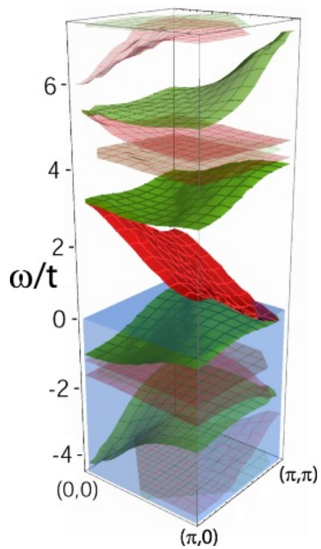
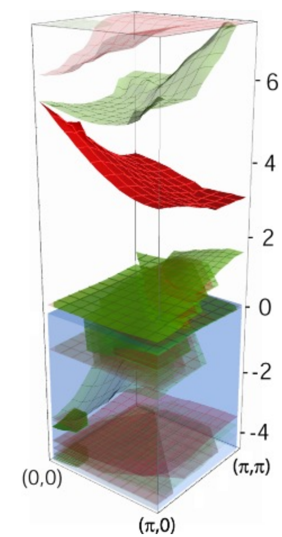
Poles and zeros of Green's function and its relevance to high-T_c cuprates

RIKEN Center for Emergent Matter Science

Shiro Sakai



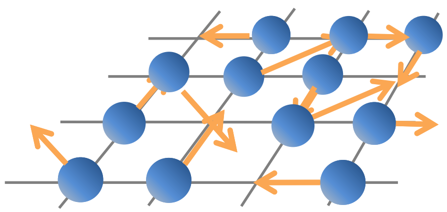


S.S, Y. Motome and M. Imada, PRL **102**, 056404 (2009); PRB **82**, 134505 (2010)

Strongly Correlated electron systems

Kinetic energy $K \sim$ Interaction energy I

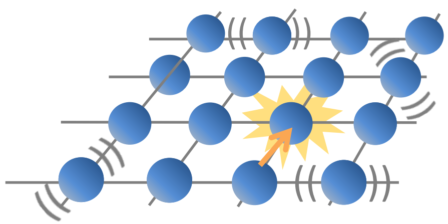
- $K >> I$



Metal (Fermi liquid)

Itinerancy

- $I >> K$

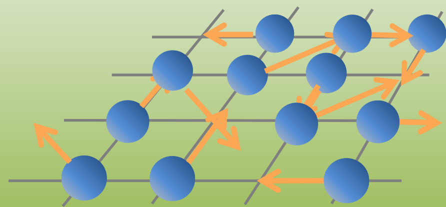


Mott insulator

Locality

Dual nature of strongly correlated electron

Itinerancy



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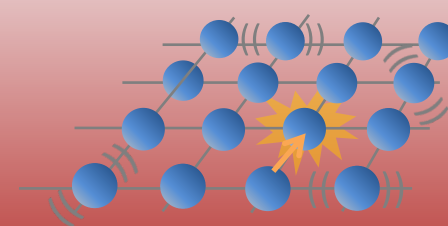


Mott insulator

Mean free path is

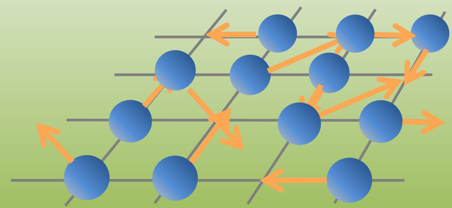
long / **short**

Effective mass is

light / **heavy**

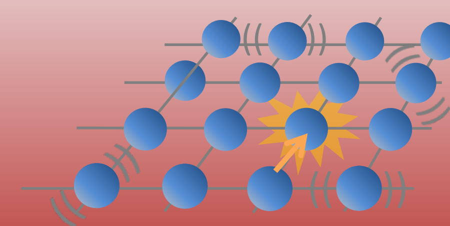
Dual nature of strongly correlated electron

Itinerancy



Metal (Fermi liquid)

Locality



Mott insulator

Mean free path is

long / **short**

Effective mass is

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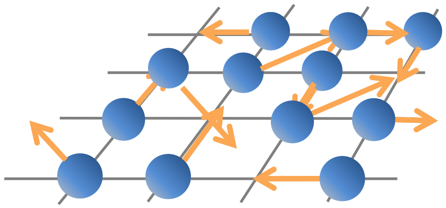
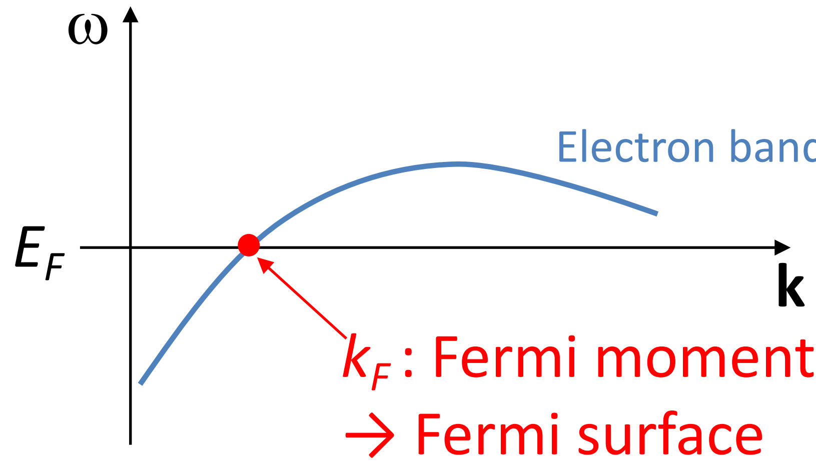
Any more fundamental and microscopic representation?

Microscopic representation of itinerancy



Metal (Fermi liquid)



Metal = (Existence of Fermi surface)
= (Band crosses E_F)

<u>Band</u>

Solution of quasiparticle eq. $\omega - \varepsilon_{\mathbf{k}} - \mathrm{Re}\Sigma(\mathbf{k},\omega)=0$: $\omega=\omega(\mathbf{k})$

Σ: self-energy

<u>Green's function</u>

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

ReG^{-1} → QP eq.

ImG^{-1} → 1/(lifetime of QP)

Itinerancy = (pole of G)

Itinerancy = (Existence of Fermi surface)

= (Band crosses E_F)

= ($\omega - \varepsilon_{\mathbf{k}} - \mathrm{Re}\Sigma = 0$ has a solution at $\omega = E_F$ & QP exists)

= ($^{\exists}\mathbf{k}$ s.t. $G(\mathbf{k}, E_F)^{-1} = 0$)

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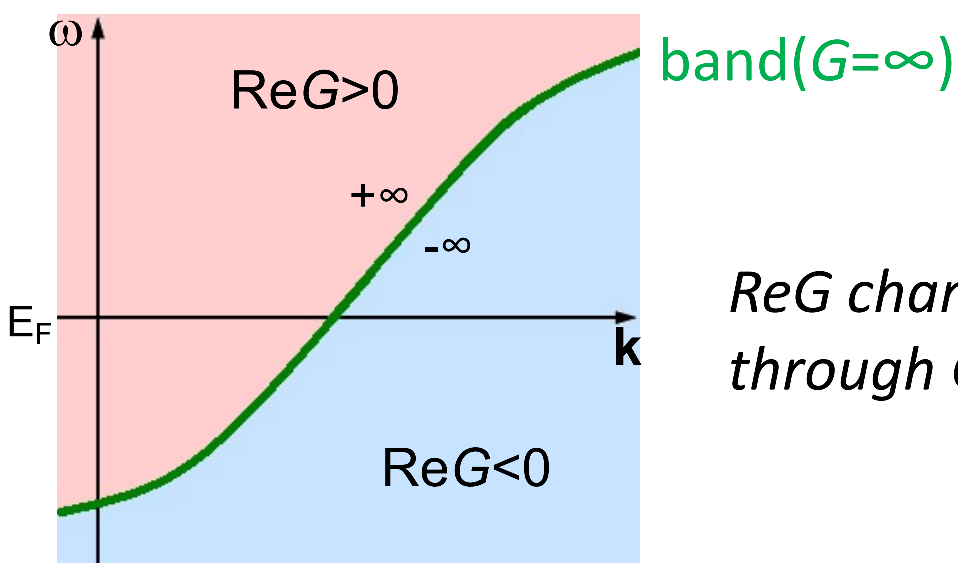
= ($\omega - \varepsilon_{\mathbf{k}} - \mathrm{Re}\Sigma = 0$ has a solution at $\omega = E_F$ & QP exists)

