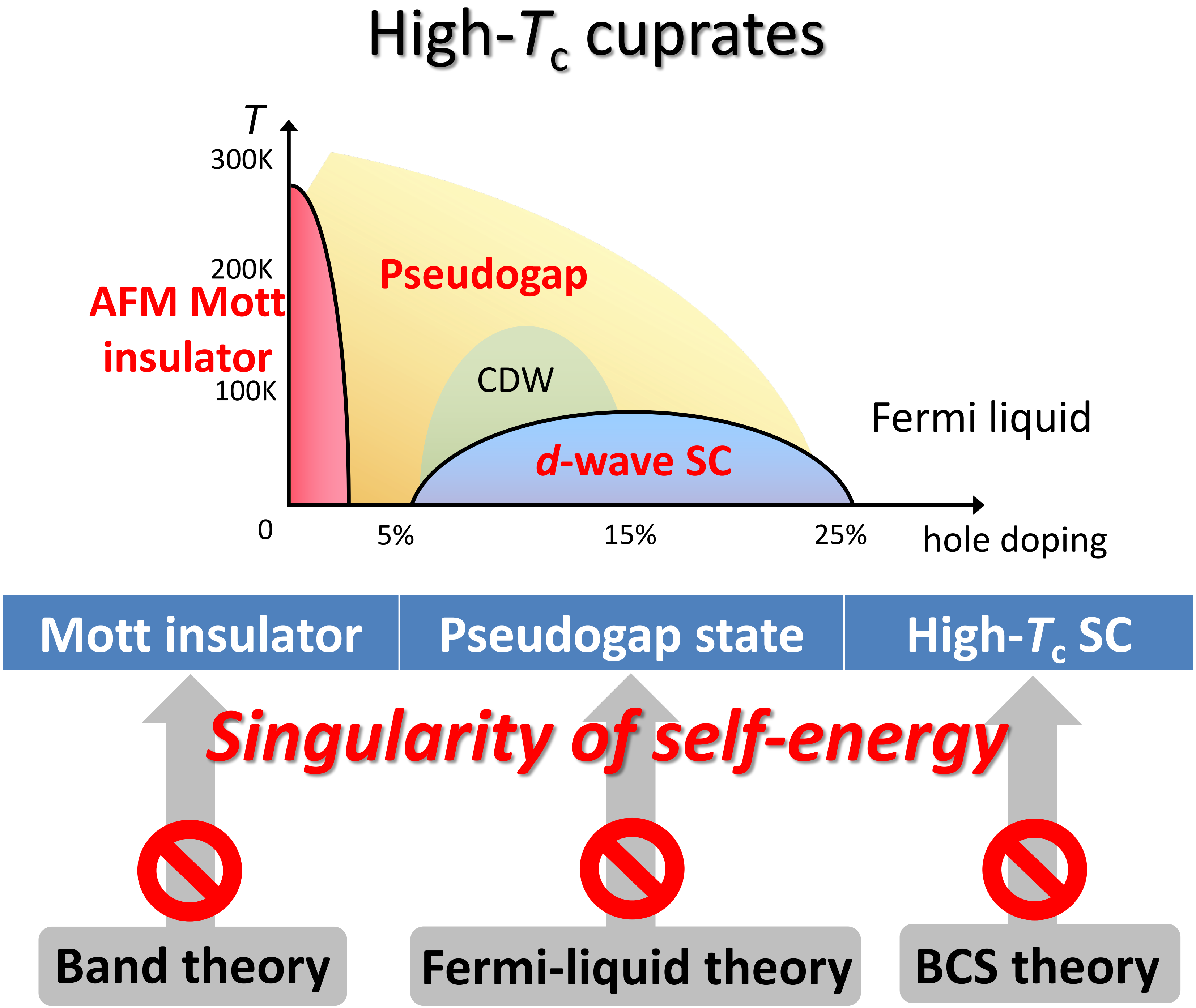
July 18, 2019

High-T_c cuprates



High-T_c cuprates




High-T_c cuprates
T
300K
200K
100K
0
AFM Mott insulator
Pseudogap
CDW
d-wave SC
Fermi liquid
5%
15%
25%
hole doping
Mott insulator
Pseudogap state
High-T_c SC
Singularity of self-energy
Band theory
Fermi-liquid theory
BCS theory

Singularity (pole) of self-energy

1-electron Green's function

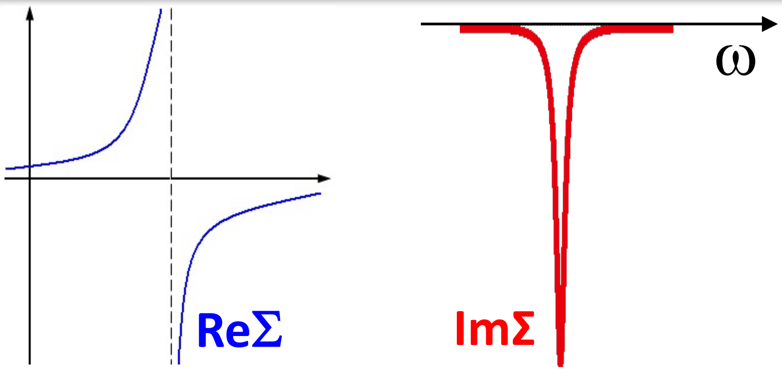
$$G(\mathbf{k},\omega) = \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)}$$

ω dependence is a key.

$\Sigma(\mathbf{k},\omega)=\infty$ ⇔ $G(\mathbf{k},\omega)=0$, $A(\mathbf{k},\omega)=0$ ⇔ *No electron at* $(\mathbf{k},\omega)$ *i.e., gap.*

(in normal state)

$$\Sigma \sim \frac{1}{\omega - p}$$



Need to go beyond one-particle & perturbative theories

Numerical simulations can

go beyond [**Band theory** / **Fermi-liquid theory** / **BCS theory**]

<u>Cluster dynamical mean-field theory</u>

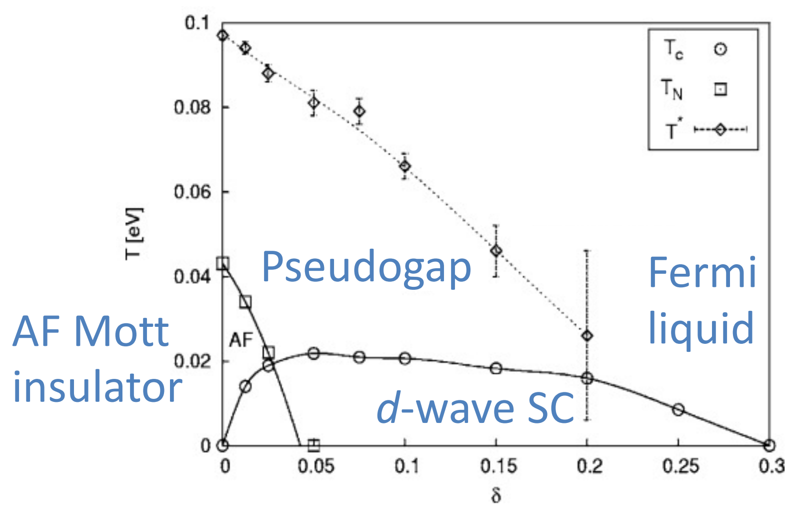
[Hettler *et al*., PRB'98; Kotliar *et al*., PRL'01]

- Capable to describe
  the singularity of Σ
- *Full* short-range correlations
  - Unbiased

- Indeed reproduces cuprates' phase diagram!

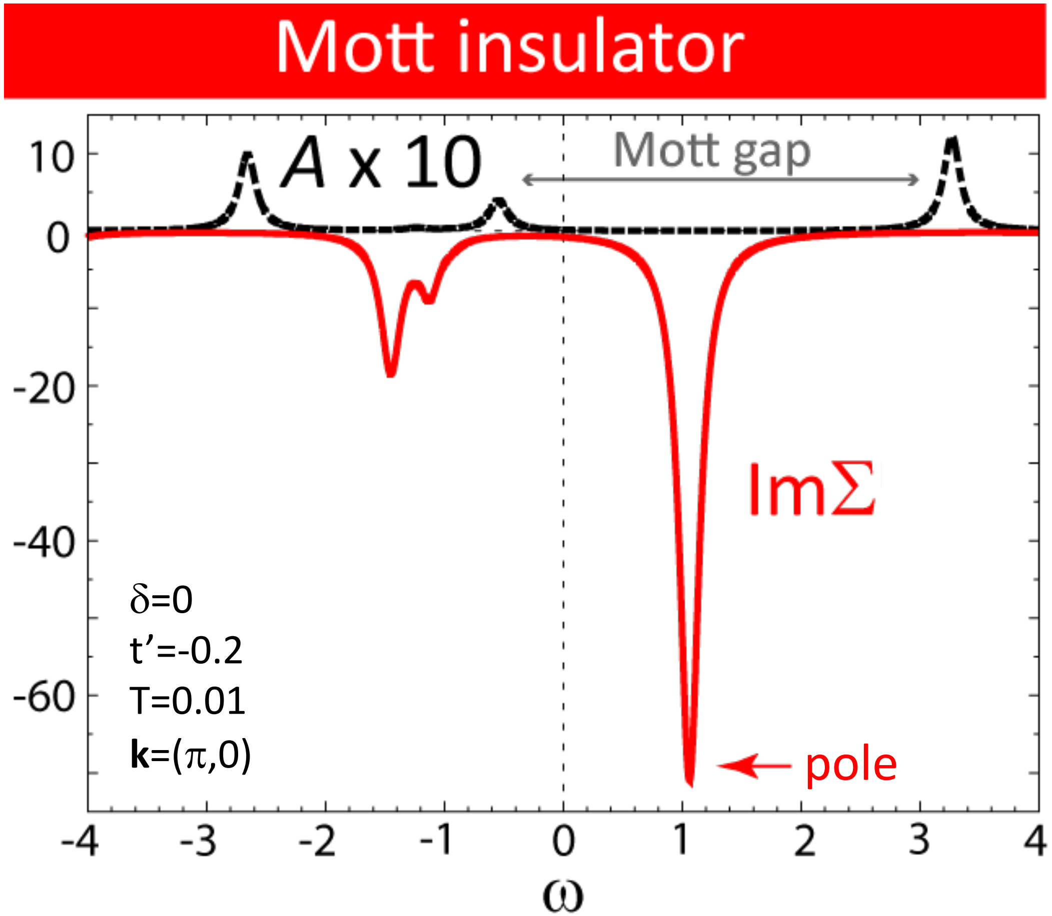
Sordi *et al*., PRL'12; Gull *et al*., PRL'13; …

