KITP Program: "*Frustrated Magnetism and Quantum Spin Liquids: From Theory and Models to Experiments*"
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Transport Criticality near the Mott Transition

Hirokazu Tsunetsugu (ISSP, Univ. of Tokyo)

東京大学
THE UNIVERSITY OF TOKYO

in collaboration with
Toshihiro Sato (ISSP, Univ. Tokyo)
Kazumasa Hattori (ISSP, Univ. Tokyo)

Frustration

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Motivation

(A) What is unconventional behavior of frustrated electron systems?

- Mott transition is a metal-insulator transition not accompanied by any symmetry breaking and spin frustration is essential to it.
  What is characteristic to Mott transition?

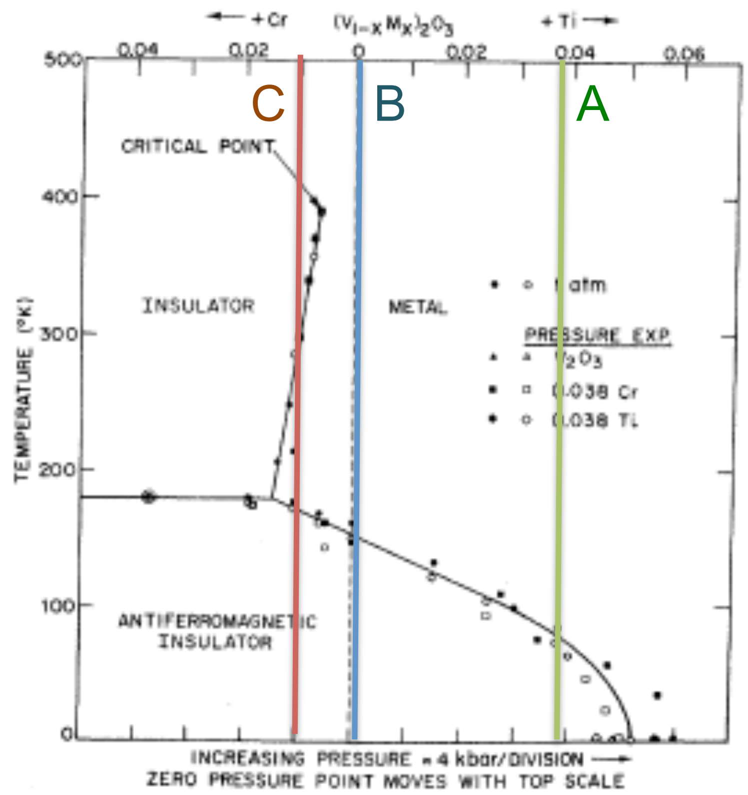
(B) Mystery in experimental works on singular electric conductivity near the Mott transition

⇒

Let us try direct numerical calculations of electric conductivity near the Mott transition and determine its critical exponent

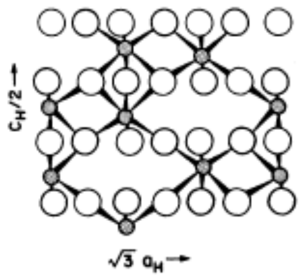
[Ref: Sato, Hattori and Tsunetsugu, J. Phys. Soc. Jpn. **81**, 083703 (2012);
full paper submitted to Phys. Rev. B]

V_2O_3 – Mott insulator

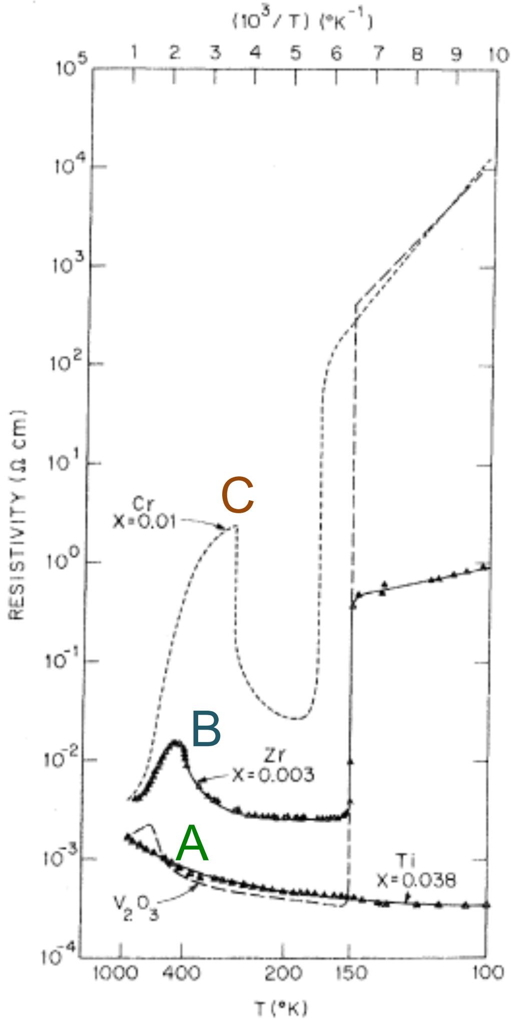


[McWhan et al, (1971, 1973)]

Transition from PMI to PMM



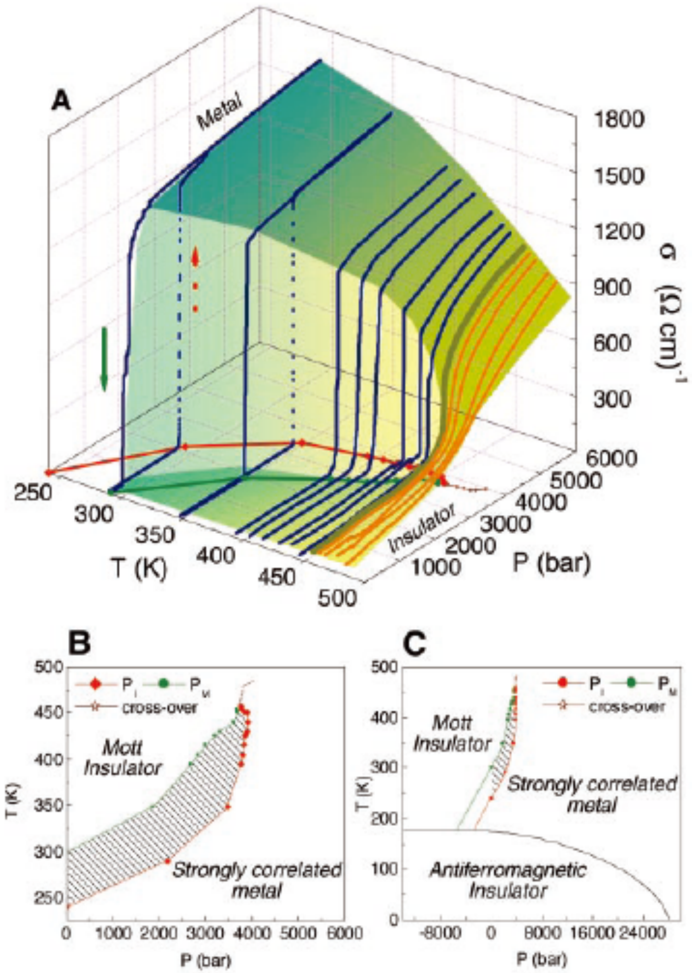
Electric resistivity

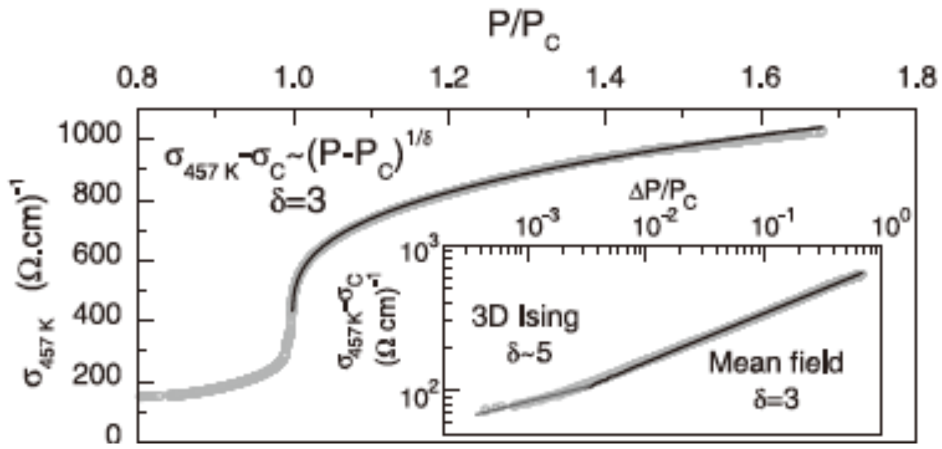


low T

Strongly correlated metal
- large specific heat
- large susceptibility

V_2O_3 – DC conductivity at T_c





[Limelette et al, Science (2003)]

Mott metal-insulator transition takes places inside the paramagnetic region, and is not accompanied by any symmetry breaking.