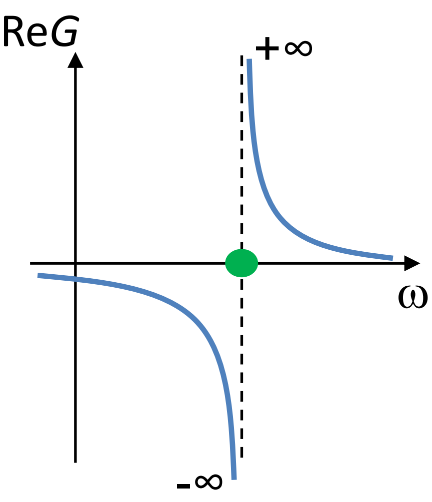
= ($^{\exists}\mathbf{k}$ s.t. $G(\mathbf{k}, E_F)^{-1} = 0$)

= (G has a pole at $\omega = E_F$)

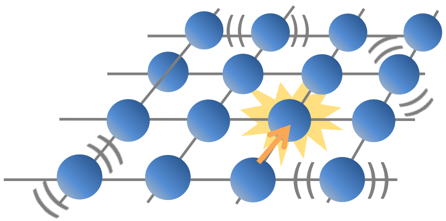


ReG changes sign through G=∞!

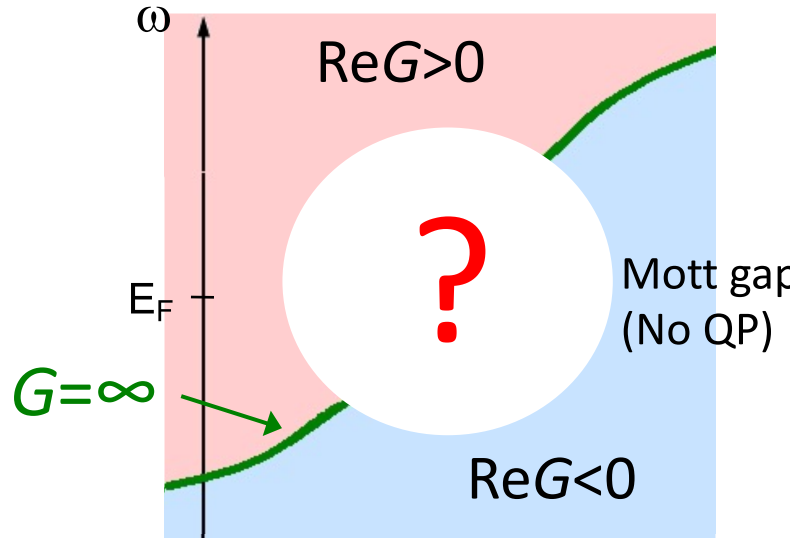
At fixed k



Locality = (pole of Σ)



Mott insulator

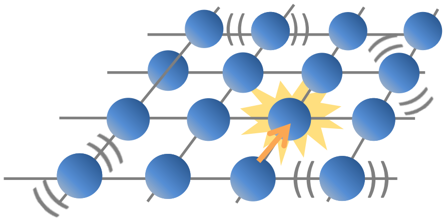


$$G = \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma}$$

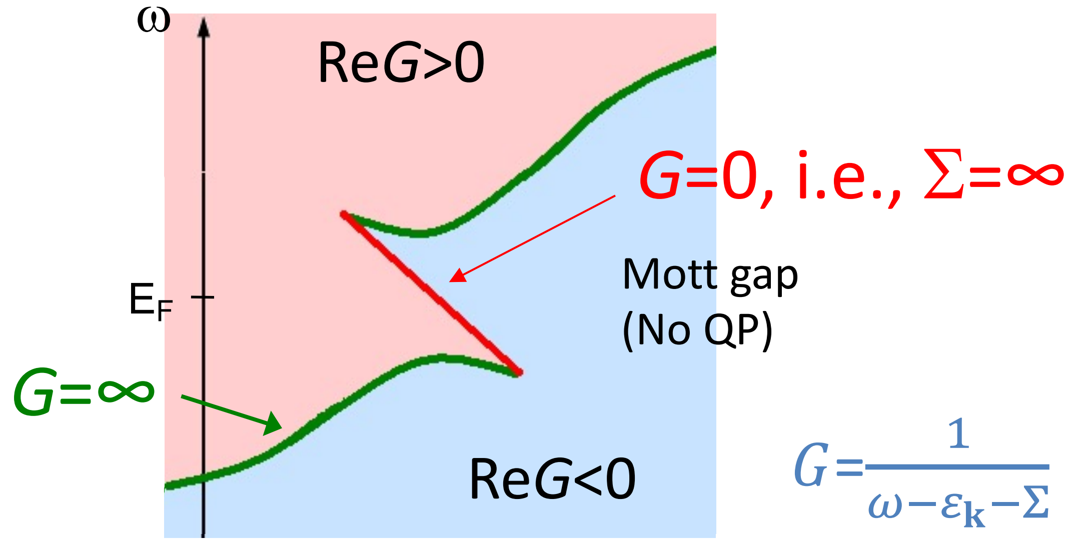
Gapped = (No pole of G around E_F)

→ How does ReG change sign
without going through G=∞?

Locality = (pole of Σ)

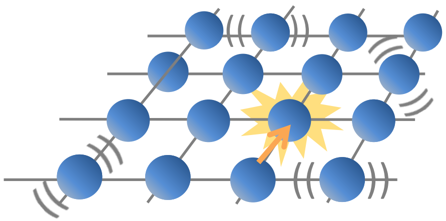


Mott insulator

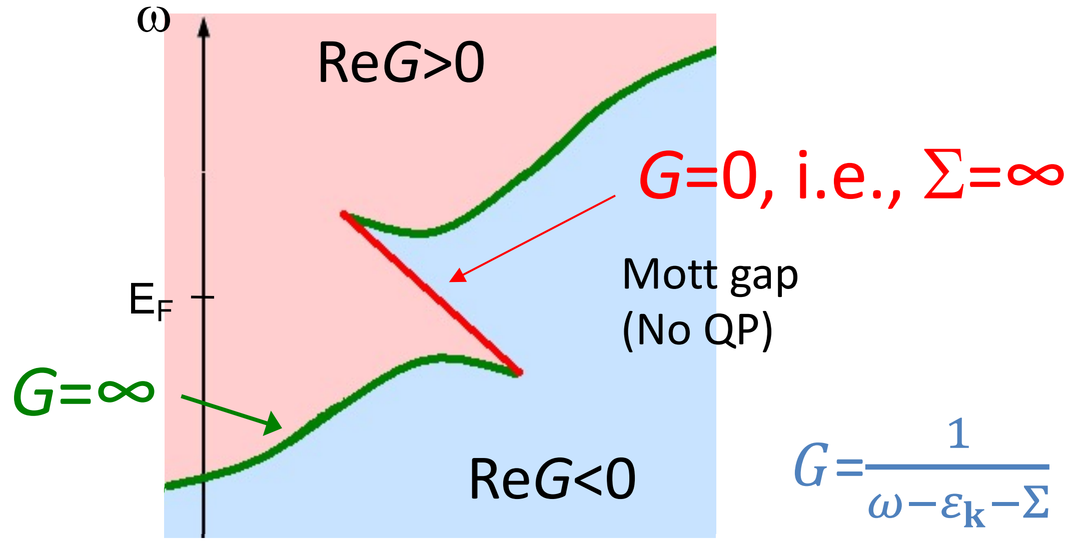


$$G = \frac{1}{\omega - \varepsilon_{\mathbf{k}} - \Sigma}$$

Locality = (pole of Σ)