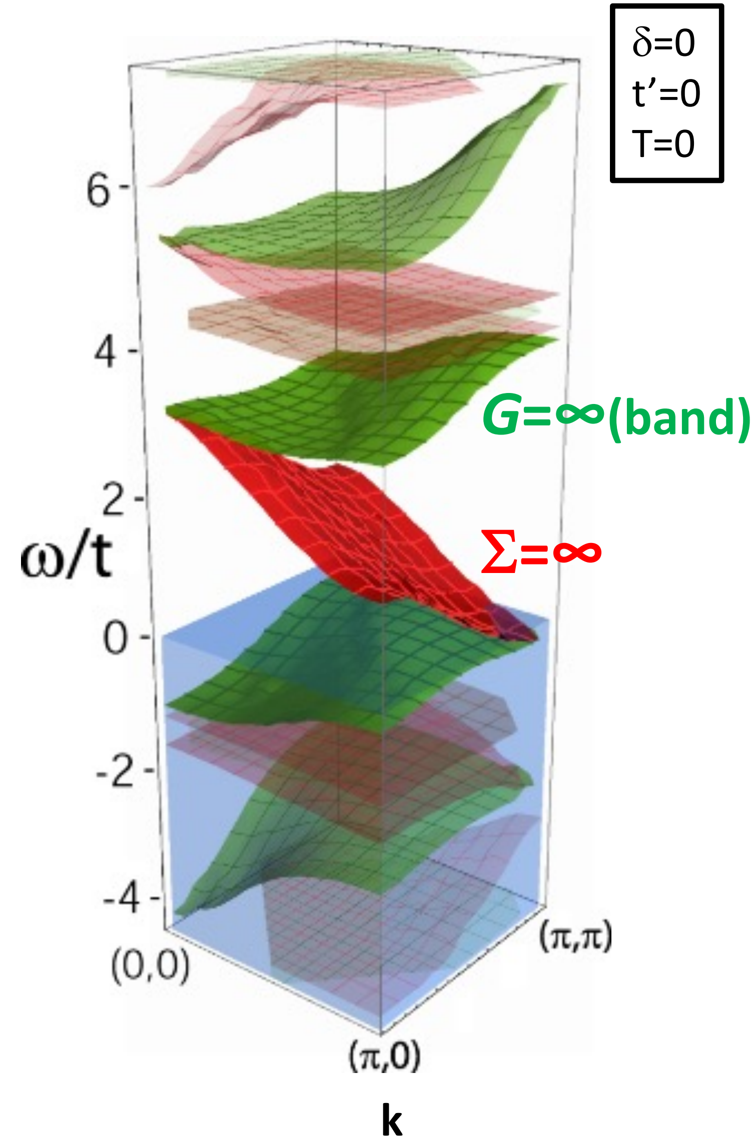
2D Hubbard model



[Maier *et al*., RMP'05]

Self-energy pole generating the Mott gap





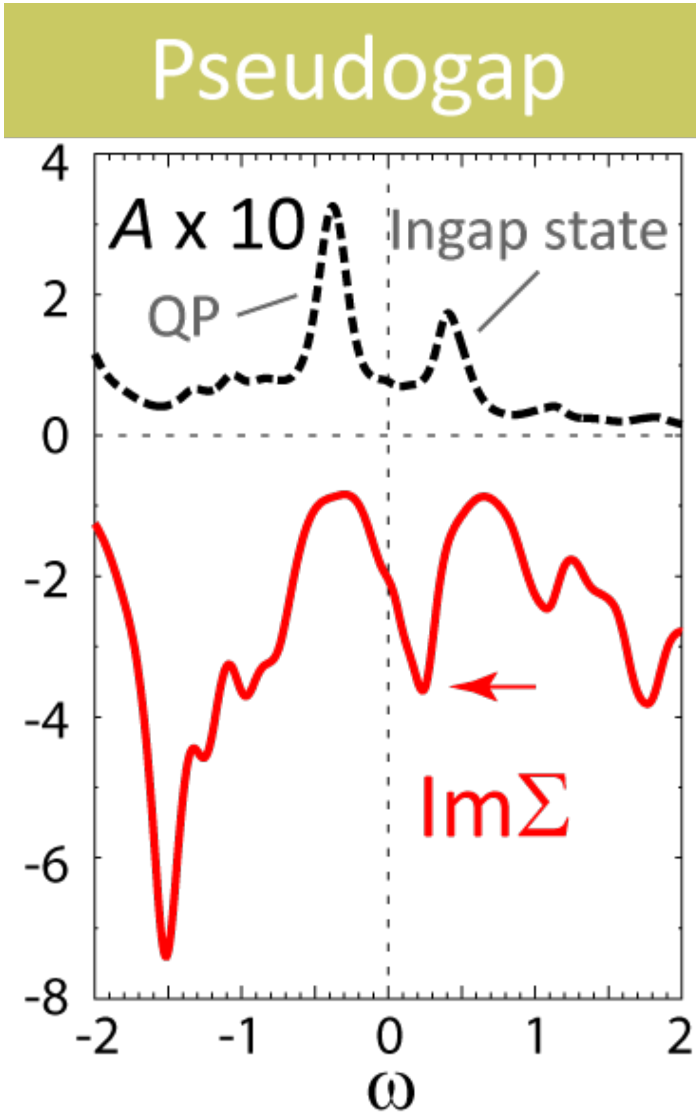
SS, Y. Motome and M. Imada, PRL**102**, 056404 (2009).

CDMFT for 2D Hubbard *t*=1 & *U*=8

$$A = -\frac{1}{\pi}\mathrm{Im}G$$

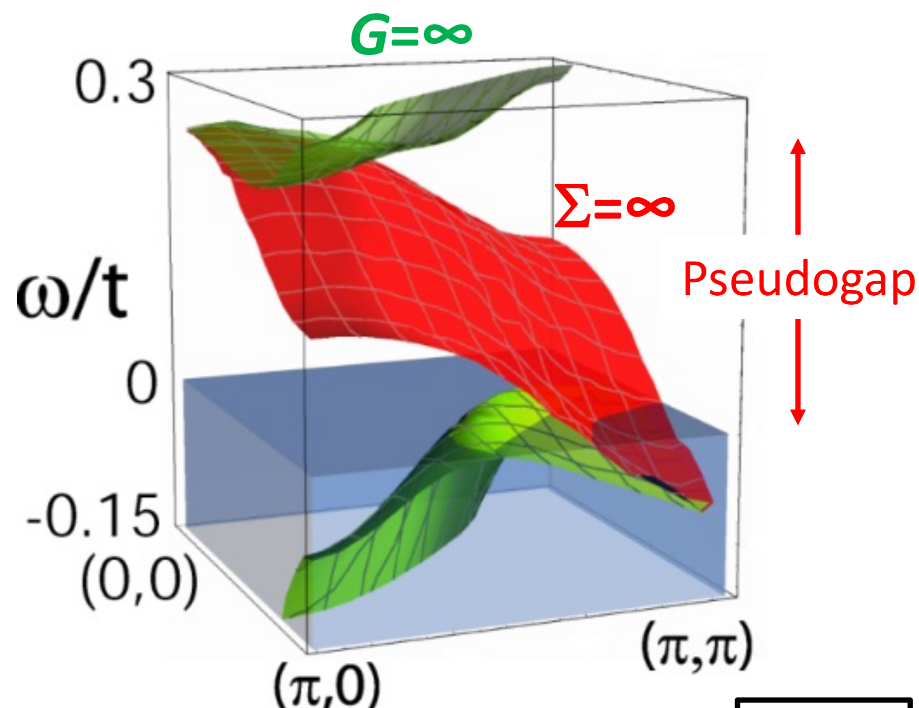
$$G = \frac{1}{\omega - \varepsilon_k - \Sigma}$$

Self-energy pole generating the pseudogap



δ=0.05
t'=-0.2
T=0.06
k=(π,0)

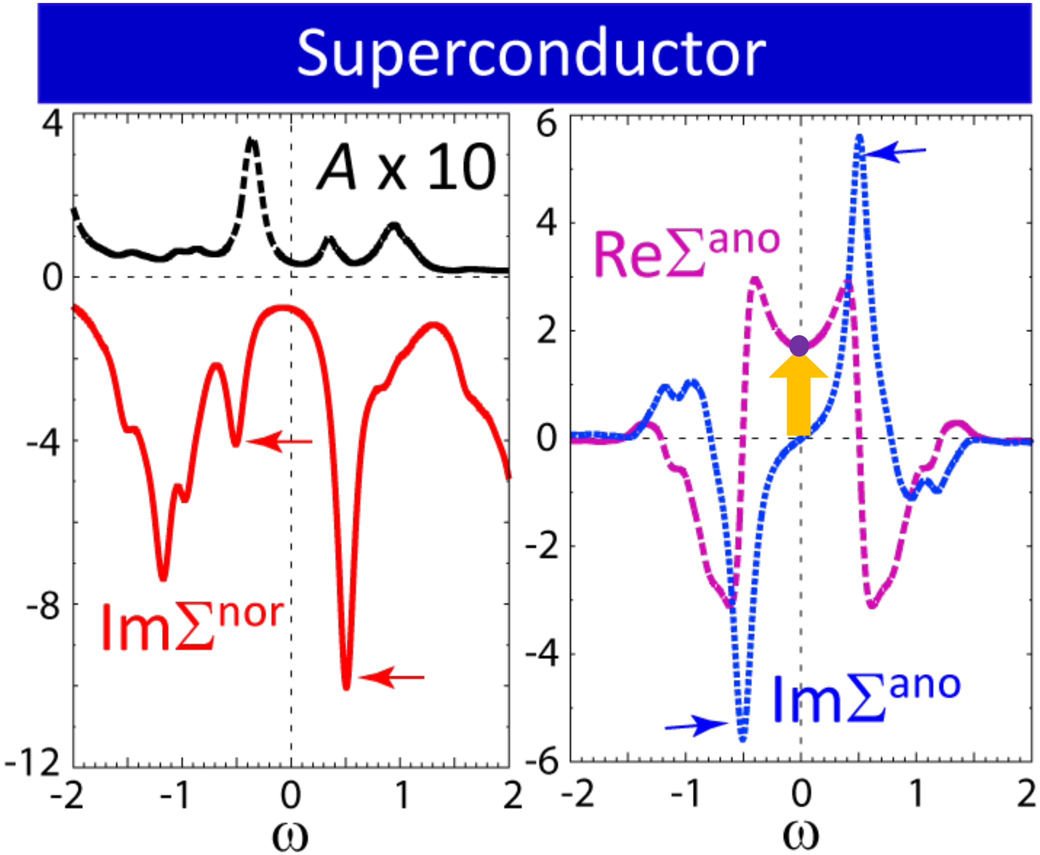
Normal-state solution at *T*=0



δ=0.09
t'=0
T=0

SS, Y. Motome and M. Imada, PRL**102**, 056404 (2009).