This is similar to liquid-gas transition, which belongs to Ising universality class.

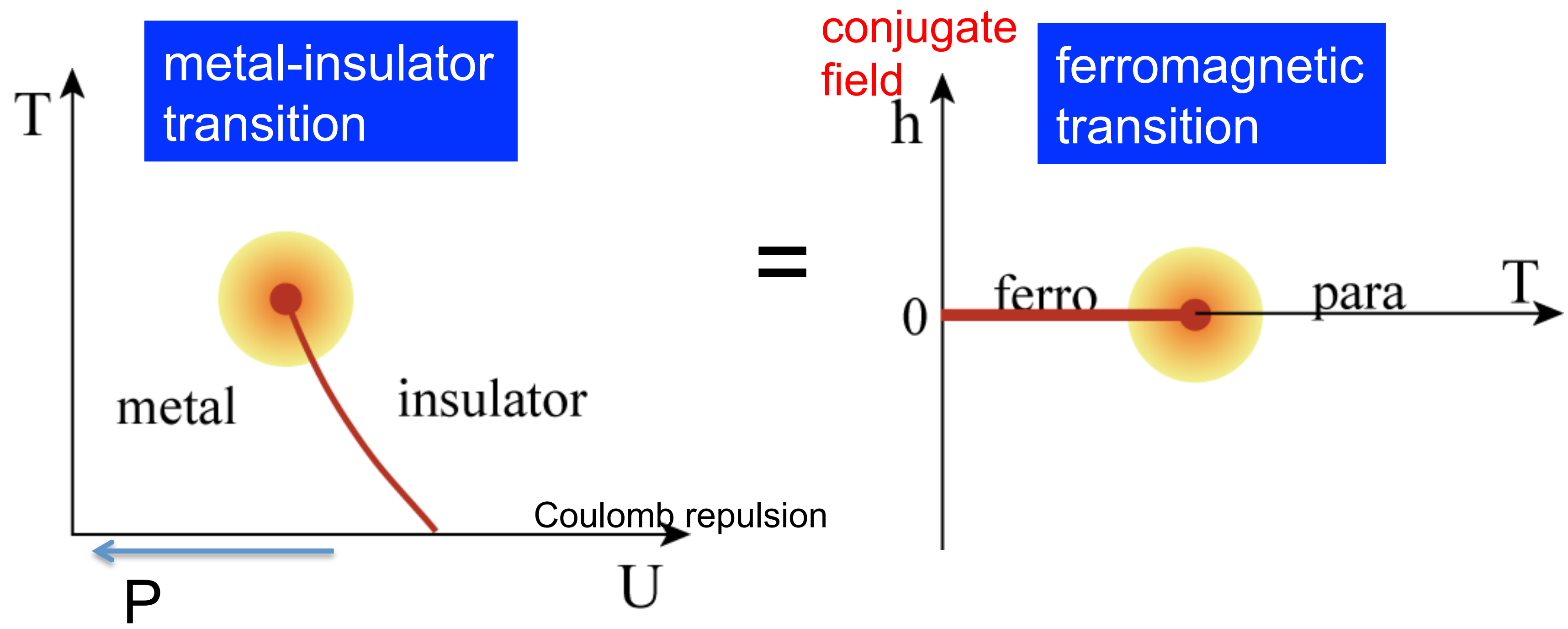
Observe Ising criticality in $\sigma(T,P)$

$$\Delta\sigma \sim |\Delta P|^{1/\delta}$$

$1/\delta = 1/3 \rightarrow 1/5$ crossover

Mott transition: Ising universality class

double occupancy *d* is the order parameter of Mott transition
→ scalar ϕ^4 field theory → Ising universality class



correspondence

d, $\delta\sigma$?	m
δT	δT
δU, $-\delta P$	h

Scaling

- Ferromagnetic transition

$$m(\delta T, h) = |h|^{1/\delta} f\left(\frac{h}{|\delta T|^{\delta\beta}}\right)$$

$$m = |h|^{1/\delta} \text{ (at } T = T_c)$$

$$\Delta m = |\delta T|^{\beta} \ (T < T_c)$$

- Metal-insulator transition (naive expectation)

$$\sigma(\delta T, \delta U) - \sigma_c \approx \sigma_{\text{sing}}(\delta T, \delta U) = |\delta U|^{1/\delta} f\left(\frac{\delta U}{|\delta T|^{\delta\beta}}\right)$$

$$\boxed{\Delta\sigma = |\delta U|^{1/\delta} \text{ (at } T = T_c)}$$

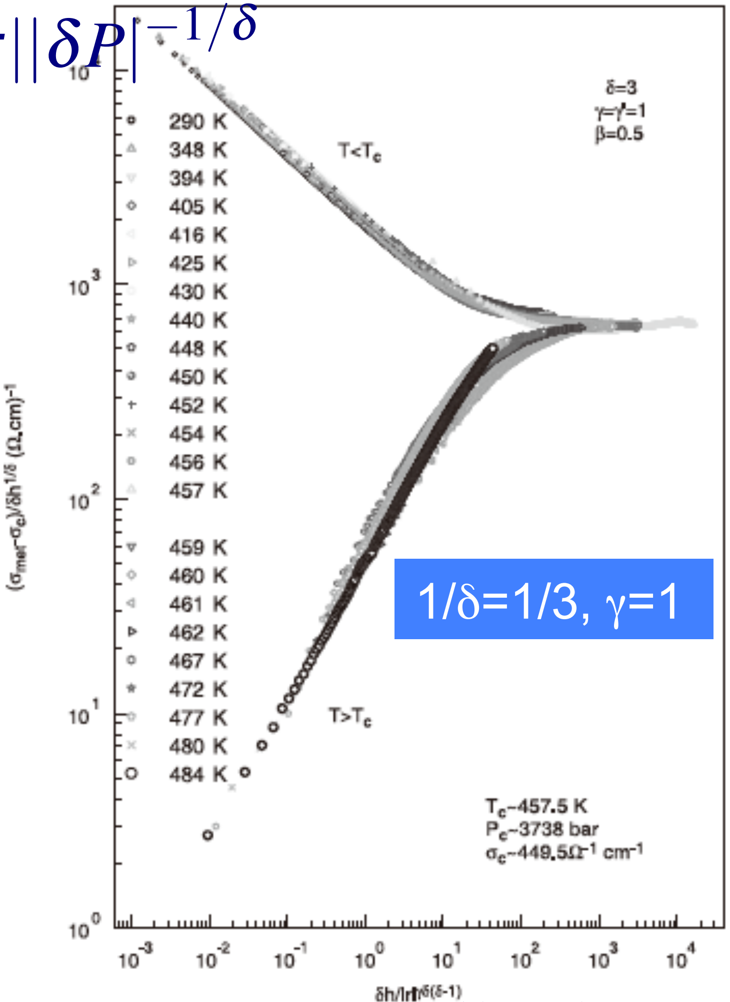
$$\Delta\sigma = |\delta T|^{\beta} \ (T < T_c)$$

scaling relation $\gamma = \beta(\delta - 1)$

V_2O_3 - Scaling of DC conductivity

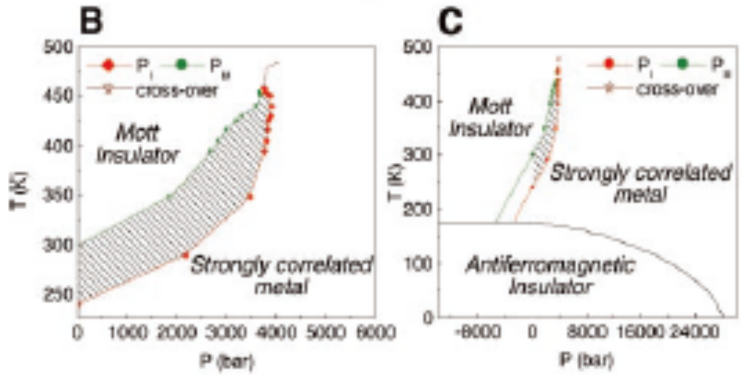
[Limelette et al, Science (2003)]

$$|\delta\sigma||\delta P|^{-1/\delta}$$



$$|\delta P||\delta T|^{-\gamma\delta/(\delta-1)}$$

more systematic scaling



$$\delta U = -\delta P$$

$$\sigma(\delta T, \delta U) - \sigma_c = |\delta U|^{1/\delta} f\left(\frac{\delta U}{|\delta T|^{\gamma\delta/(\delta-1)}}\right)$$

$$\delta\sigma \sim -|\delta U|^{1/\delta}\mathrm{sgn}\,\delta U \quad (\text{at } T = T_c)$$