Mott insulator



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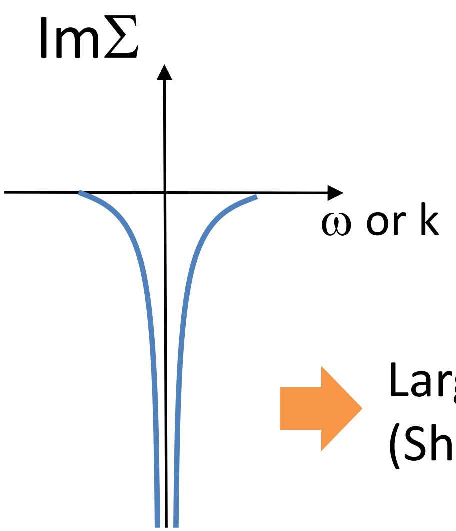
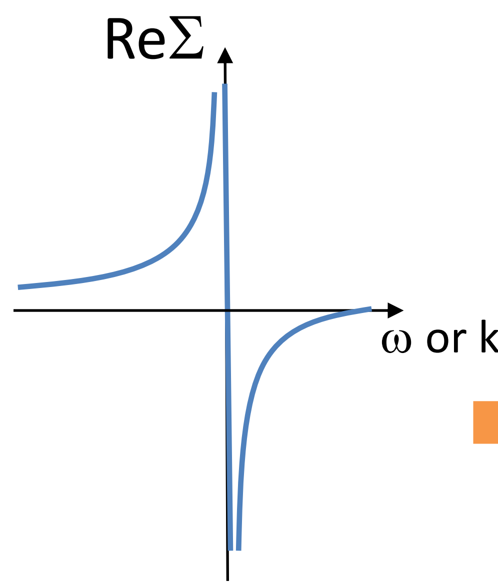
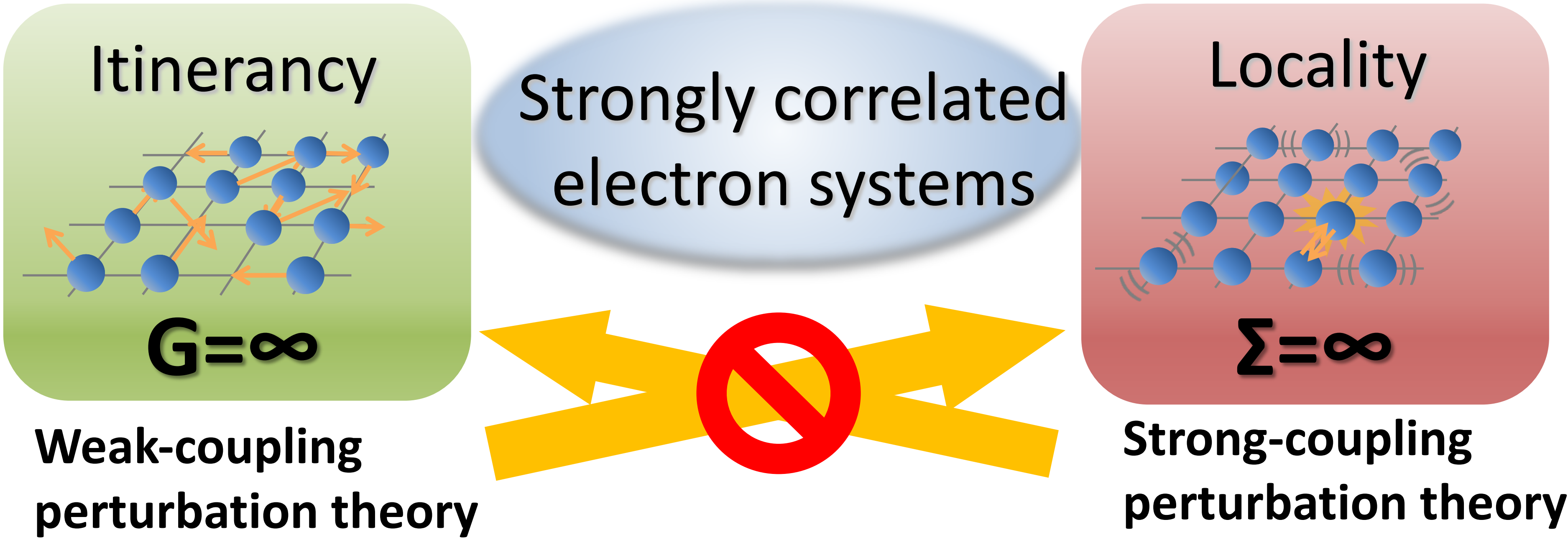


Large scattering
(Short lifetime)