Self-energy pole making the SC "high-T_c"



δ=0.05
t'=-0.2
T=0.01
k=(π,0)

$$\hat{\Sigma} = \begin{pmatrix} \Sigma^{\mathrm{nor}} & \Sigma^{\mathrm{ano}} \\ \Sigma^{\mathrm{ano}} & -\Sigma^{\mathrm{nor}}(-\omega)^* \end{pmatrix}$$

Both Σ^{nor} and Σ^{ano} have poles at the same ω.

$$\mathrm{Re}\Sigma^{\mathrm{ano}}(\mathbf{k}, \omega = 0) = \frac{2}{\pi}\int_0^\infty \frac{\mathrm{Im}\Sigma^{\mathrm{ano}}(\mathbf{k}, \omega')}{\omega'} d\omega'$$ (Kramers-Kronig relation)

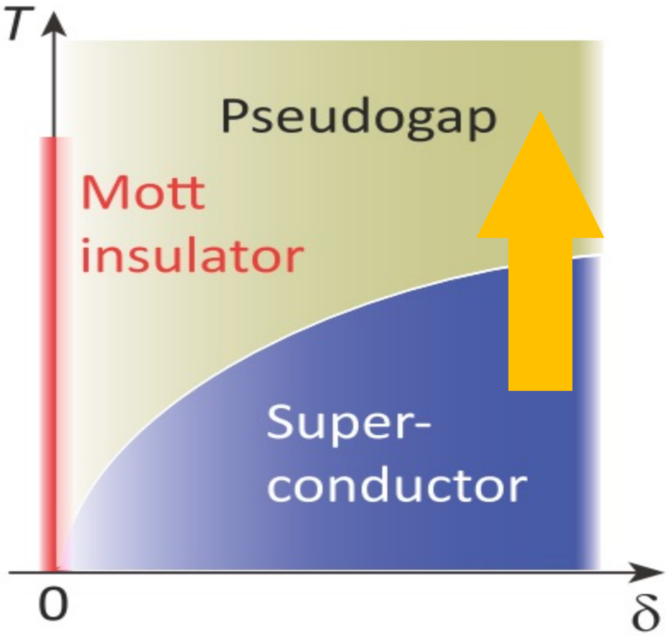
The peak of $\mathrm{Im}\Sigma^{\mathrm{ano}}$ enhances $\mathrm{Re}\Sigma^{\mathrm{ano}}(\omega=0)$ (～gap) by 5-10 times.

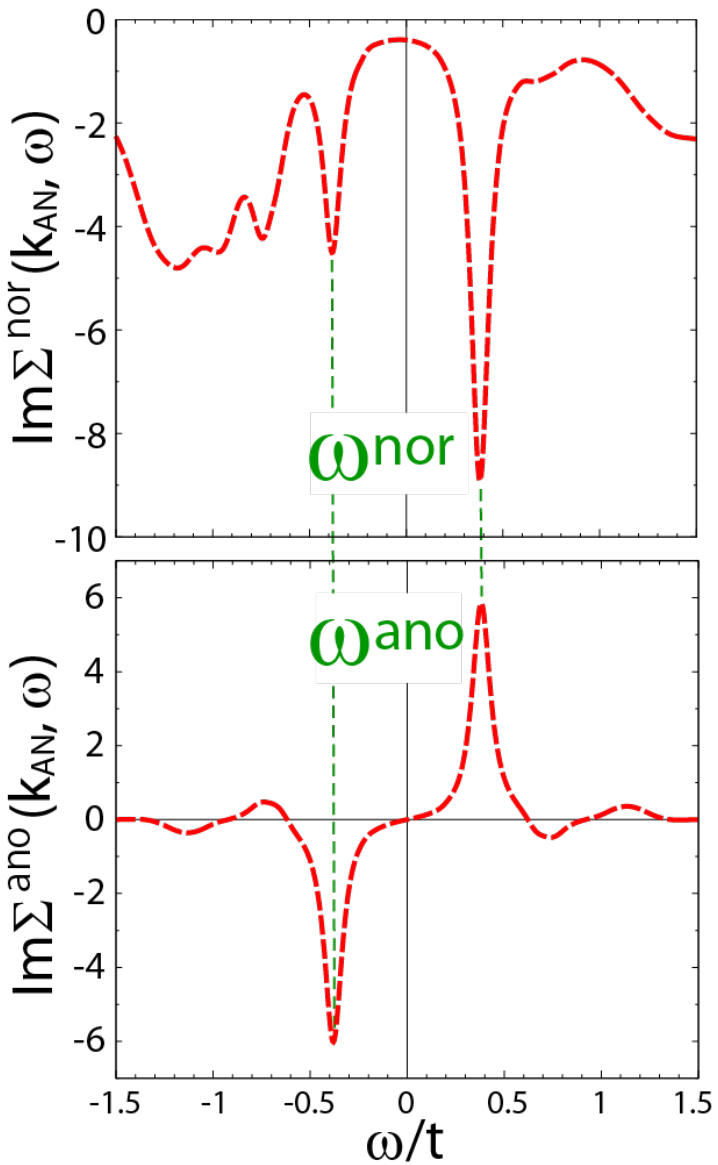
→ Origin of high T_c

[Maier *et al.*, PRL **100**, 237001 (2008)]

Poles of SC and PG are continuously connected!

SS, M. Civelli and M. Imada, PRL **116**, 057003 (2016)





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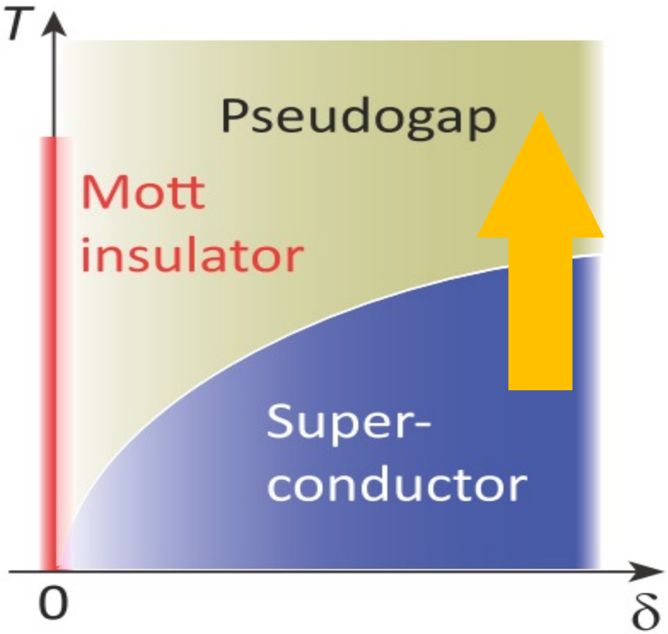