Basic Hypothesis behind this scaling

This kind scaling analysis is based on an implicit assumption that
conductivity is a regular function of the order parameter
in the vicinity of the critical end point.

$$\sigma(T,U) = \sigma_{regular} + \sigma_{singular}$$

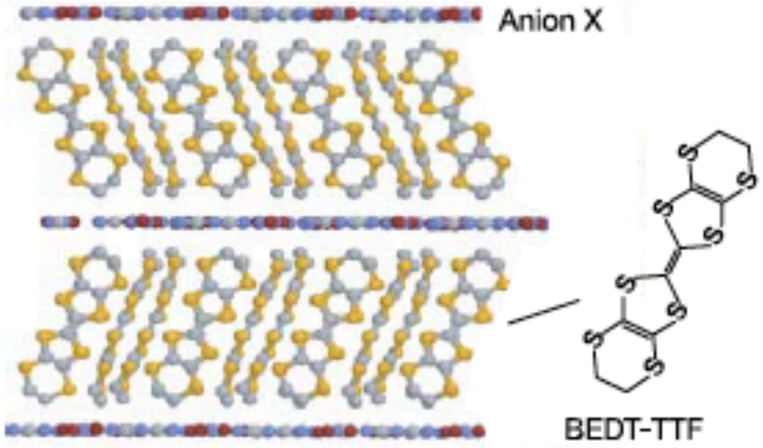
$$\sigma_{singular}(\delta T, \delta U) = A_1 \langle d(\delta T, \delta U)\rangle + A_2 \langle d(\delta T, \delta U)^2\rangle + \ldots$$

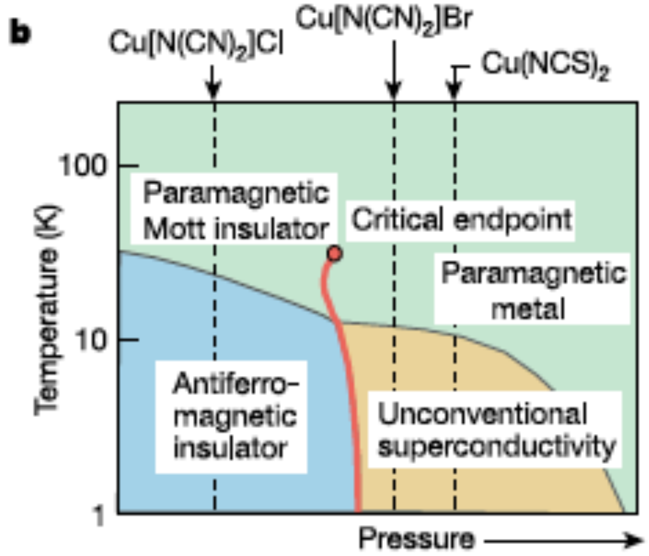
order parameter

However, this is highly nontrivial.

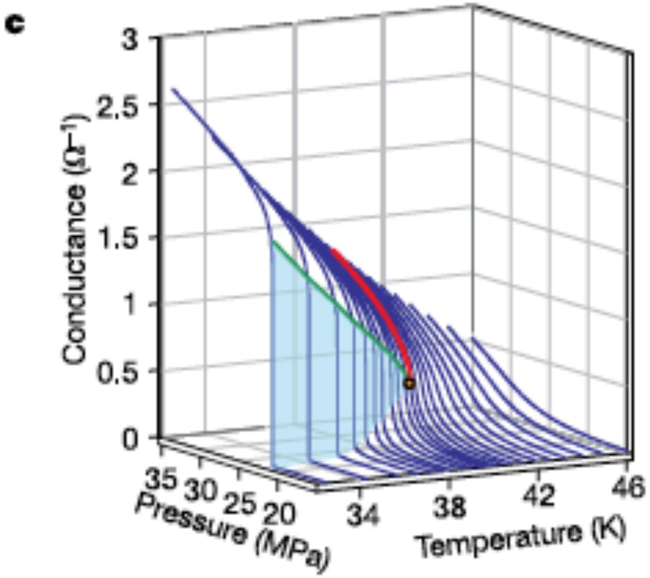
κ-type organic – DC conductivity

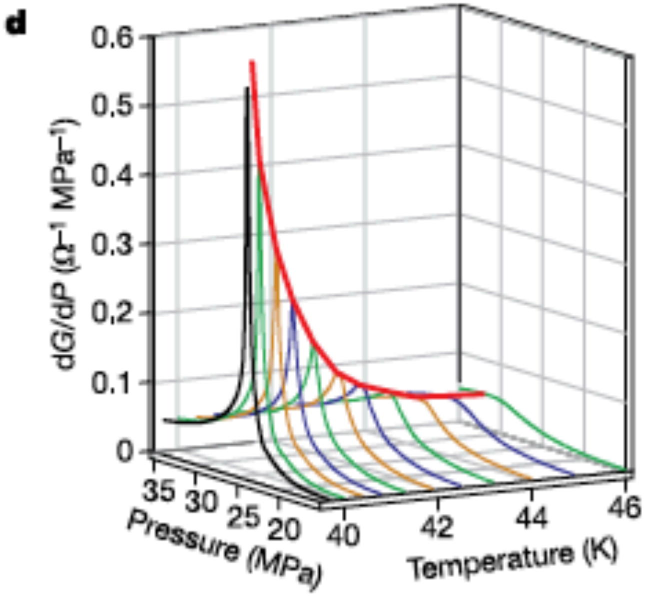
triangular lattice of ET dimers





κ-$(ET)_2Cu[N(CN)_2]Cl$



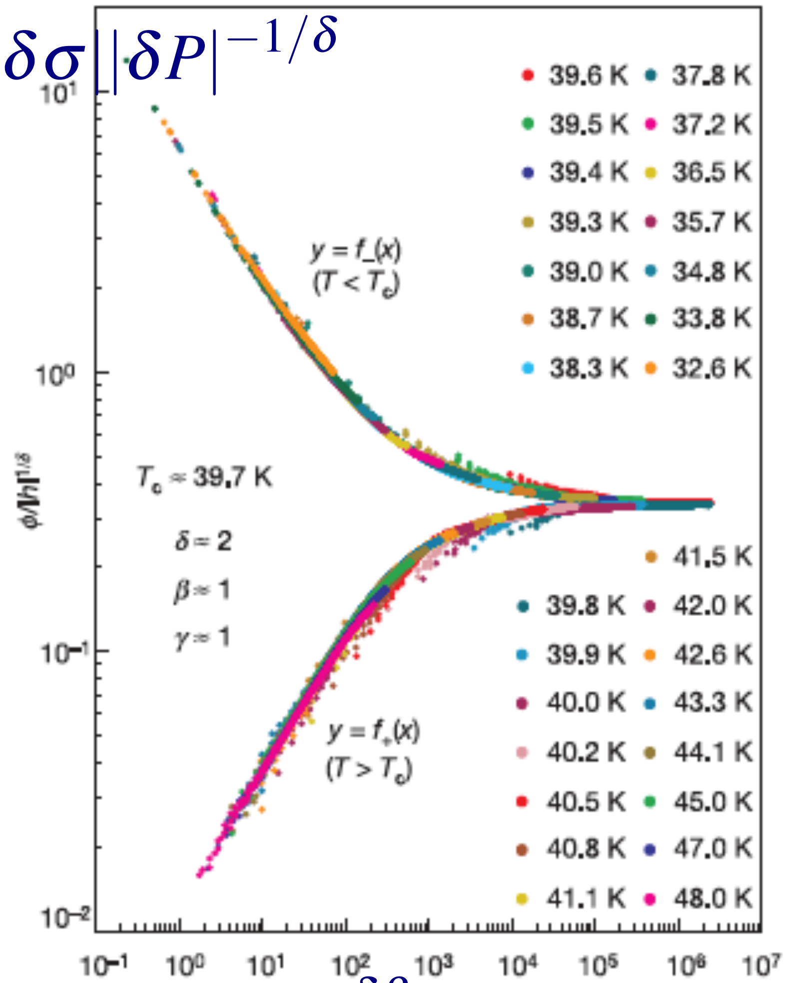


[Kagawa et al, Nature (2005)]