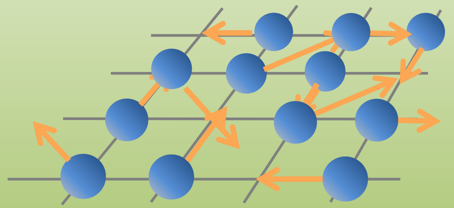
Diverging mass

Poles of G and Σ



Poles of G and Σ

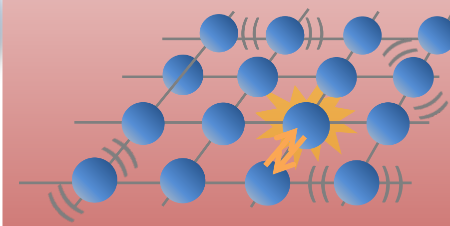
Itinerancy



G=∞

Strongly correlated electron systems

Locality



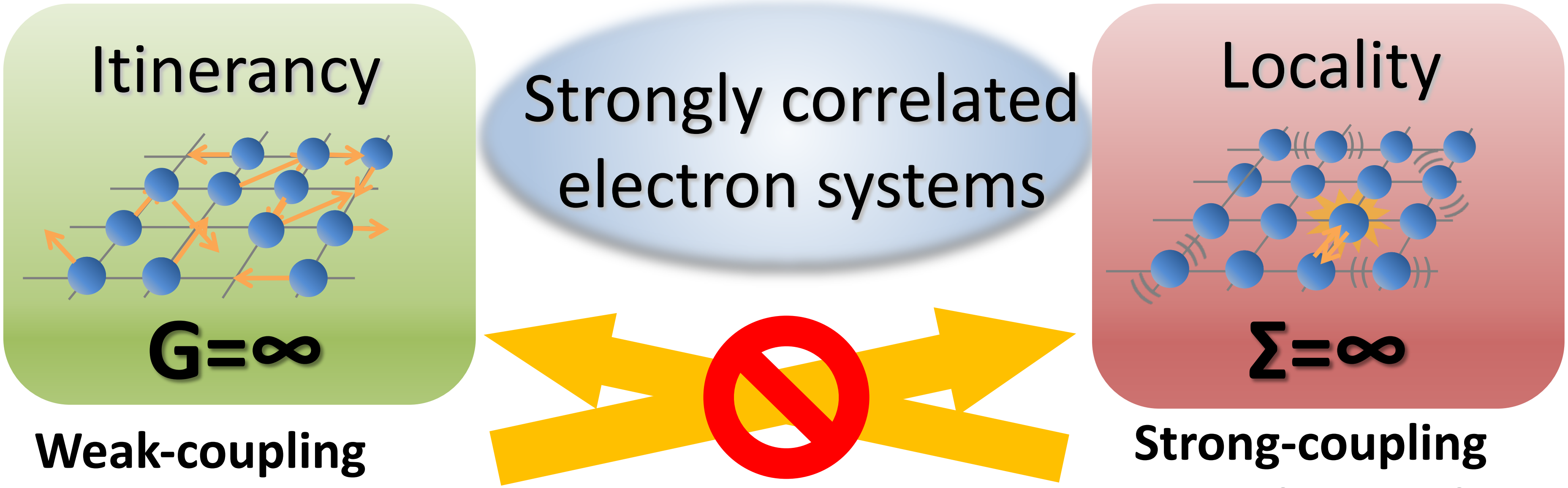
Σ=∞

Weak-coupling perturbation theory

Strong-coupling perturbation theory

Nonperturbative theory is necessary

Poles of G and Σ



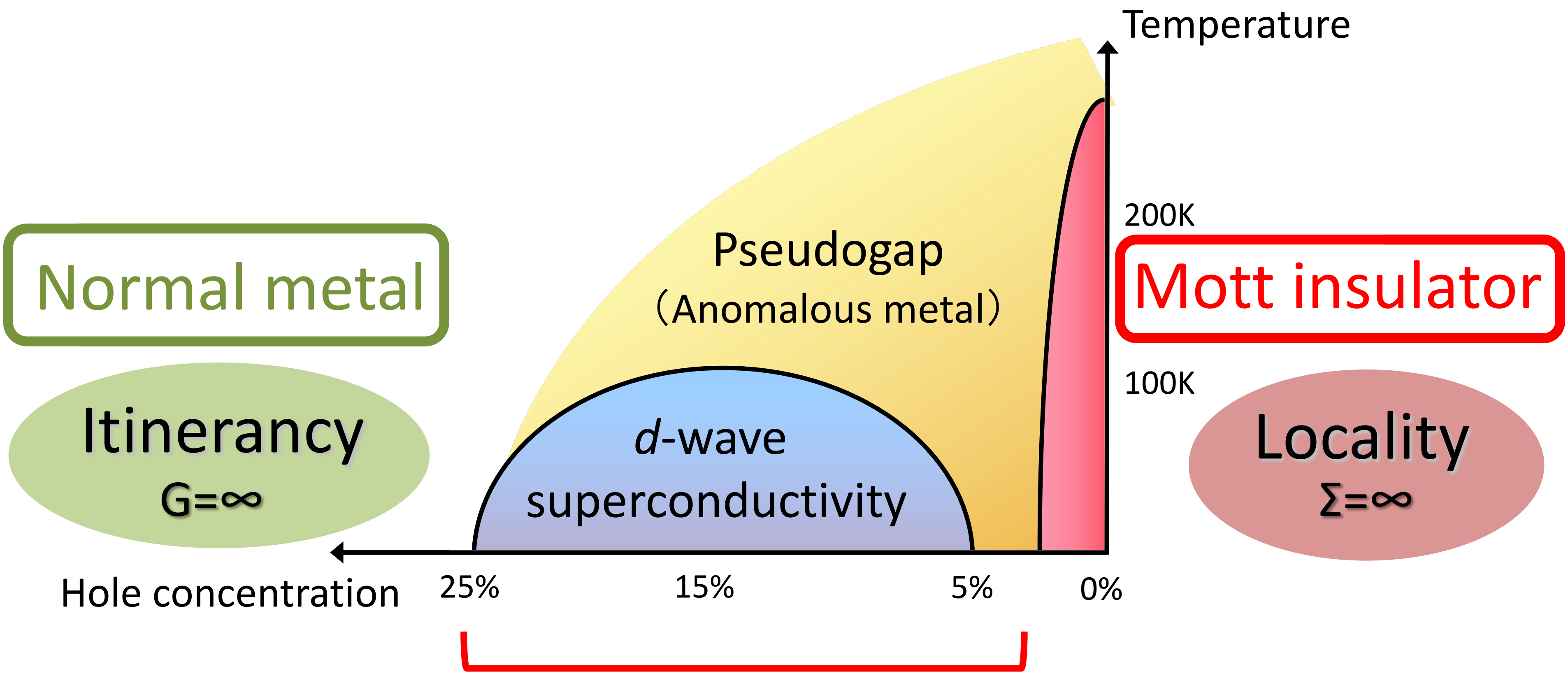
Weak-coupling perturbation theory

Strong-coupling perturbation theory

Nonperturbative theory is necessary

Can G=∞ and Σ=∞ coexist? If so, what happens?

High-T_c cuprates



G=∞ and Σ=∞ coexist??

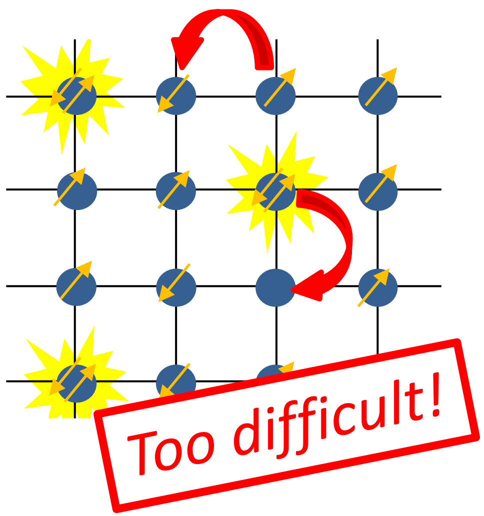
Cluster Dynamical Mean-Field Theory (CDMFT)

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

2D Hubbard model

(Standard model for cuprates)

$$H = -\sum_{ij\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



Map

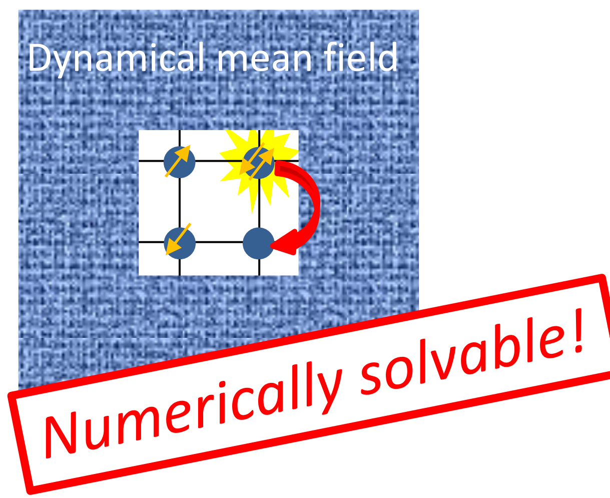
Σ_{ij}

Effective cluster model

A few interacting sites (cluster)

+

Dynamical mean field



Full short-range correlations

- Unbiased & nonpertabative!