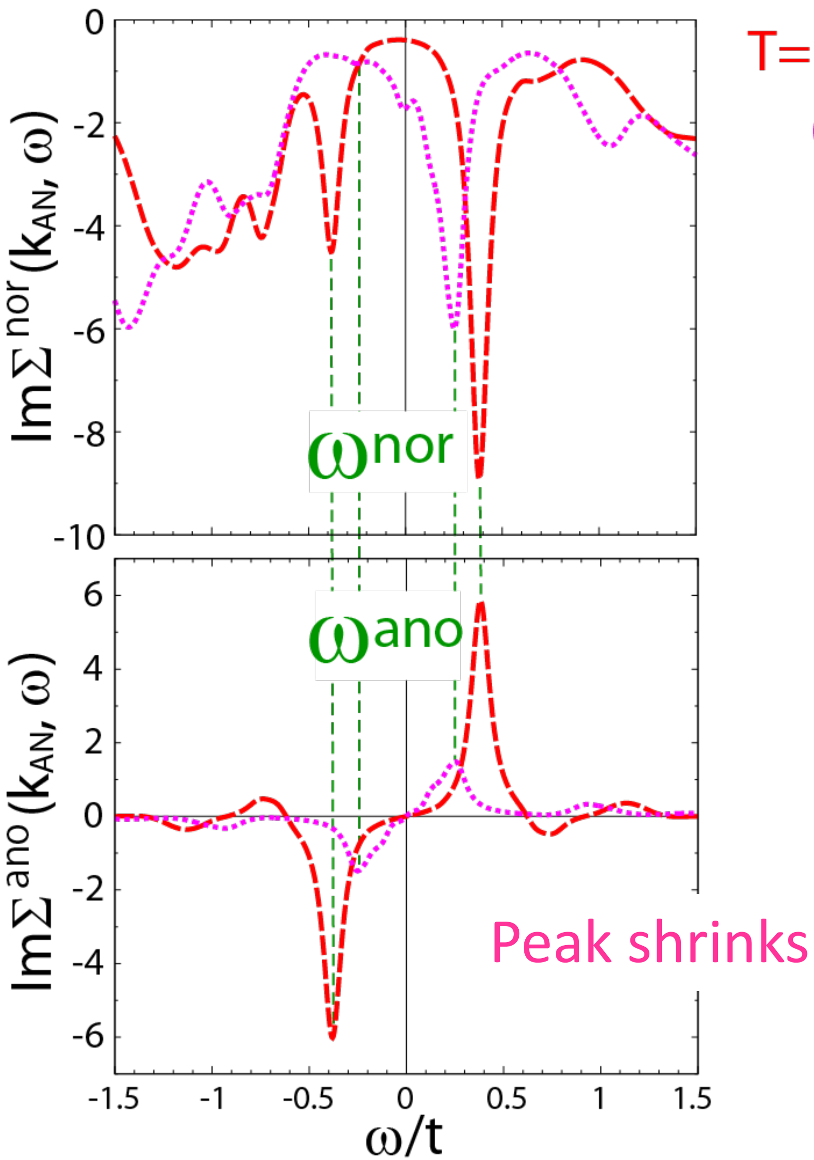

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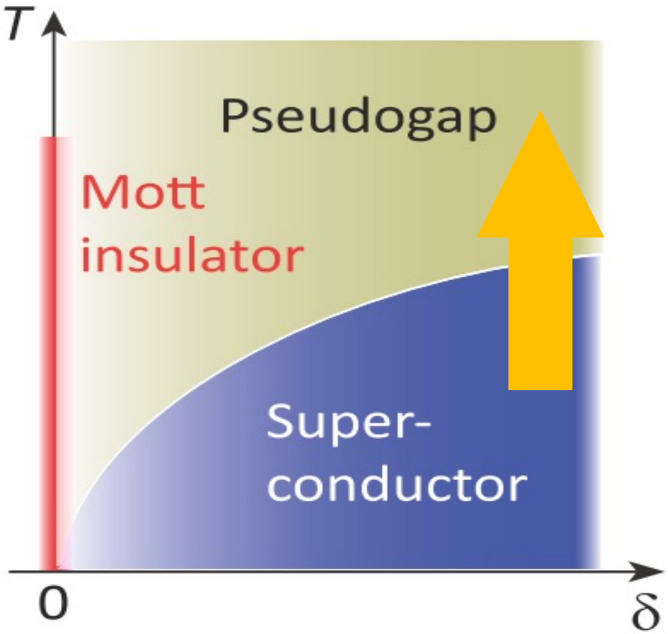
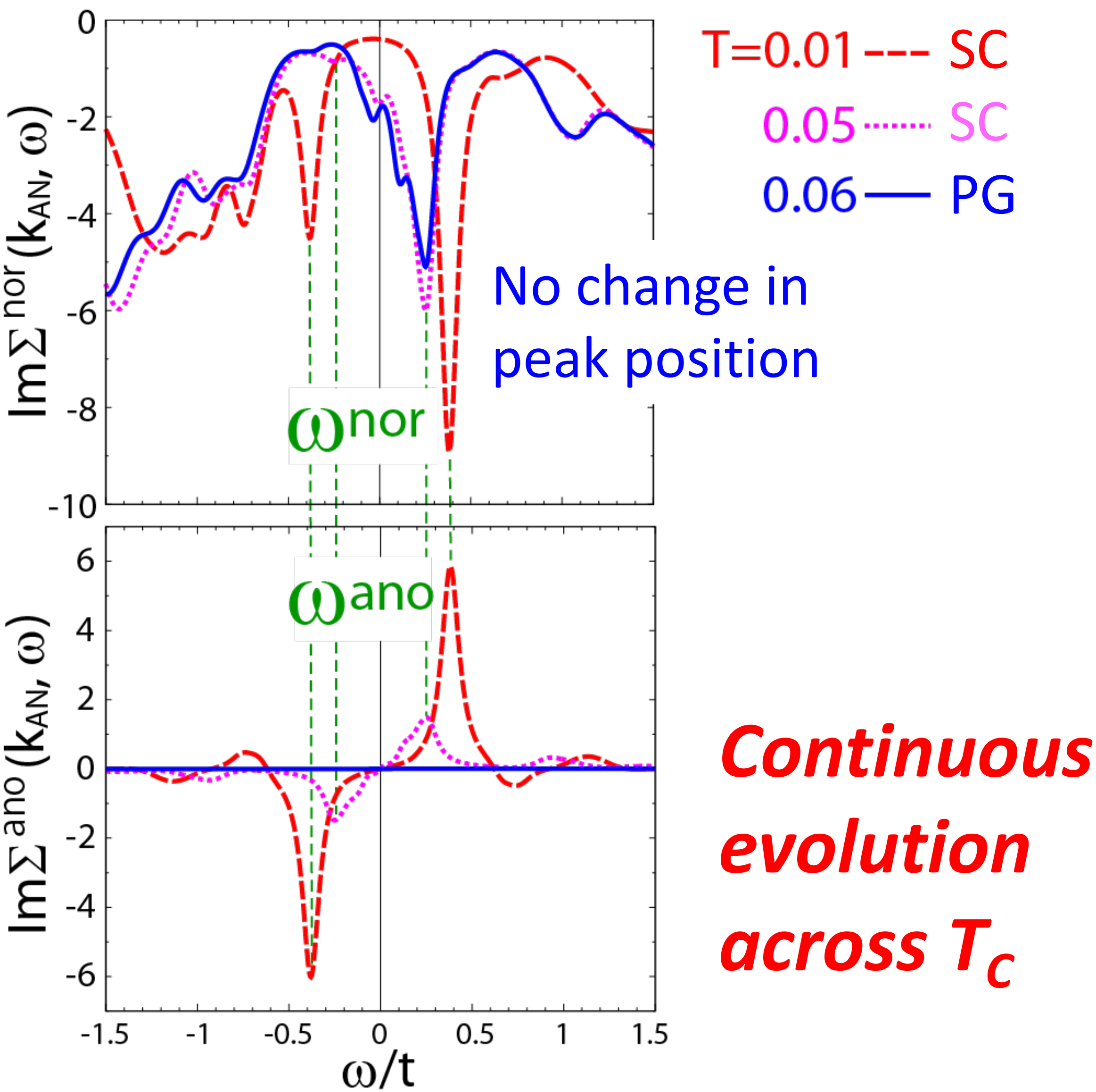
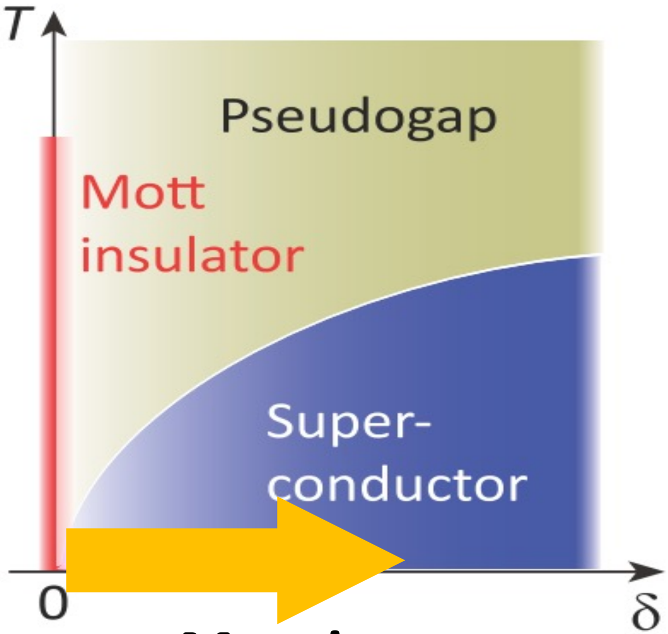




Poles of SC and MI are continuously connected!

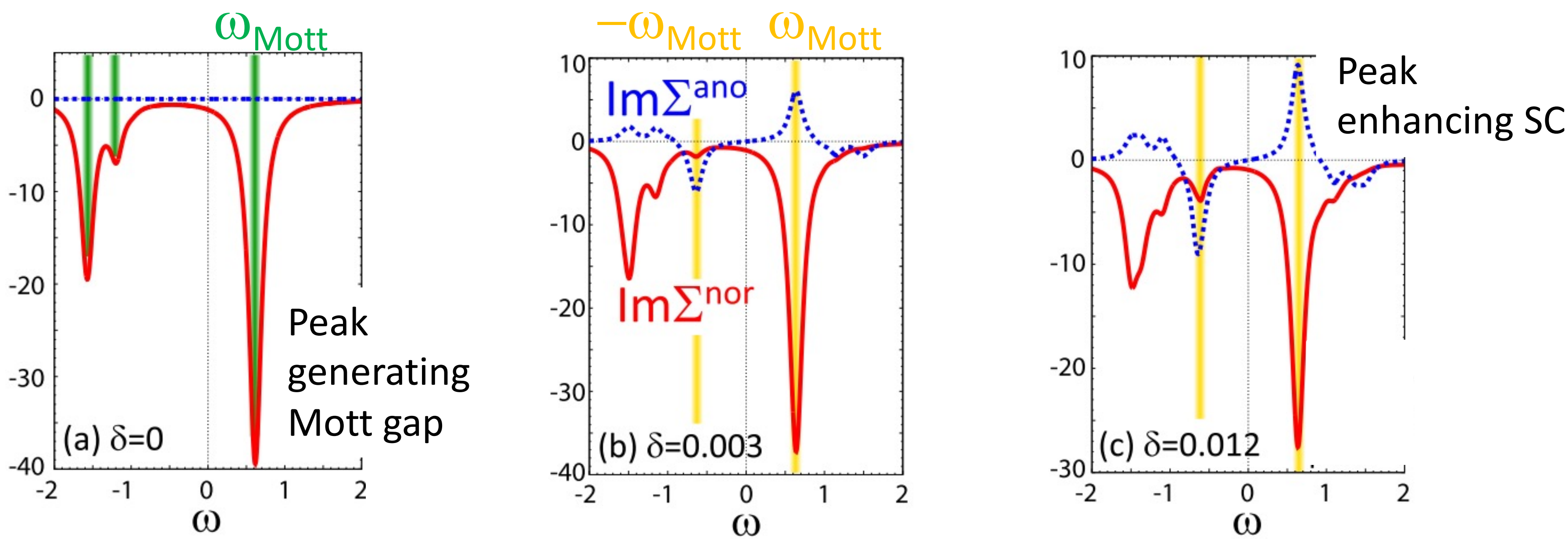
SS, M. Civelli and M. Imada, PRB **98**, 195109 (2018)

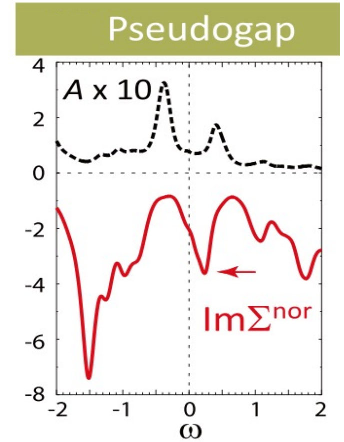


Continuous evolution with doping

- Peak enhancing SC emerges at ω_{Mott} , which characterizes the Mott gap.

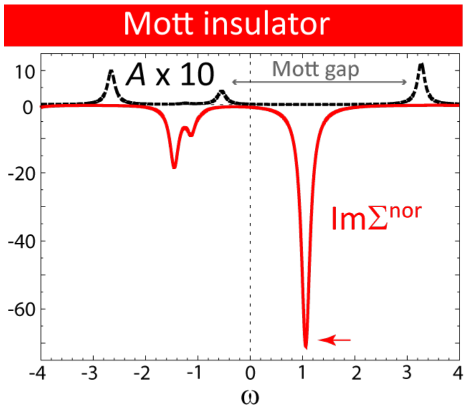
Mott ins. **SC** **SC**



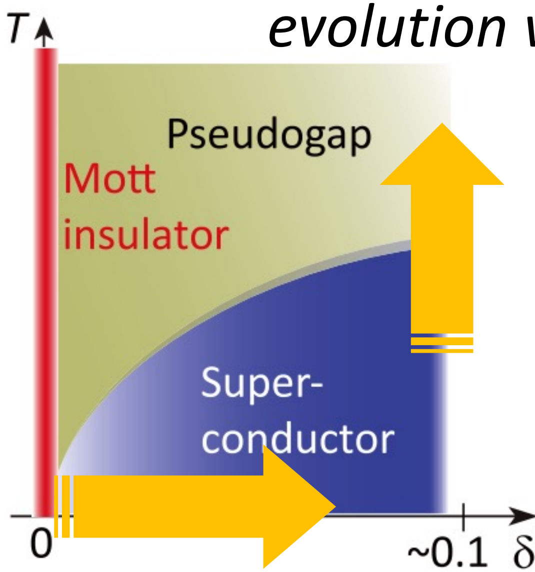


Generating pseudogap

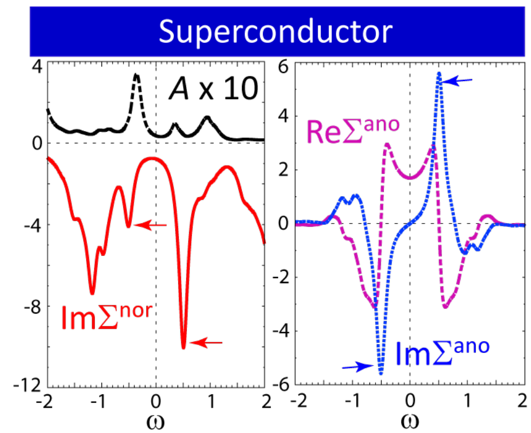
Continuous evolution with T



Generating Mott gap



Continuous evolution with δ



Enhancing T_c

These poles are essentially the same!