κ-type organic - Scaling of DC conductivity

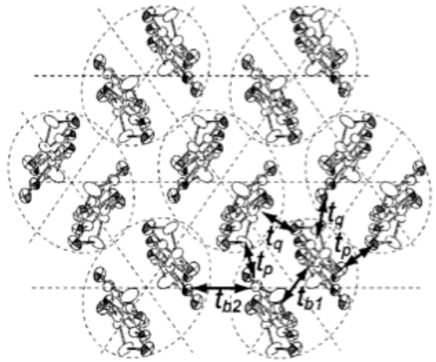
[Kagawa et al, Nature (2005)]

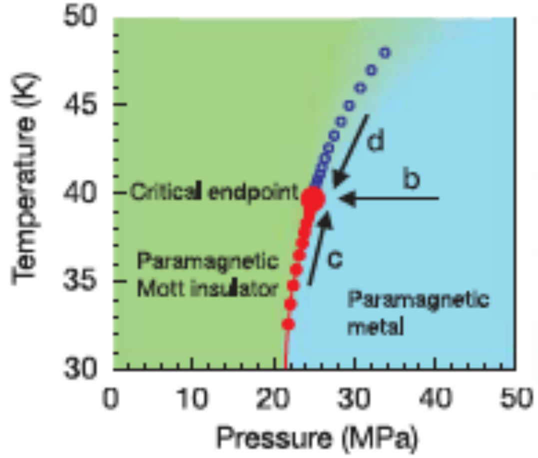
$|\delta\sigma||\delta P|^{-1/\delta}$



$|\delta P||\delta T|^{-\delta\beta}$

κ-(ET)$_2$Cu[N(CN)$_2$]Cl





$$\delta U = -\delta P$$

$$\sigma(\delta T, \delta U) - \sigma_c = |\delta U|^{1/\delta} f\left(\frac{\delta U}{|\delta T|^{\delta\beta}}\right)$$

$$\delta\sigma \sim -|\delta U|^{1/\delta}\mathrm{sgn}\,\delta U \quad (\text{at } T = T_c)$$

unconventional exponent

$1/\delta=1/2$ [cf 1/3 (MF), 1/15 (2D Ising), ~1/5 (3D Ising)]

$\gamma=1$, $\beta=1$ scaling relations are satisfied.

Theories for unconventional exponents

triangular-lattice organic compound

κ-$(ET)_2Cu[N(CN)_2]Cl$

unconventional exponents

$1/\delta=1/2$ [cf 1/3 (MF), 1/15 (2D Ising), ~1/5 (3D Ising)]

$\beta=1$ [cf 1/2 (MF), 1/8 (2D Ising), ~5/16 (3D Ising)]

(1) Marginally quantum critical region in 2 dimensions

$\beta=d/2$, $1/\delta=d/4$

(Imada, PRB, 2005)

(2) 2D-Ising universality, but response to energy density

$\beta=1$, $1/\delta=8/15$

(Papanikolaou et al, PRL, 2008)

Both approaches are phenomenological, and also based on the assumption that some thermodynamic critical exponent appears in transport singularity.

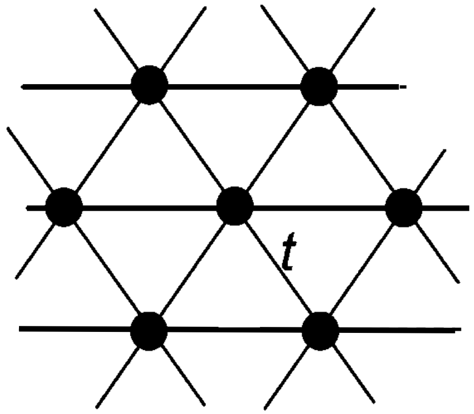
(1) Let us calculate electric conductivity directly for a microscopic model near the Mott transition.

(2) Compare its criticality to the criticality of order parameter.

Model and Method

Model: Hubbard model on triangular lattice

- half filling n=1
- t~t'~50 [meV] (Shimizu, PRL 2003)



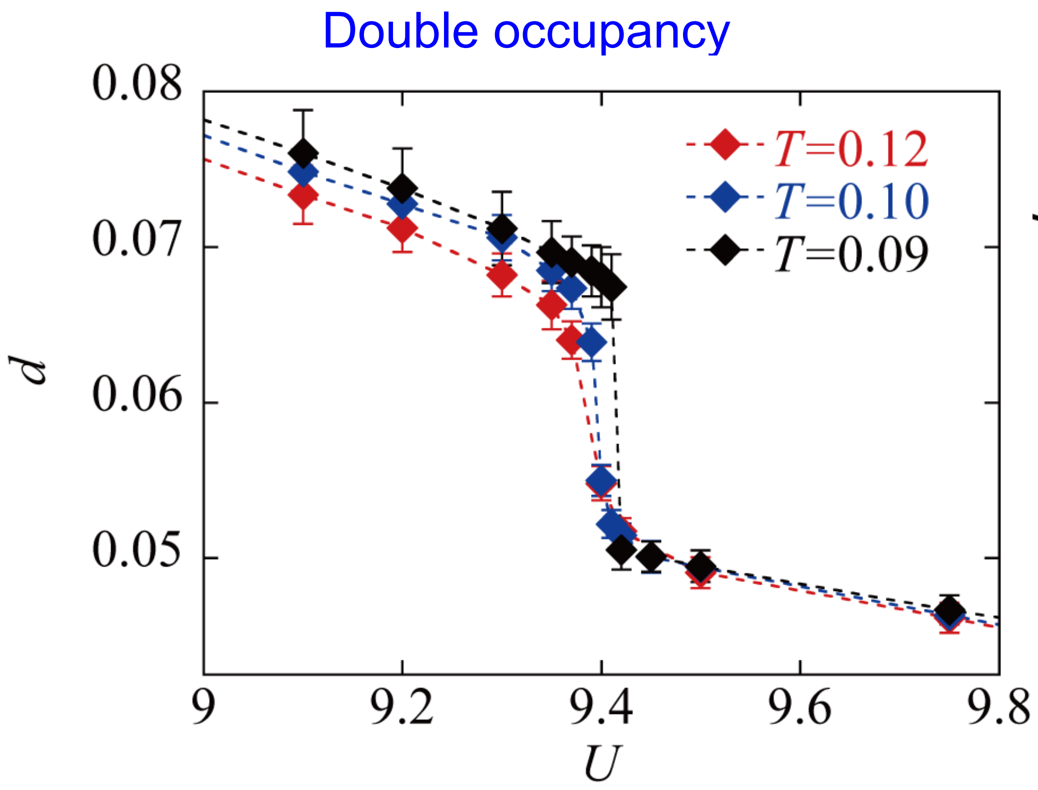
$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.}) - \mu \sum_{j\sigma} c_{j\sigma}^{\dagger} c_{j\sigma} + U \sum_{j} n_{j\uparrow} n_{j\downarrow}$$