Mott transition at half filling

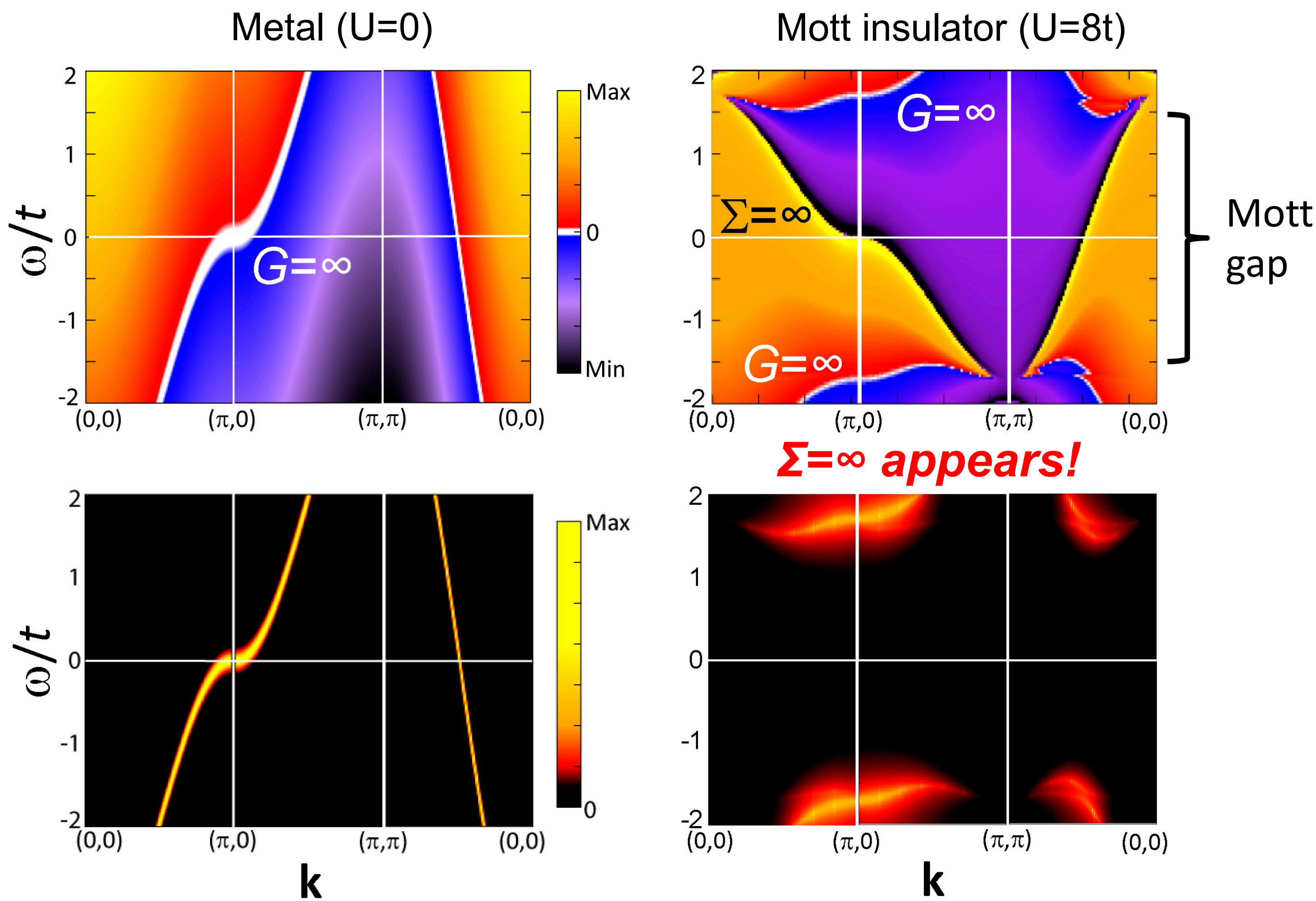
- Square lattice at T=0
- Paramagnetic solution