- ***Mott physics yields high-T_c SC and pseudogap.***
- ***Relation between high-T_c SC and pseudogap.***

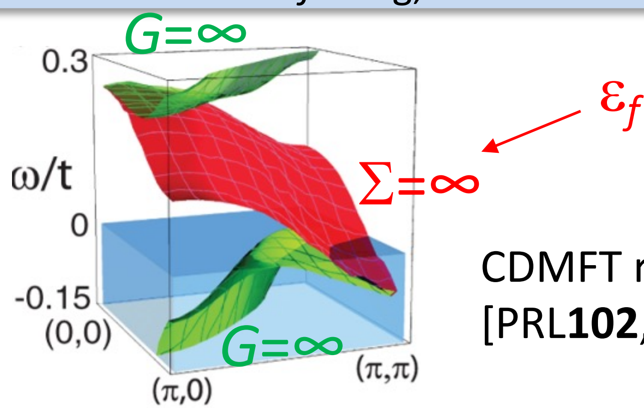
What does the self-energy pole mean?

Self-energy pole = Hidden Fermion

In Mott-insulating or pseudogap state,

$$\Sigma^{\mathrm{nor}}(\mathbf{k},\omega) \simeq \frac{V(\mathbf{k})^2}{\omega - \varepsilon_f(\mathbf{k})} \qquad \omega \to \omega + i\eta \qquad (1)$$

cf. Yang, Rice and Zhang, PRB 73, 174501 (2006)



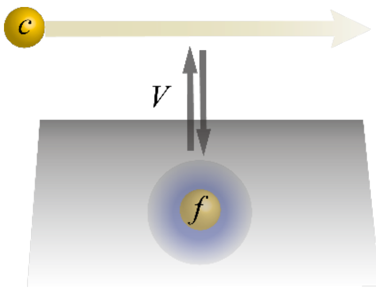
CDMFT result for Hubbard model
[PRL**102**, 056404 (2009)]

Phenomenological model:

$$H = \sum_{\mathbf{k}\sigma} \left[\varepsilon_c(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \varepsilon_f(\mathbf{k}) f^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + V (c^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + f^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}) \right]$$

c : Bare electron

f : Hidden fermion (emergent from strong correlation)



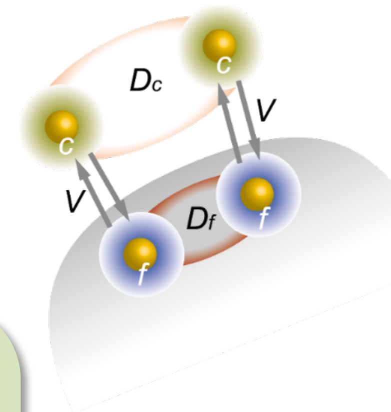
Integrating out f → Eq. (1)

Self-energy pole = Hidden Fermion

Extension of the model to SC state:

$$H = \sum_{\mathbf{k}\sigma} \left[\varepsilon_c(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \varepsilon_f(\mathbf{k}) f^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + V (c^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + f^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}) \right]$$

$$- \sum_{\mathbf{k}} \left[D_c(\mathbf{k}) c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} + D_f(\mathbf{k}) f_{\mathbf{k}\uparrow} f_{-\mathbf{k}\downarrow} + \text{h.c.} \right]$$



Integrating out *f*

$$\frac{1}{Z^{\text{eff}}} \exp(-S^{\text{eff}}[c^\dagger, c]) = \frac{1}{Z} \int \mathcal{D}f^\dagger \mathcal{D}f \exp(-S[c^\dagger, c, f^\dagger, f])$$

$$\Sigma^{\text{nor}}(\mathbf{k},\omega) = \frac{V(\mathbf{k})^2(\omega + \varepsilon_f(\mathbf{k}))}{\omega^2 - \varepsilon_f(\mathbf{k})^2 - D_f(\mathbf{k})^2}$$

$$\Sigma^{\text{ano}}(\mathbf{k},\omega) = D_c(\mathbf{k}) - \frac{V(\mathbf{k})^2 D_f(\mathbf{k})}{\omega^2 - \varepsilon_f(\mathbf{k})^2 - D_f(\mathbf{k})^2}$$

Self-energy pole = Hidden Fermion

Extension of the model to SC state:

$$H = \sum_{\mathbf{k}\sigma} \left[\varepsilon_c(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \varepsilon_f(\mathbf{k}) f^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + V (c^\dagger_{\mathbf{k}\sigma} f_{\mathbf{k}\sigma} + f^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}) \right]$$

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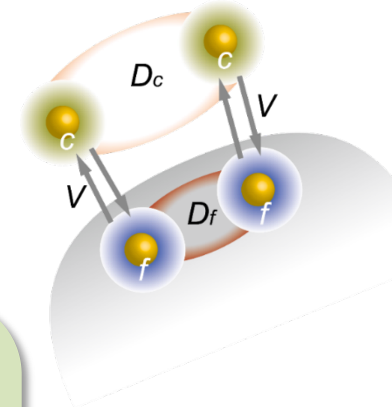

Integrating out *f*

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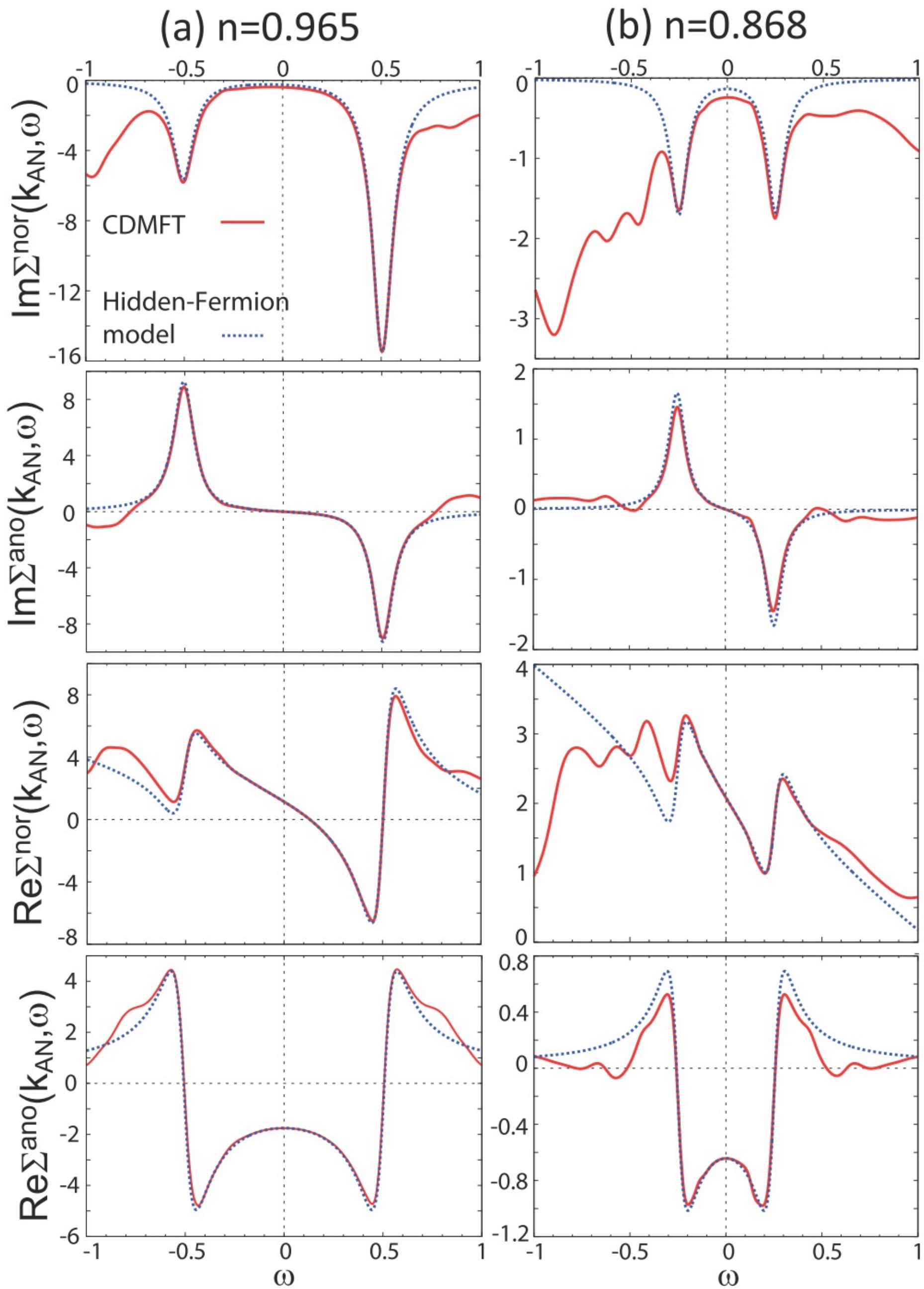
$$\Sigma^{\mathrm{ano}}(\mathbf{k}, \omega) = D_c(\mathbf{k}) - \frac{V(\mathbf{k})^2 D_f(\mathbf{k})}{\omega^2 - \varepsilon_f(\mathbf{k})^2 - D_f(\mathbf{k})^2}$$

← Poles due to D_f

Poles at the same ω's, in consistency with CDMFT.