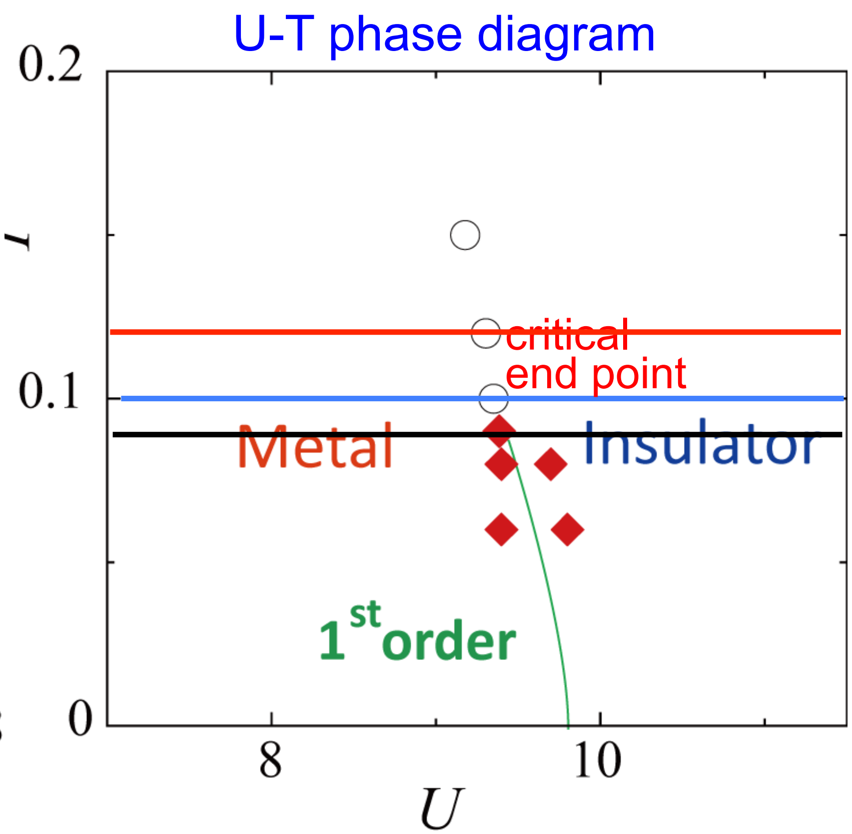
Method: Cluster Dynamical Mean Field Theory (CDMFT)

Kotliar
Lichtenstein
Werner
…

- 3-site cluster
  correctly describe Mott transition
  take into account short-range quantum&thermal fluctuations
- continuous-time quantum Monte Carlo (CTQMC) hybridization expansion
  effective for large U
- Kubo formula for $\sigma(\omega)$ (inc. vertex corrections inside cluster)

U-T Phase diagram



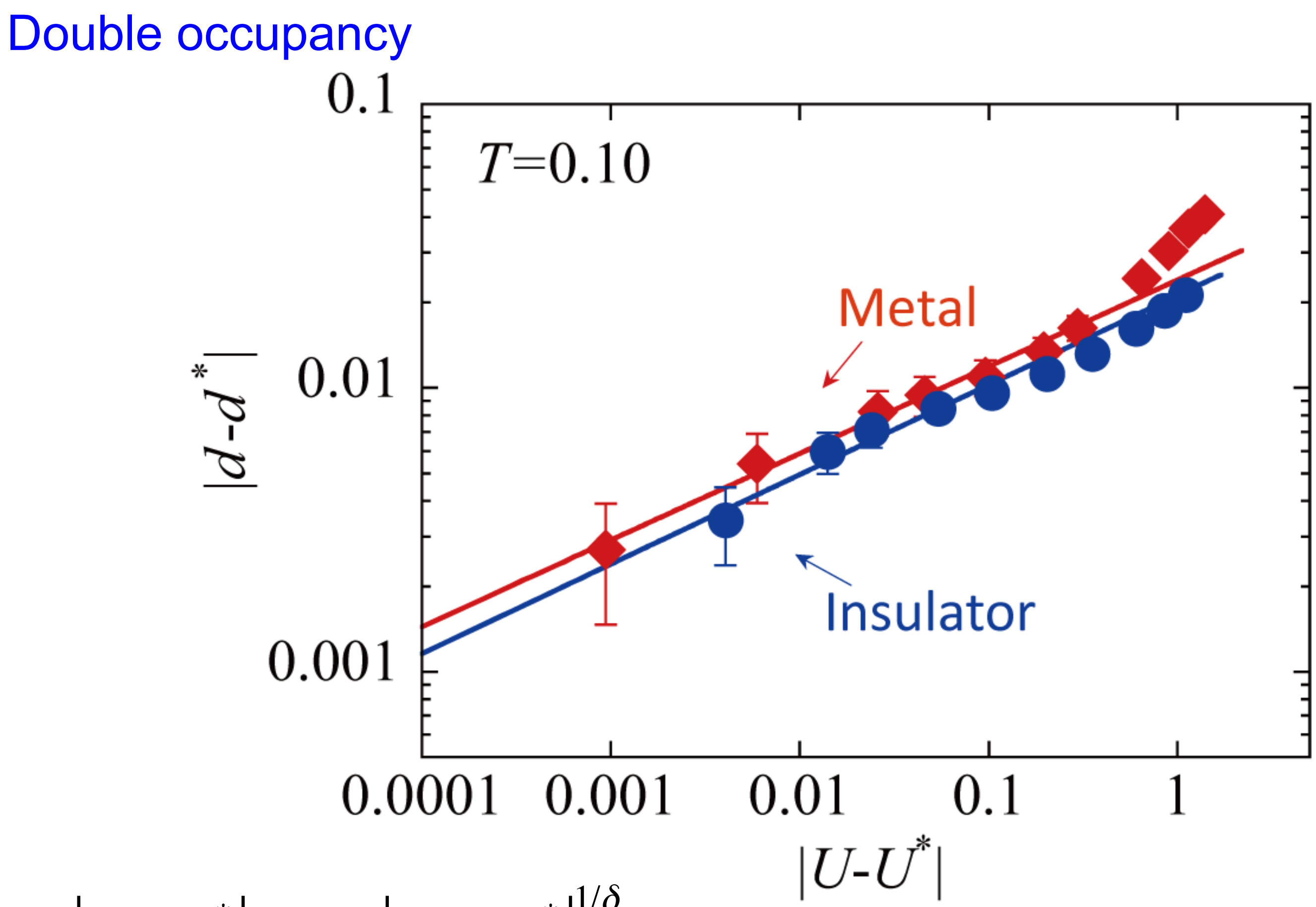


Double occupancy is the order parameter
representing thermodynamic criticality of Mott transition.