Re*G*$^{-1}$

$=\omega+\mu-\varepsilon_k-\mathrm{Re}\Sigma$

***A*(k,ω)**

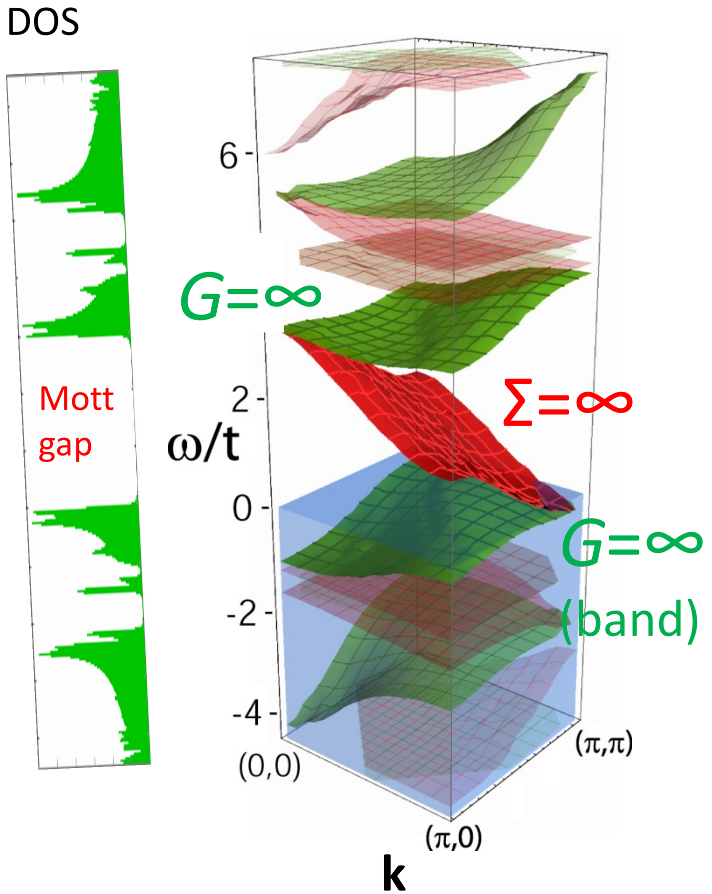
$=-\mathrm{Im}G/\pi$



Evolution of pole structure across the Mott transition

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

Mott insulator



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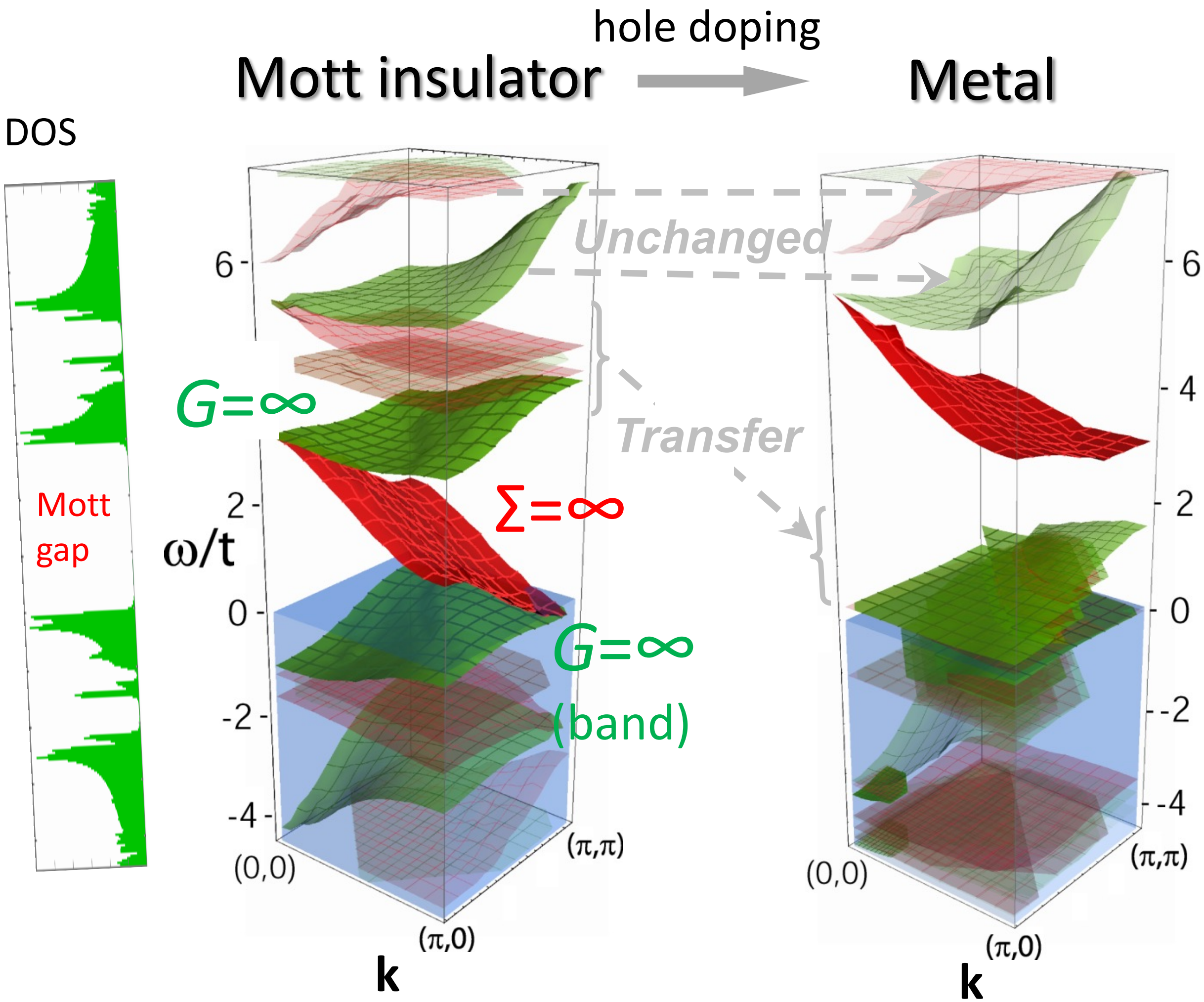

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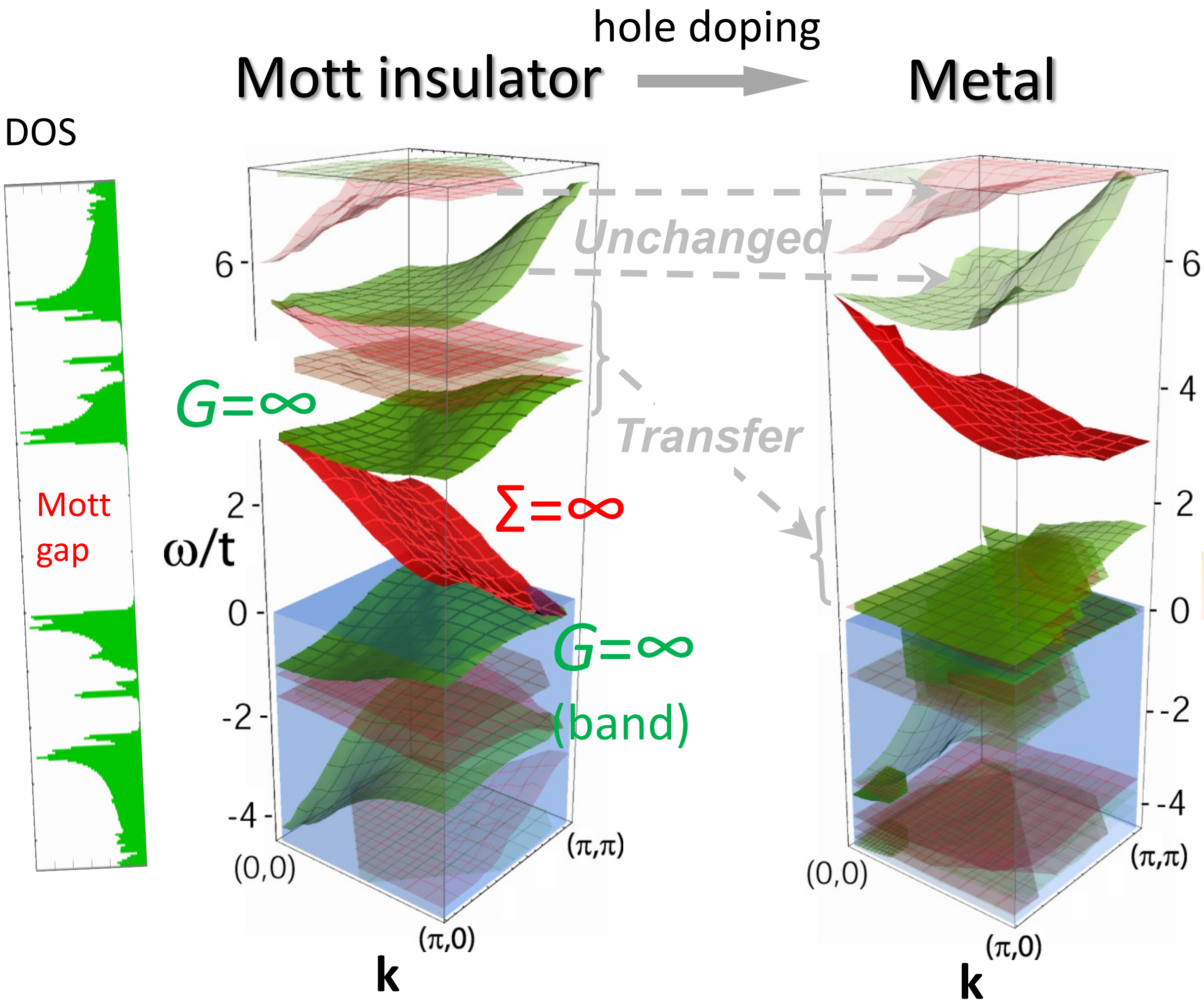