Fitting of low-energy part of self-energy

U=8t
t'=-0.2t
T=0.01
$\mathbf{k}=\mathbf{k}_{AN}=(\pi,0)$



SS, M. Civelli and M. Imada, PRB **94**, 115130 (2016)

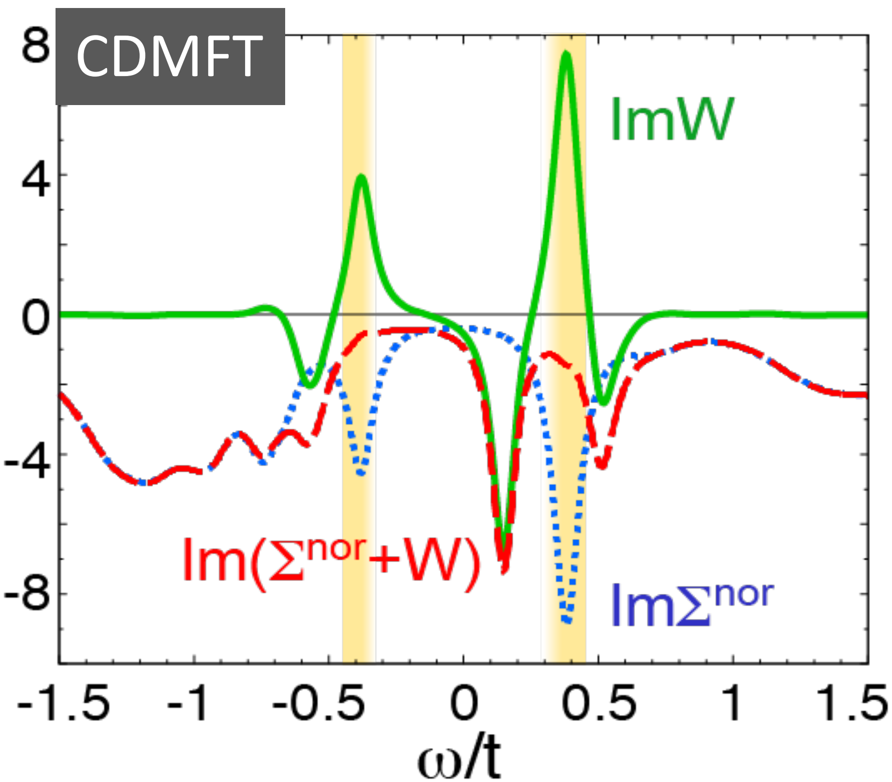
Low-energy part is well fitted by hidden-fermion model.

Pole-to-pole cancellation in *G*

SS, M. Civelli and M. Imada, PRL **116**, 057003 (2016)

$$G(\mathbf{k},\omega)=\left[\omega+\mu-\varepsilon_{\mathbf{k}}-\Sigma^{\mathrm{nor}}(\mathbf{k},\omega)-W(\mathbf{k},\omega)\right]^{-1}$$

$$W(\mathbf{k},\omega)=\frac{\Sigma^{\mathrm{ano}}(\mathbf{k},\omega)^2}{\omega-\mu+\varepsilon_{\mathbf{k}}+\Sigma^{\mathrm{nor}}(\mathbf{k},-\omega)^*}$$



Σ^{nor} cancels with *W*

Residues at the poles in hidden-fermion model

$$\mathrm{Res}_{\Sigma^{\mathrm{nor}}}=\frac{V^2}{2}\left(1\pm\frac{\varepsilon_f}{\sqrt{\varepsilon_f^2+D_f^2}}\right)$$

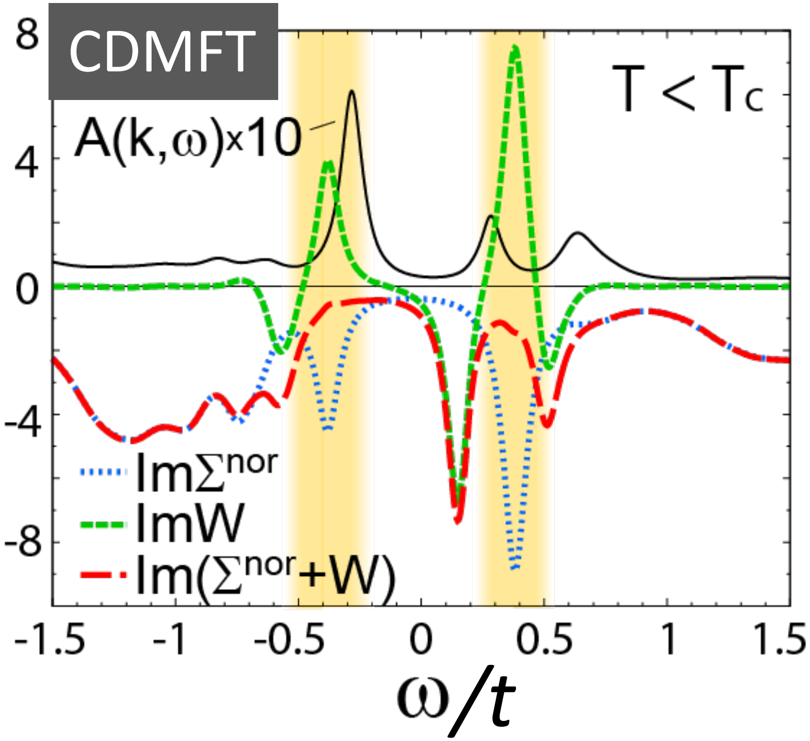
$$=-\mathrm{Res}_W$$

Fully consistent!

What do these results mean?

Pole-to-pole cancellation

SS, M. Civelli and M. Imada, PRL **116**, 057003 (2016)



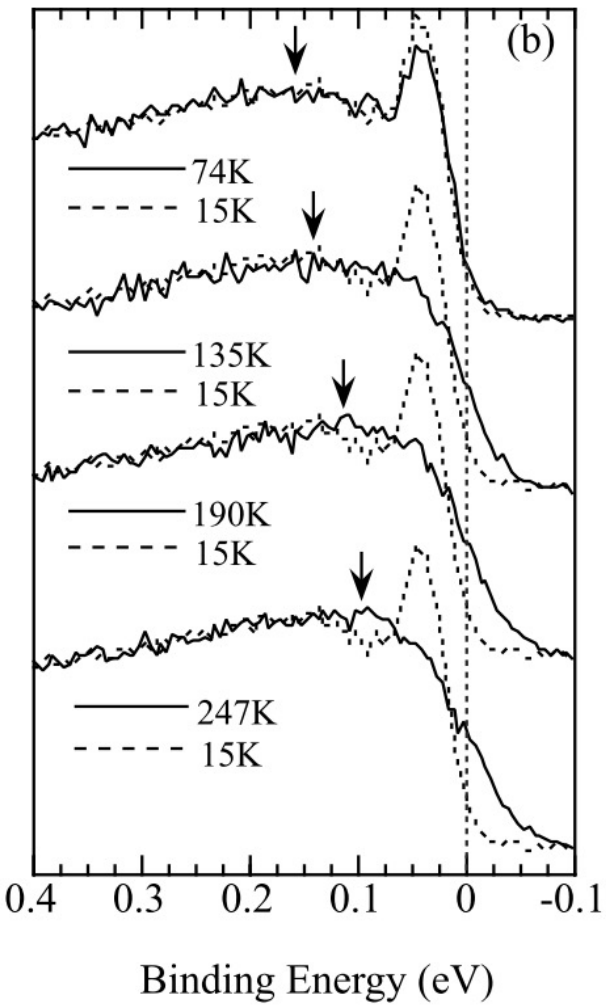
Σ^{nor} cancels with *W*

Self-energy peaks are invisible in *G* (and hence in spectra).

This explains why the self-energy peak has eluded an experimental detection.

Recently detected by ARPES+Machine learning! [Y. Yamaji *et al*., arXiv: 1903.08060]

Bogoliubov peak can emerge from broad spectra



ARPES for Bi2212, UD89K, **k**=(π,0)
Campuzano *et al*., PRL **83**, 3709 (1999)

How can a coherent Bogoliubov peak emerge from a broad spectrum lacking quasiparticles?

➡ Cancellation, i.e.,

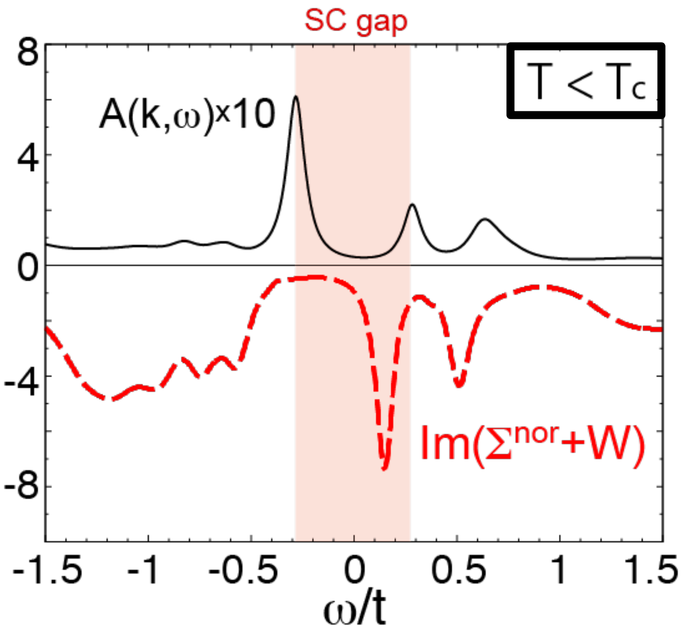
- ***T* > *T*c**
  Large ImΣ^{nor} → Pseudogap & broad spectra

- ***T* < *T*c**
  Σ^{nor} is canceled with *W*.
  → Sharp Bogoliubov peak.