✧ ***T/t* = 0.09** ⇒ 1st order transition
***T/t* = 0.12** ⇒ crossover

K. Kanoda, J. Phys. Soc. Jpn. **75**. 051007 (2006)
Y. Furukawa (private communication)

Scaling of double occupancy



$$\left|d - d^*\right| \approx A_\pm \left|U - U^*\right|^{1/\delta_\pm}$$

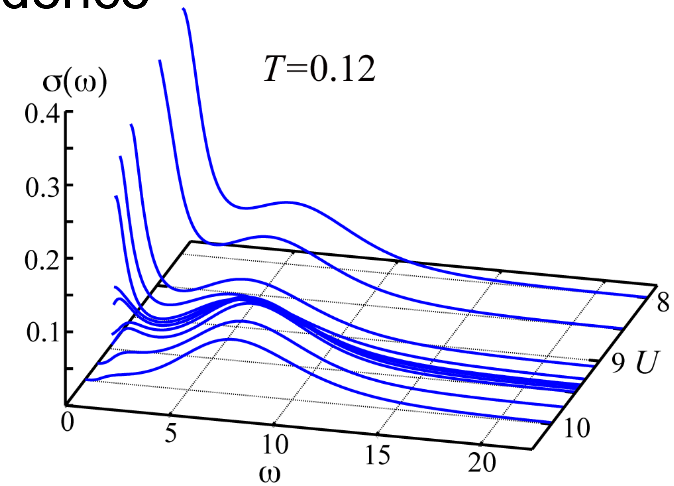
$$1/\delta_- = 0.32 \pm 0.05$$

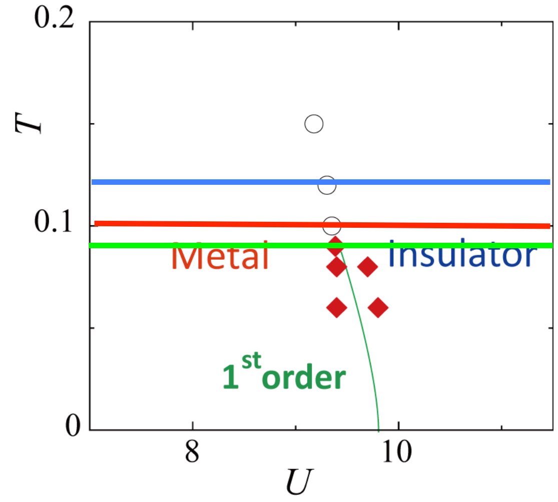
$$1/\delta_+ = 0.30 \pm 0.04$$

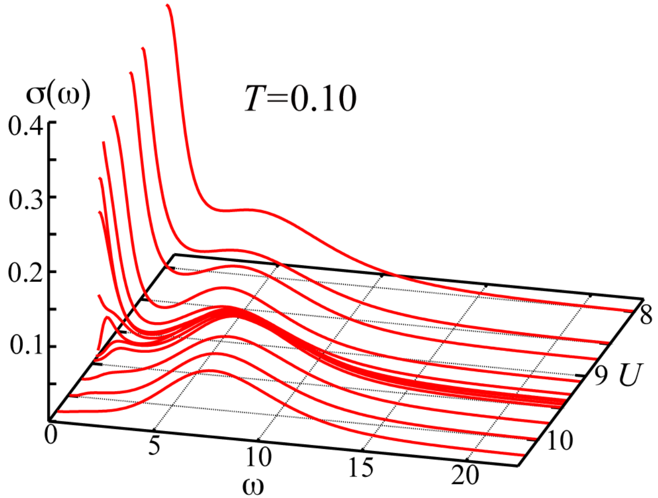
This value is consistent with
the mean-field exponent of Ising order parameter
$1/\delta = 1/3$

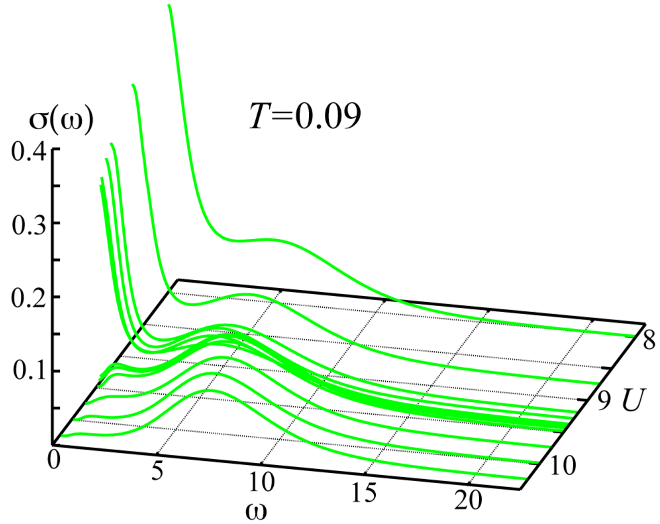
Optical conductivity σ(ω)

U-dependence





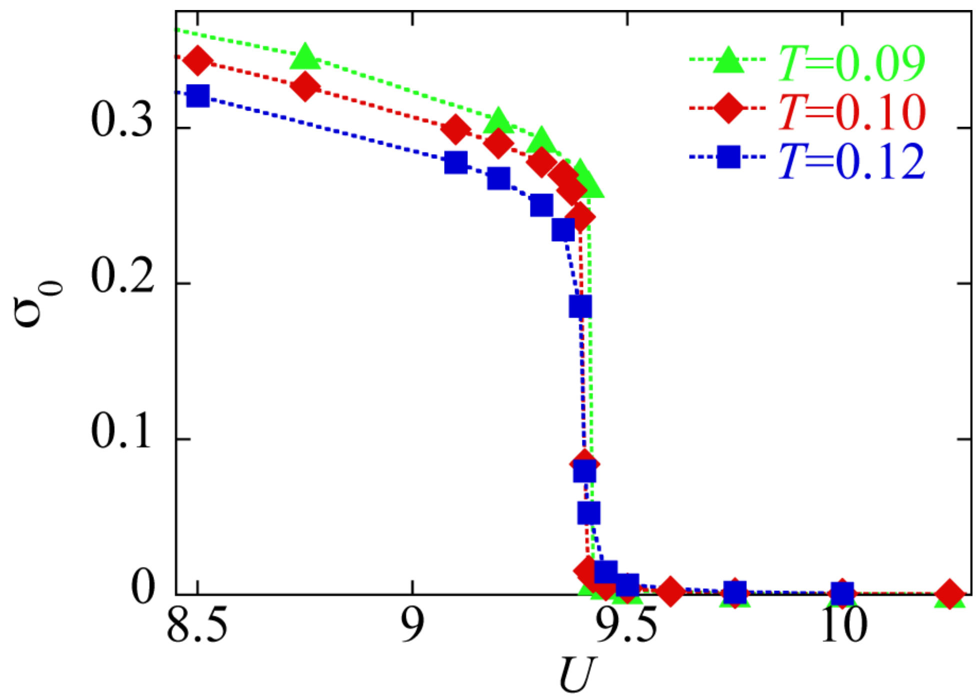




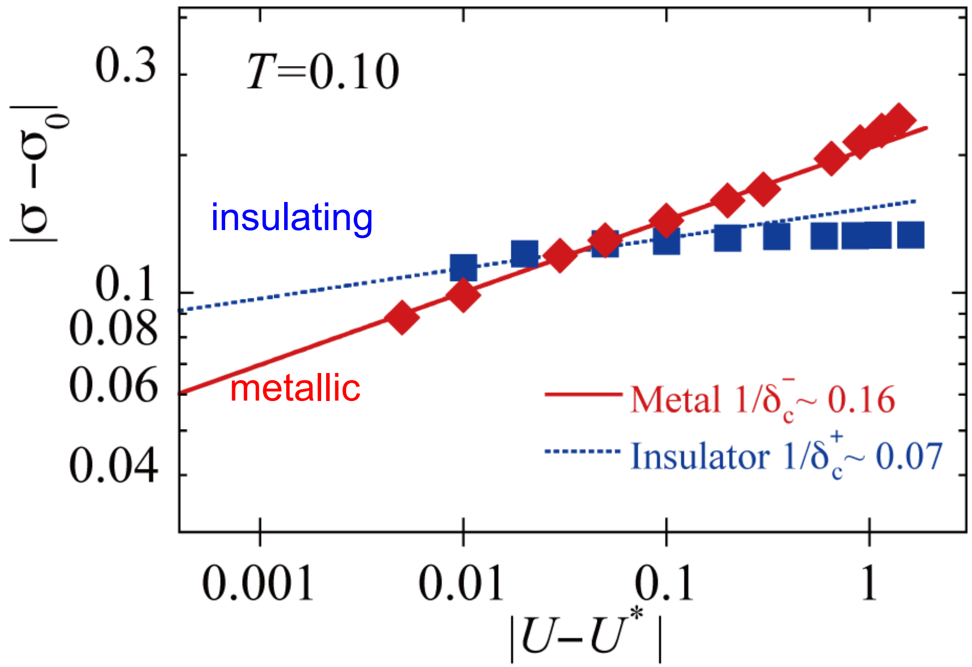
- High-ω incohent peak is robust and correspond to excitations to the Hubbard bands
- Low-ω Drude peak appears in the metallic region
- *U*-dependence is continuous but exhibits a singularity around *U/t*=9.4, *T/t*=0.10

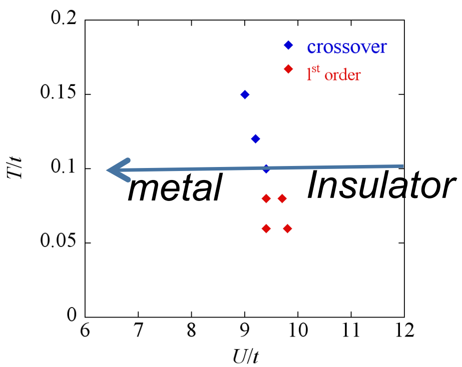
DC Conductivity and its Scaling

DC conductivity



$$|\sigma_0 - \sigma_0^*| = A_\pm |U - U^*|^{1/\delta\pm}$$





U-dependence of DC conductivity
is continuous,
But the singularity does not have the same exponent
on the both sides of the transition.