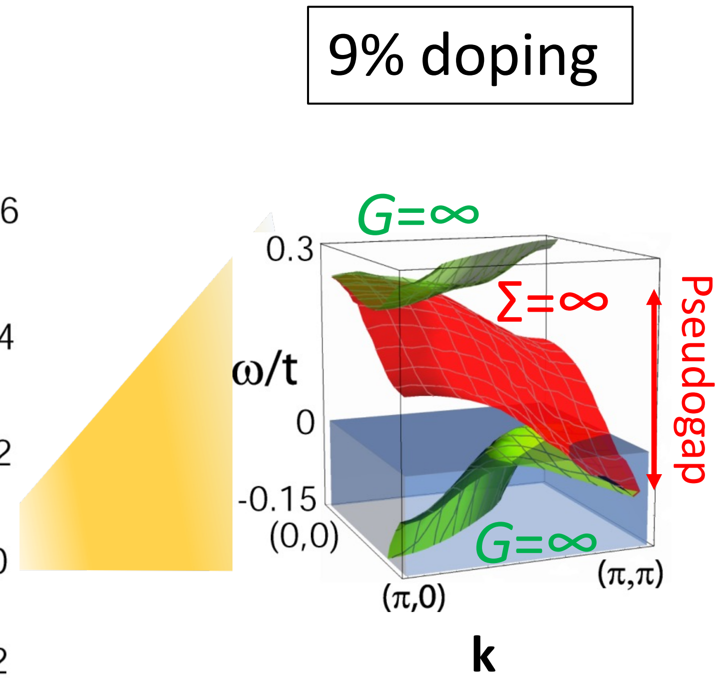

Similar structure but in much smaller energy scale

Evolution of pole structure across the Mott transition

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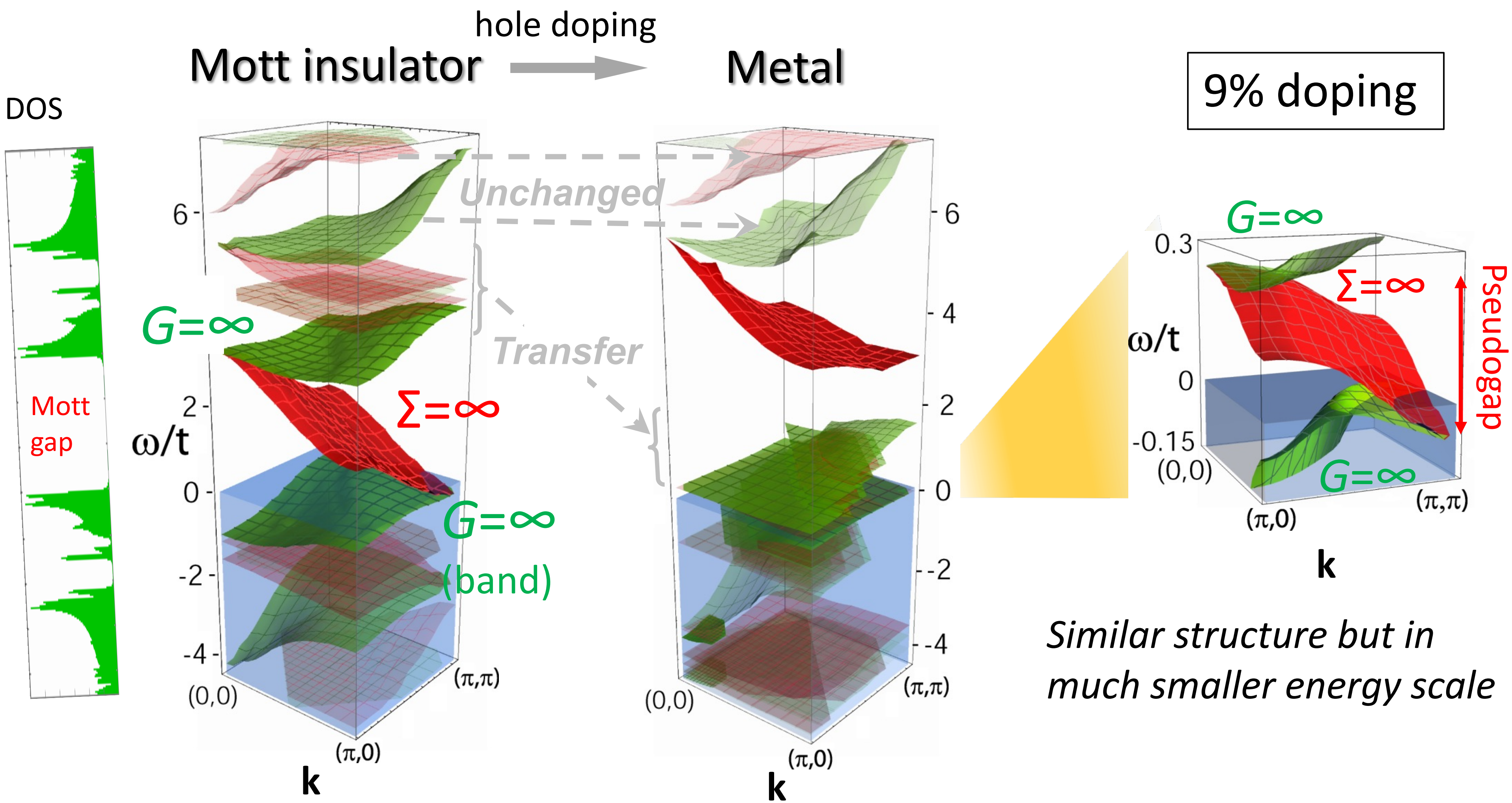
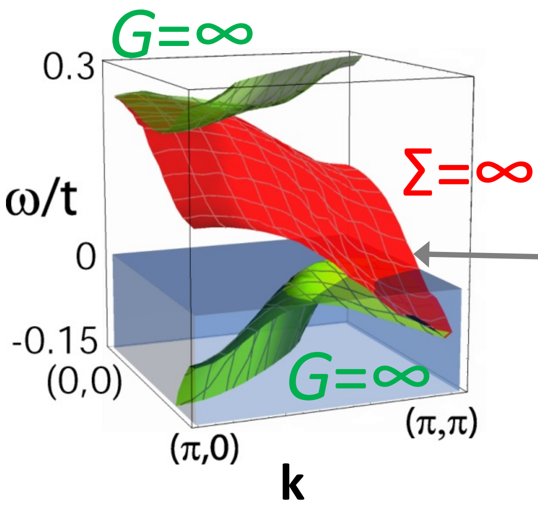


Visualization of $G=\infty$ and $\Sigma=\infty$ in SCES. ⟺ *Band ($G=\infty$) structure of weakly interacting system.*

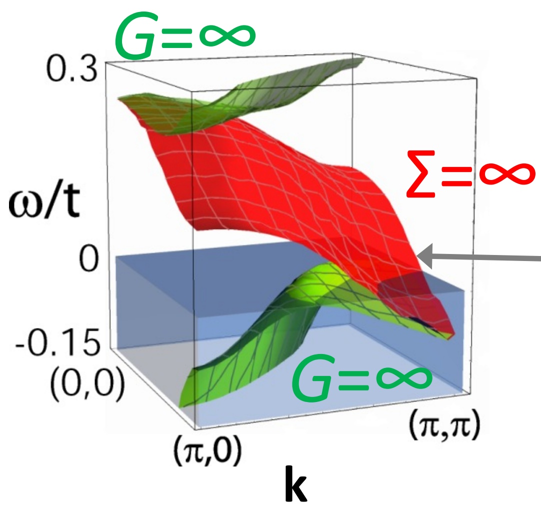
Structure of G=∞ and Σ=∞ in pseudogap state



G=∞ & Σ=∞ coexist at low ω !

Σ=∞ surface pushes down G=∞ surface (pocket appears without symmetry breaking)