Another consequence: Peak-dip-hump
[PRL **116**, 057003; PRL **116**, 197001 (2016)]

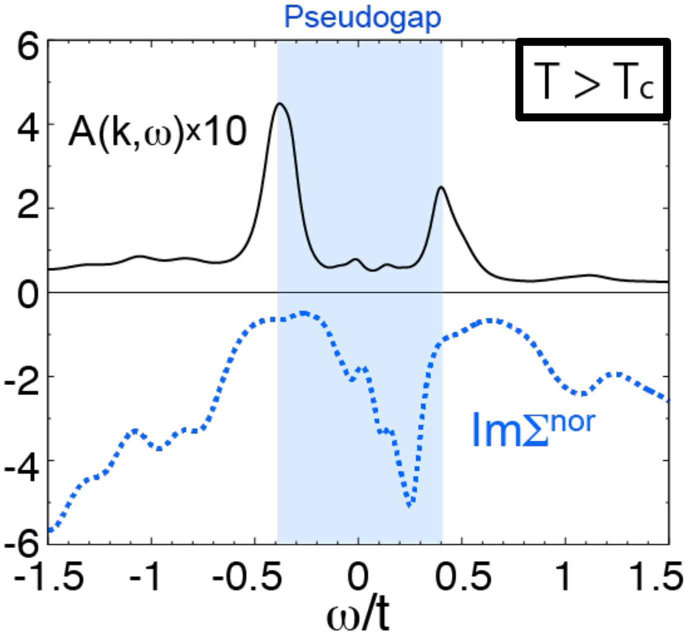
PG and SC gap involve different singularities

i.e., mathematically different!



$$G(\mathbf{k},\omega)=\left[\omega+\mu-\varepsilon_{\mathbf{k}}-\Sigma^{\mathrm{nor}}(\mathbf{k},\omega)-W(\mathbf{k},\omega)\right]^{-1}$$

$$W(\mathbf{k},\omega)=\frac{\Sigma^{\mathrm{ano}}(\mathbf{k},\omega)^2}{\omega-\mu+\varepsilon_{\mathbf{k}}+\Sigma^{\mathrm{nor}}(\mathbf{k},-\omega)^*}$$



SC state

Gap (G=0) ⟷

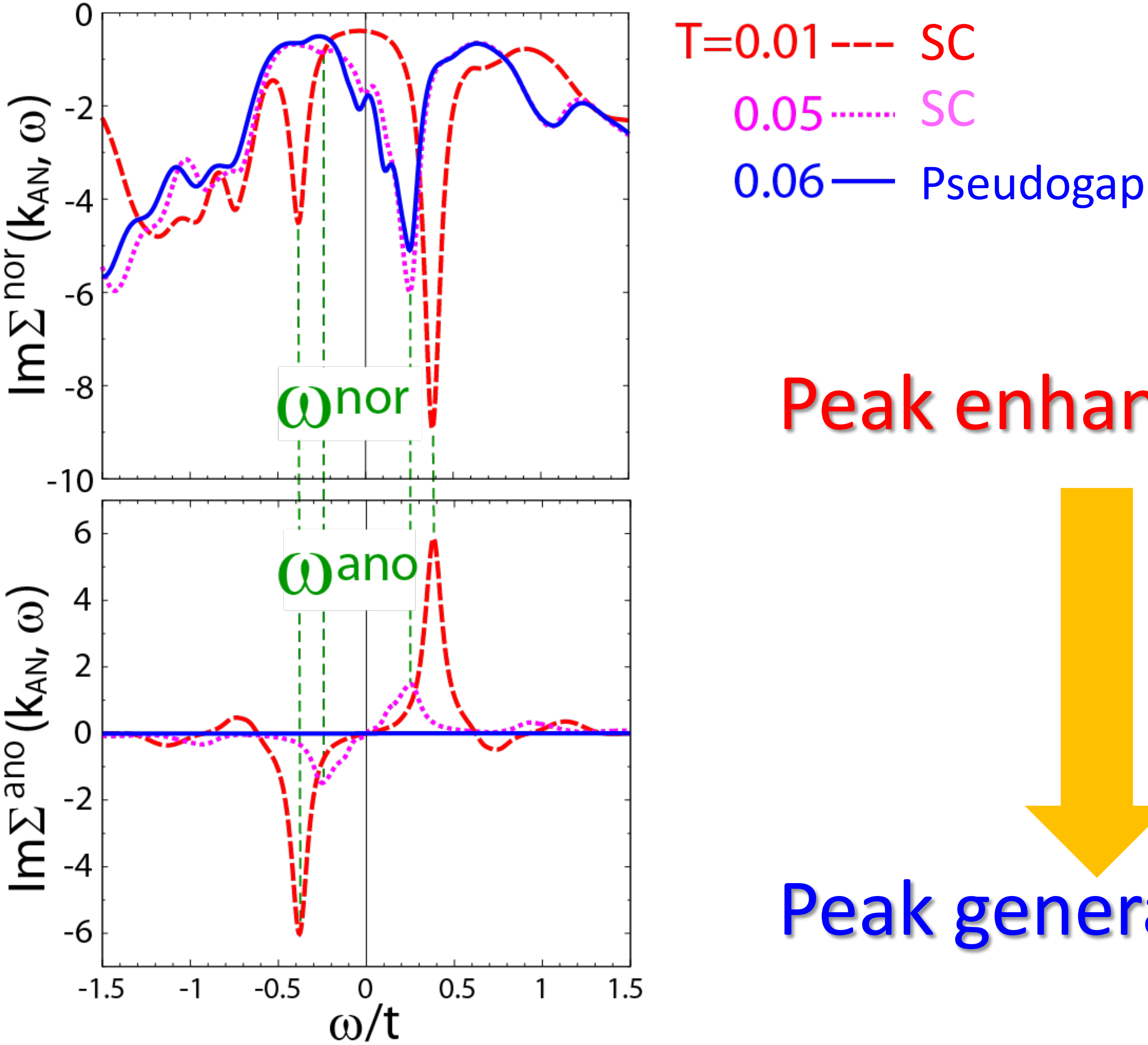
$\Sigma^{\mathrm{nor}}(\mathbf{k},\omega)=\infty$
or
$\Sigma^{\mathrm{ano}}(\mathbf{k},\omega)=\infty$
} *Cancelling!*
or
$\omega-\mu+\varepsilon_{\mathbf{k}}+\Sigma^{\mathrm{nor}}(\mathbf{k},-\omega)^*=0$ **SC gap**

Normal state

Σ^{ano}=W=0: No cancelation any more.

Gap (G=0) ⟷ $\Sigma^{\mathrm{nor}}(\mathbf{k},\omega)=\infty$ **Pseudogap**

However, the same hidden fermion is at the origin of both pseudogap and 'high T_c':



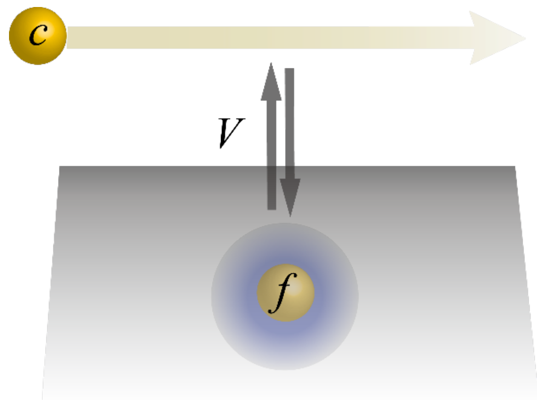
Peak enhancing SC

Continuous evolution with T

Peak generating PG

Unified understanding of pseudogap and high-T_c superconductivity

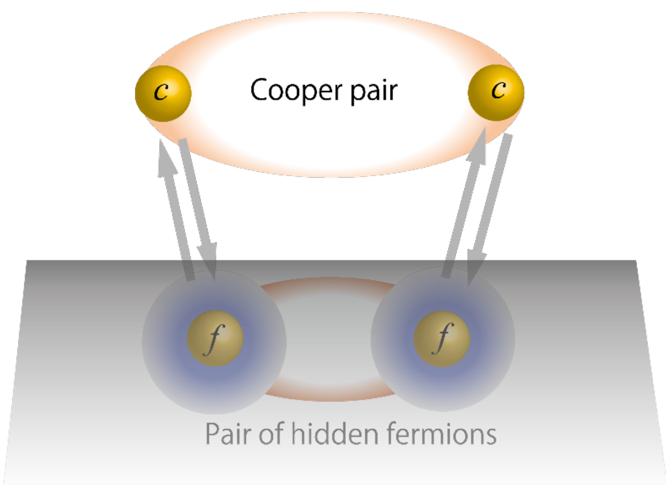
$T > T_c$



Pseudogap

= (Hybridization gap with f)

$T < T_c$



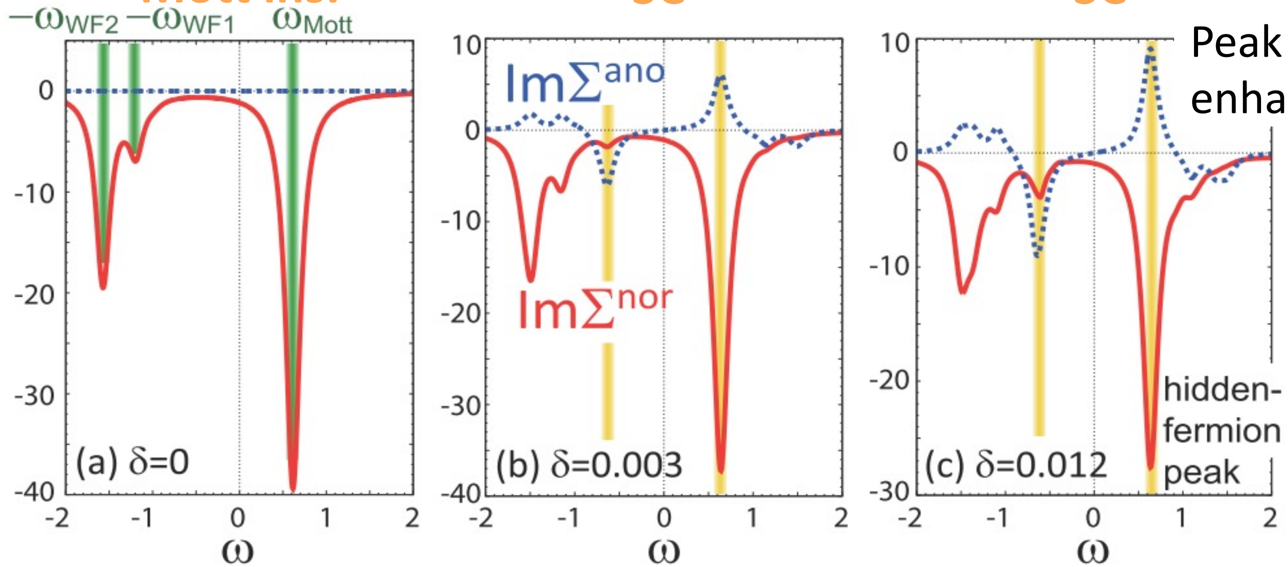
High-T_c SC

Hybridization with f

→ Pole of Σ^{ano} → High T_c

Fermionic high-T_c mechanism ⟷ Bosonic glue ("conventional")

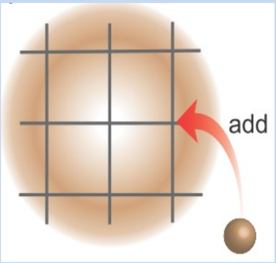
Origin of the hidden fermion *f* is in the Mott gap



Direct microscopic relation between MI and high-T_c SC.