Choice of scaling variable

Simple choice is the singular part of dc-conductivity:

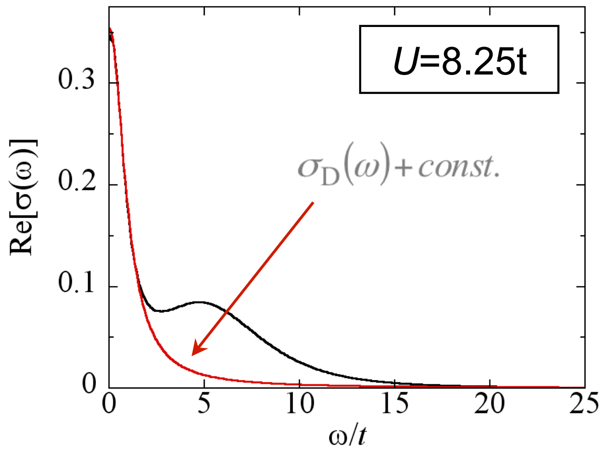
$$\sigma_0(\delta U) = \sigma_0^{\text{reg}}(\delta U) + \sigma_0^{\text{sing}}(\delta U)$$

This does not exhibit an expected conventional scaling behavior.

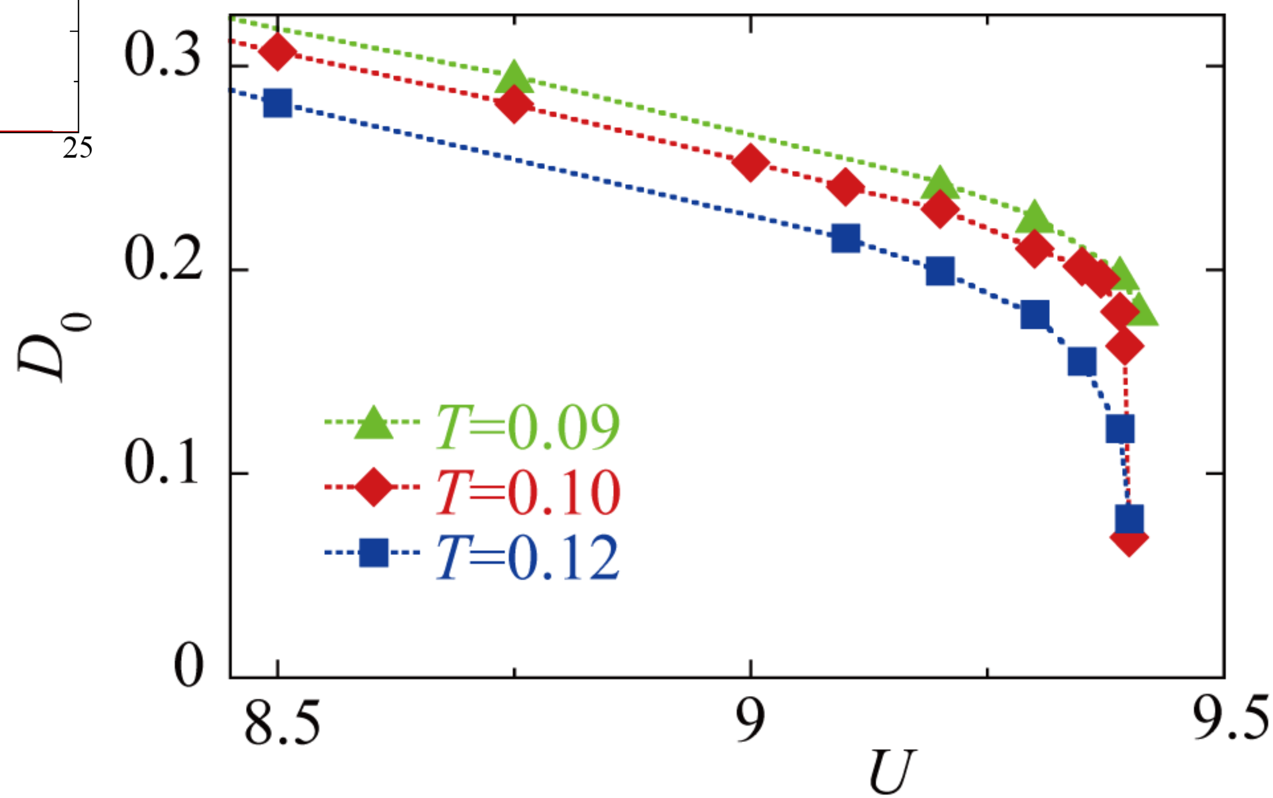
Try another quantity as a scaling variable:
$\rightarrow$ the weight of a low-energy peak in $\sigma(\omega)$

Low-ω Peak (metallic side)

➢Metal side: Drude peak

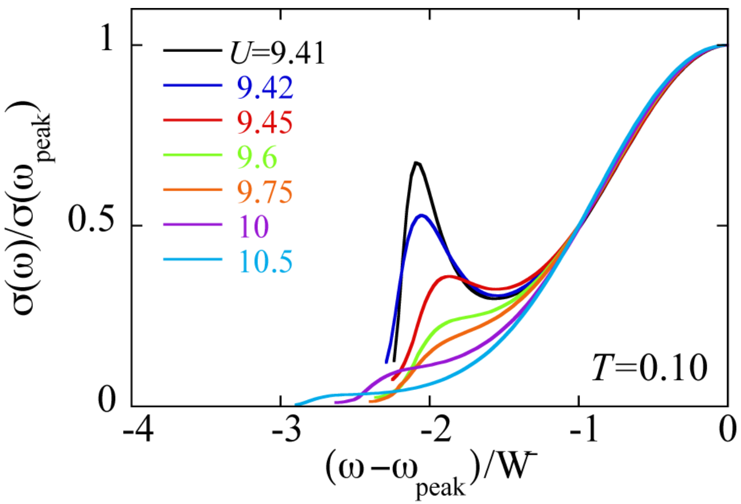


Sharp decrease of the Drude weight with approaching the critical point



Low-ω Peak (insulating side)

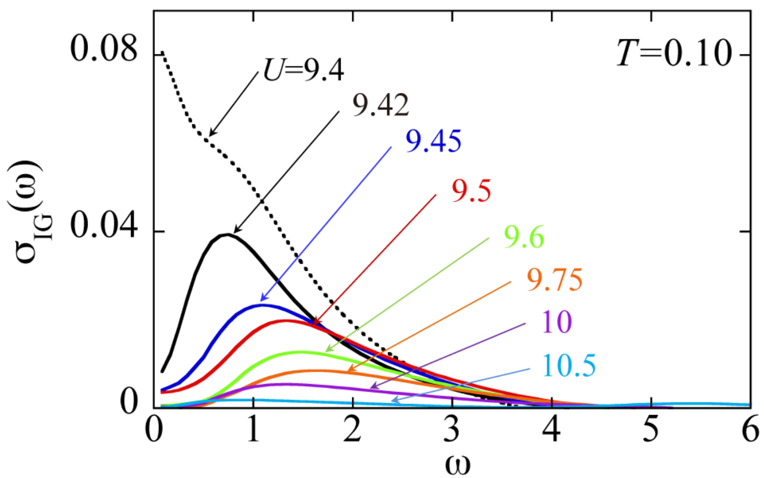
➢Insulator side: Ingap peak



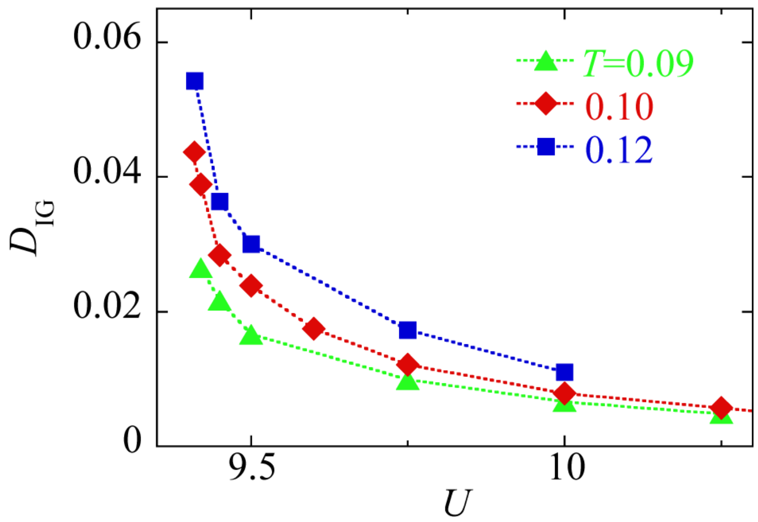
・Within the Hubbard gap, there appears an *ingap* peak.