Structure of G=∞ and Σ=∞ in pseudogap state



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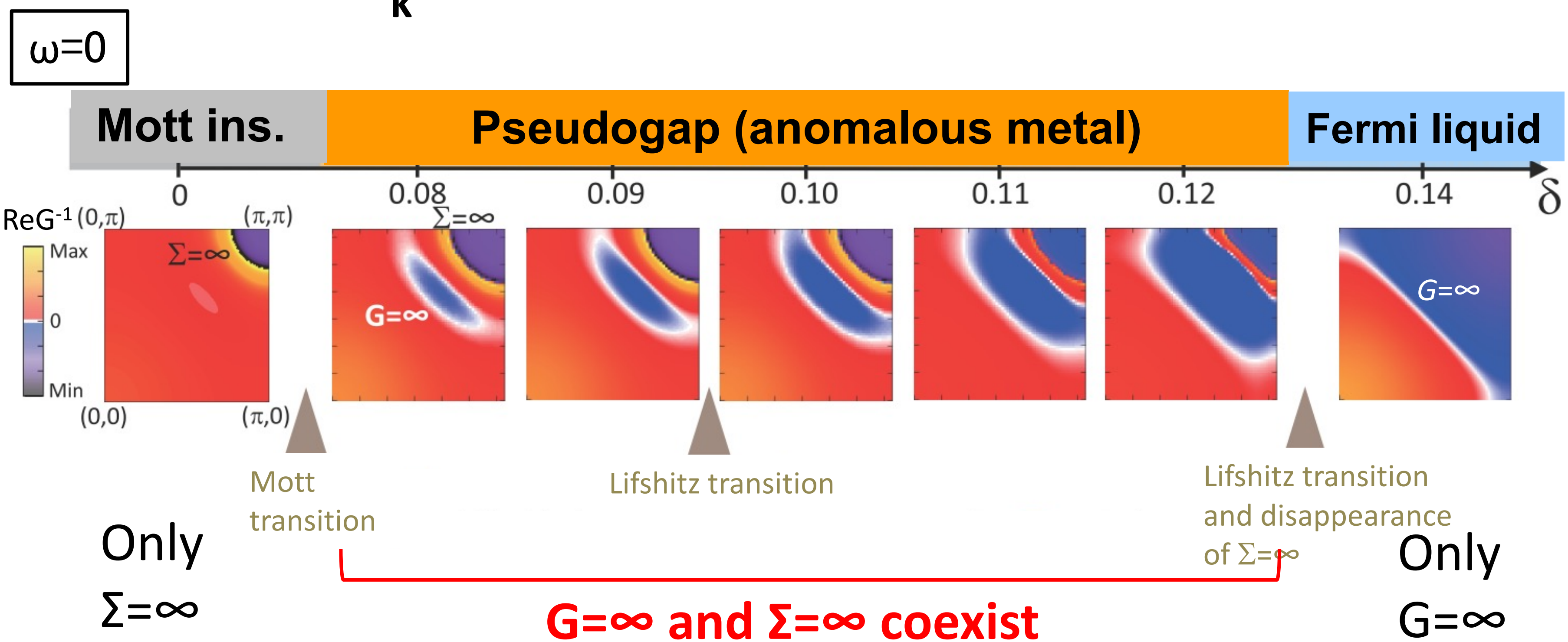
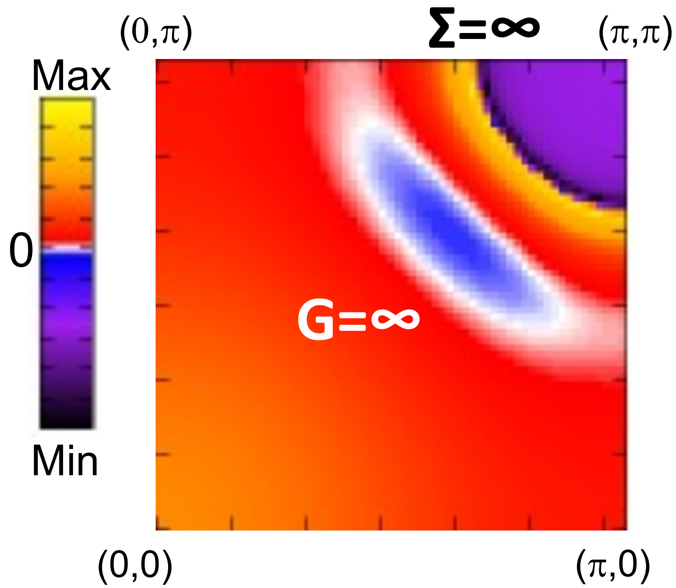


Interference between poles of G and Σ

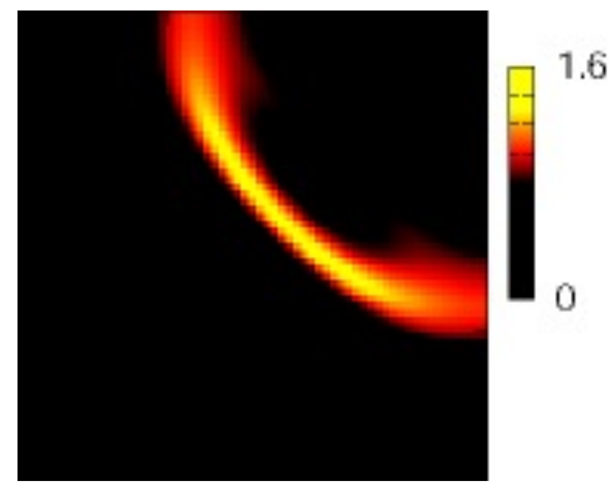
Stanescu & Kotliar, PRB **74**, 125110 (2006);
S. S., Y. Motome, and M. Imada, Physica B **404**, 3183 (2009).

$$\mathrm{Re}G^{-1}(\mathbf{k},\omega=0) = -\varepsilon_{\mathbf{k}} - \mathrm{Re}\Sigma(\mathbf{k},\omega=0)$$

$$A(\mathbf{k},\omega=0) = -\frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega=0)$$



ImΣ

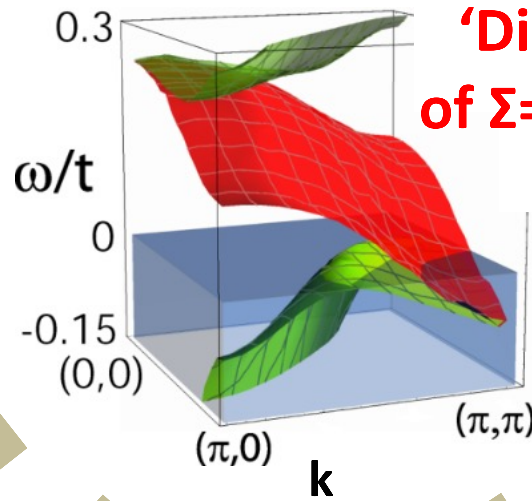


Fermi arc

Fermi arc due to the interference of G=∞ and Σ=∞

Unified understanding of spectral anomalies

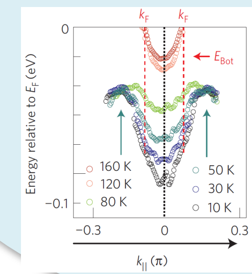
S.S, Y. Motome, M. Imada,
PRB **82**, 134505 (2010)



'Dispersion' of Σ=∞ is a key

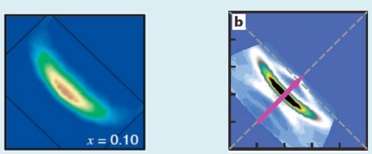
- Low-E kink, waterfall
- e-doped cuprates
- Pseudogap

Shift of back-bending point



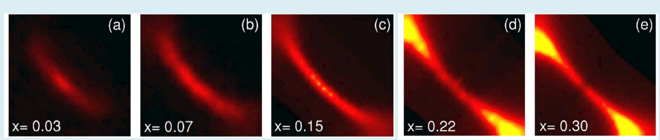
Hashimoto *et al.*, Nat. Phys.'10

Fermi arc/pocket



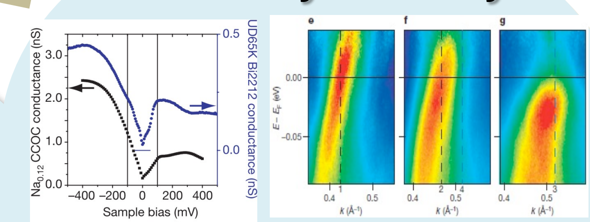
Norman *et al.*, Nature'98;
Shen *et al.*, Science'05;
Meng *et al.*, Nature'09

Doping evolution of Fermi surface



Yoshida *et al.*, PRB'06

e-h asymmetry



Hanaguri *et al.*, Nature'04;
Yang *et al.*, Nature'08