Two different low-energy excitations in doped Mott insulators

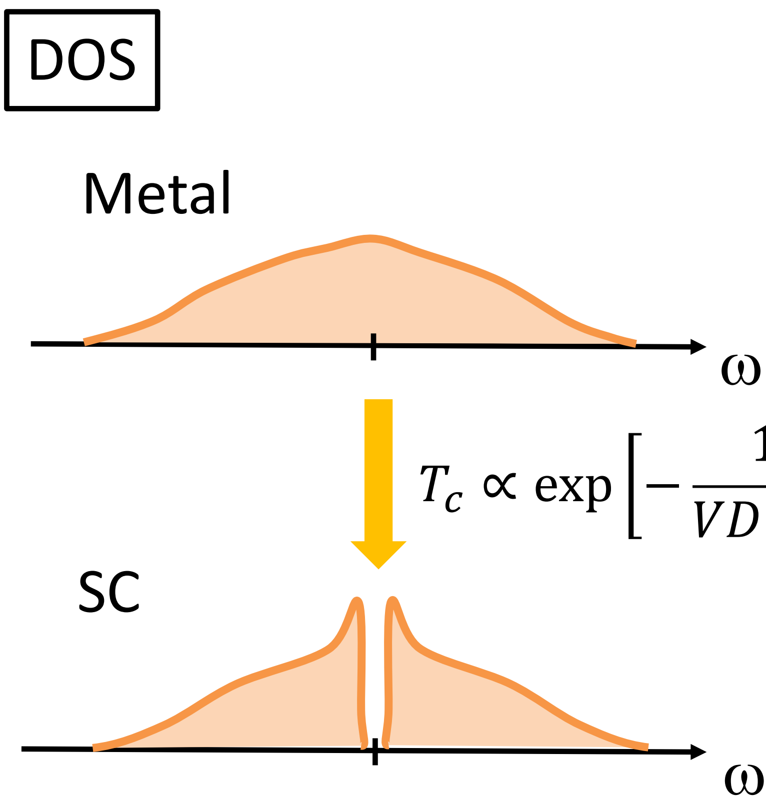
[Yamaji and Imada, PRL **106**, 016404 (2011)]



Electron
- Extended in space → Quasiparticle
- or
- Weakly bound to the hole → Hidden fermion

Conventional superconductor

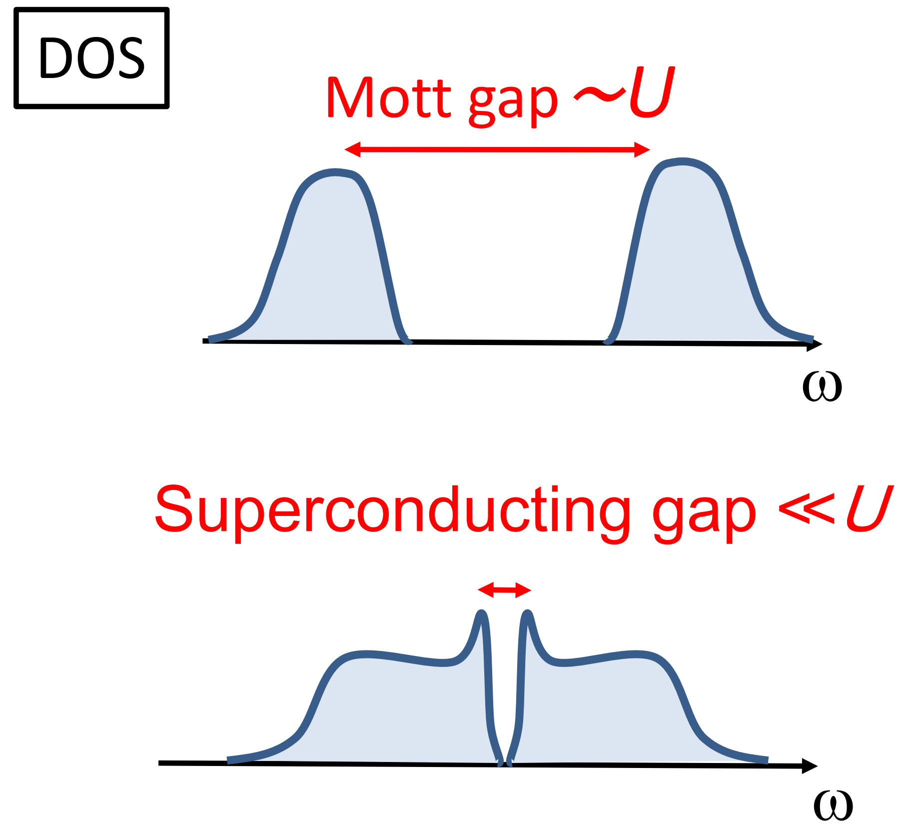
BCS theory tells a relation in the spectral function



$$T_c \propto \exp\left[-\frac{1}{VD(0)}\right]$$

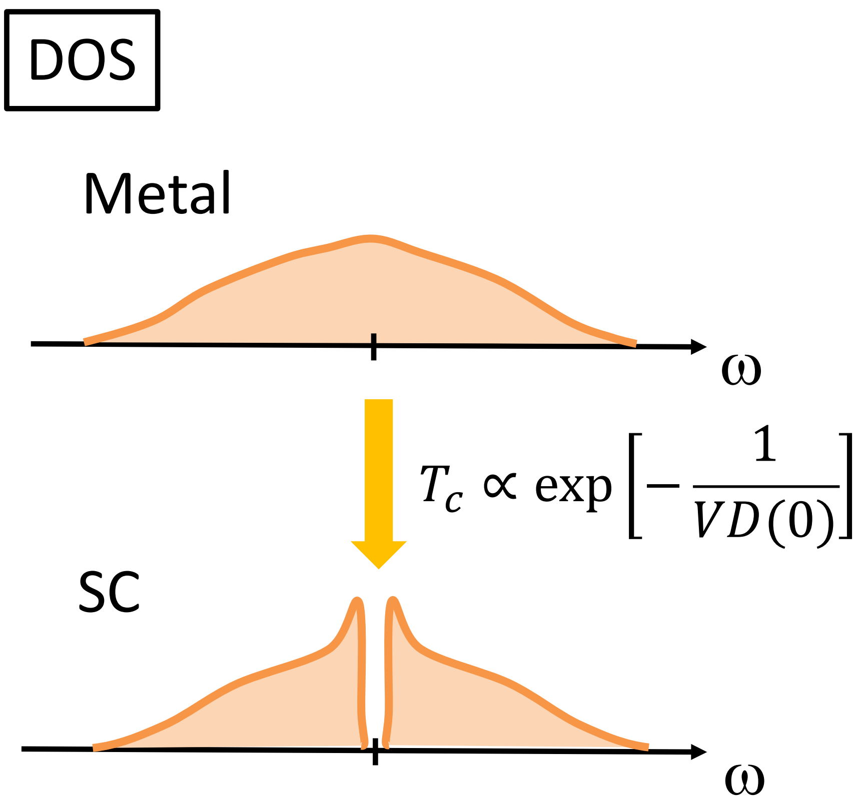
Strongly-correlated superconductor

Direct connection in spectra is hard to imagine.



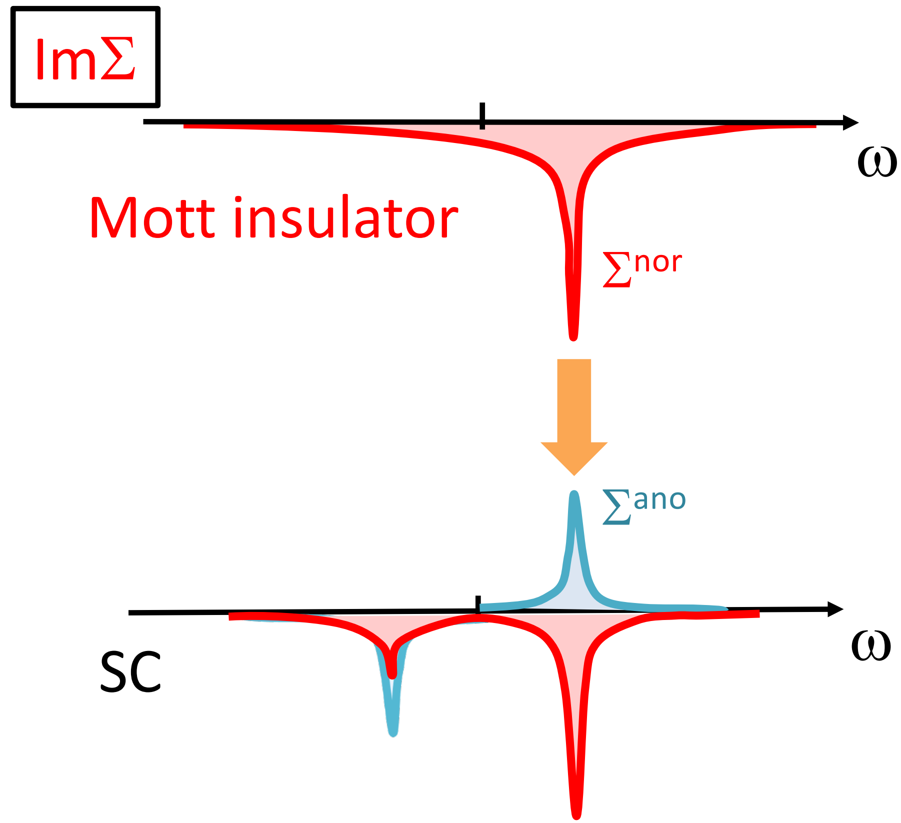
Conventional superconductor

BCS theory tells a relation in the spectral function



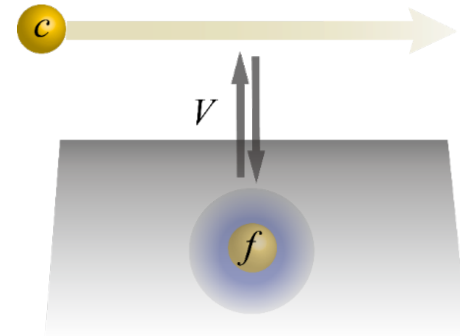
Strongly-correlated superconductor

We found a relation in the self-energy



Property of SC determined by *insulator*

Summary



Low-energy dynamics in MI, PG and SC states is governed by a self-energy pole (= hidden fermion)!

Pole of Σ^{nor} generates Mott gap

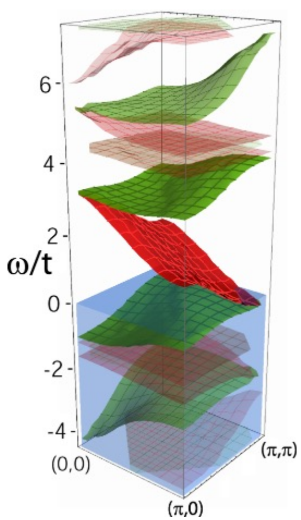
doping

Pole of Σ^{nor} generates PG

T

Σ^{ano} vanishes above T_c

Pole of Σ^{ano} enhances SC



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