・Subtract the part of high-energy peak, which is well approximated by Gaussian.

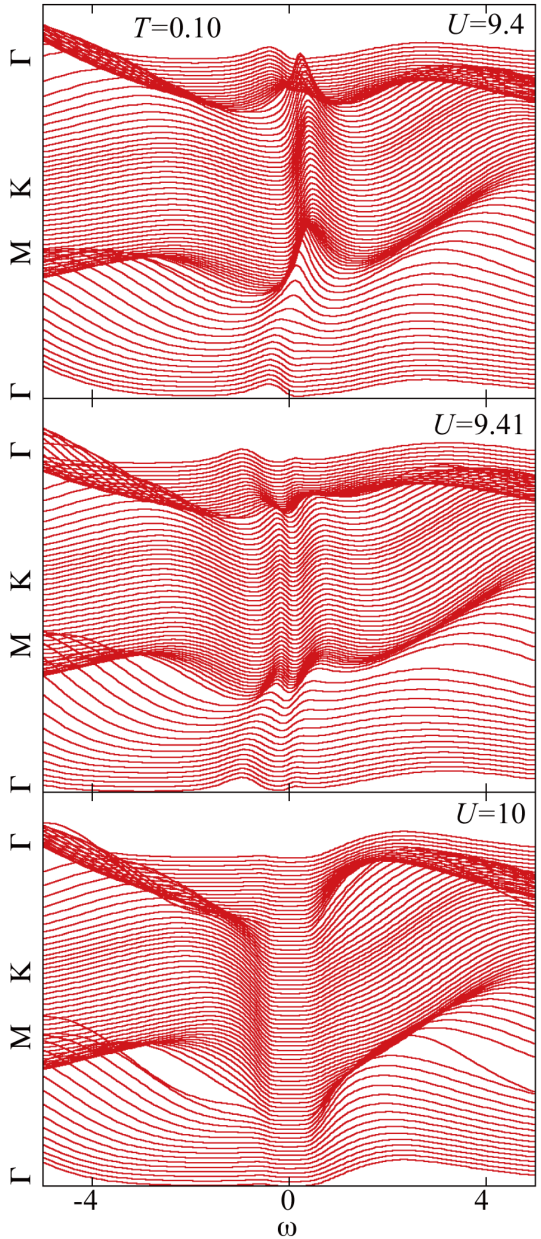
・This ingap peak evolves into the coherent Drude peak on the metallic side.



Weight of the ingap peak



Ingap peak and Electron Spectrum



metallic

heavy quasiparticle band

insulating and near the critical point

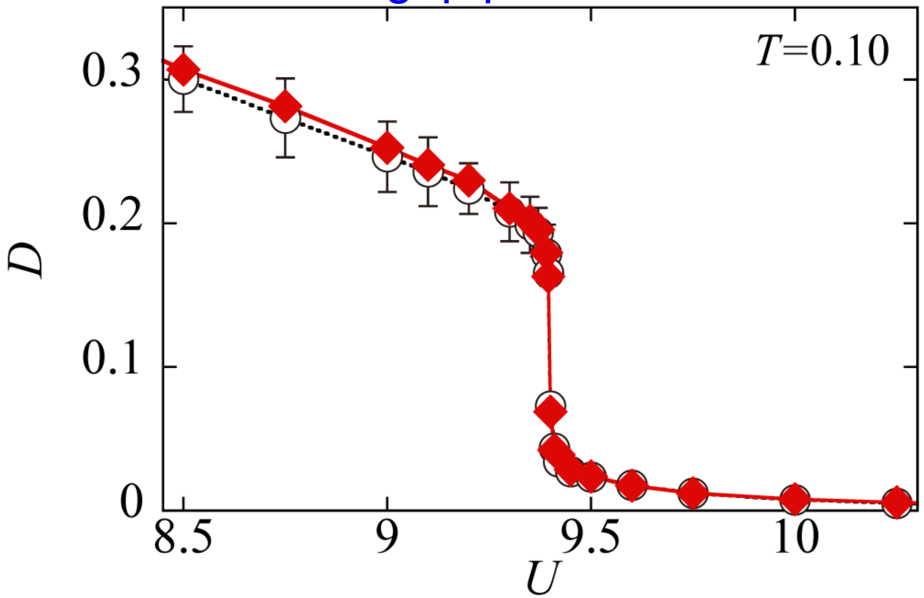
2 small peaks around ω=0
→ ingap peak in σ(ω) correspond to transition between these two

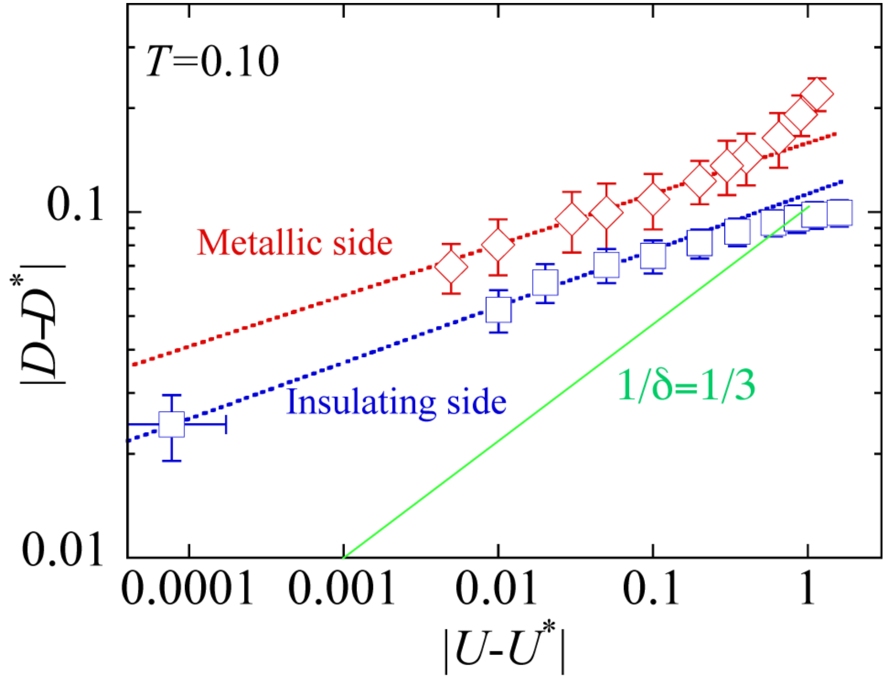
insulating

quasiparticle has dissappeared

Scaling analysis of low-ω peaks

Drude+ingap peak





$$\left|D - D^*\right| \approx A_\pm \left|U - U^*\right|^{1/\delta_c^\pm}$$

$$1/\delta_c^- = 0.15 \pm 0.08$$

$$1/\delta_c^+ = 0.16 \pm 0.05$$

a power-law singularity
with the same exponent
on both sides now

The determined transport exponent differs from
Ising universality class
the exponent of order parameter vs. conjugate field at T_c
1/δ=1/3 (MF), 1/15 (2D Ising), ~1/5 (3D Ising)

Summary

We have calculated optical conductivity $\sigma(\omega)$ of triangular-lattice Hubbard model.

Calculation is performed by Cluseter DMFT with Continuous-Time QMC solver for cluster Green's function and includes vertex corrections

(1) We have observed a critical behavior in optical weight at the Mott transition

(2) Exponent = ~0.15
does not agree with thermodynamic exponent of Ising universality class
[in any dimensions , also exclude simple expectation of mean-field exponent]

(3) A small peak emerges within the "Mott gap" with approaching crititcal point on the insulating side (INGAP peak)
(4) Ingap peak seems to evolve into the Drude peak with U↓
(5) Weight of Drude and ingap peaks are good scaling variable

Outlook

(A) How to explain the new exponent theoretically?

(B) Comparison to experimental data. Hubbard model is enough?