The Abdus Salam International Centre for Theoretical Physics

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School and Workshop on Highly Frustrated Magnets and Strongly Correlated Systems: From Non-Perturbative Approaches to Experiments

30 July - 17 August, 2007

Strongly Correlated Electrons on Frustrated Lattices

Hirokazu Tsunetsugu
University of Tokyo,
Japan

School and Workshop on *"Highly Frustrated Magnets and Strongly Correlated Systems: From Non-Perturbative Approaches to Experiments"*
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Strongly Correlated Electrons on Frustrated Lattices

(ISSP, Univ of Tokyo) Hirokazu Tsunetsugu

collab./w
(Osaka Univ.) Takuma Ohashi
(Kyoto Univ.) Norio Kawakami
(RIKEN) Tsutomu Momoi

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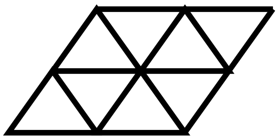
OUTLINE

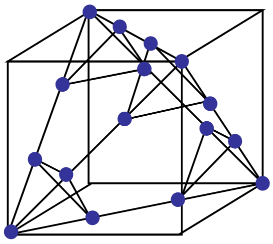
- Motivation
- [A] Kagomé Lattice Hubbard model
  - Mott transition and charge fluctuations
  - 1D-type spin correlation
  - quasiparticle
- [B] Anisotropic Triangular Lattice Hubbard Model
  *** effects of reduction of frustration **
  - slope of Mott transition line - entropy effects
  - heavy quasiparticle formation and metal-insulator transition
- Summary

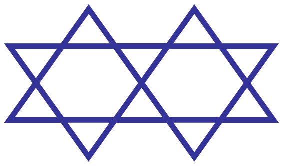
Correlated electron systems with geometrical frustration



Triangular

Pyrochlore





Kagomé

Many interesting systems:

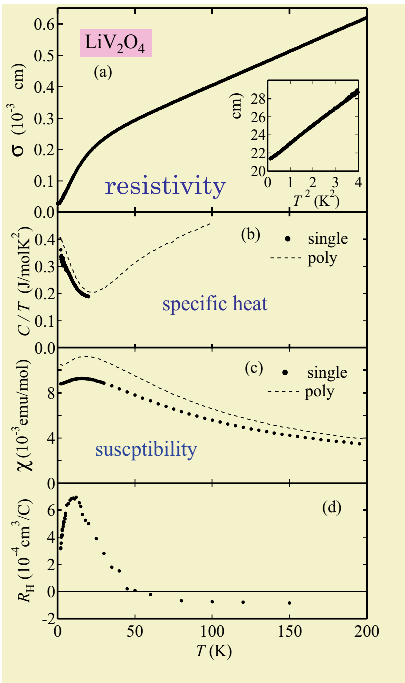
- •Superconductivity — $Na_xCoO_2 \cdot yH_2O$, AOs_2O_6
- •Heavy Fermion — LiV_2O_4, etc
- •Quantum spin liquid — κ-$(ET)_2Cu_2(CN)_3$

(Ex.) LiV_2O_4 – Heavy Fermion behavior

[Ref: Kondo et al, Urano et al.]

V ions ⇒ pyrochlore lattice

- NO f-electrons ($V^{3.5+}$:$(3d)^{1.5}$)
- Specific heat
  $\gamma \sim 200$[mJ/K^2 V-mol]
- Wilson ratio
  $R_W \sim 1.7$



Large low-energy entropy
characteristic to frustrated lattice
participate to heavy
quasiparticle formation?

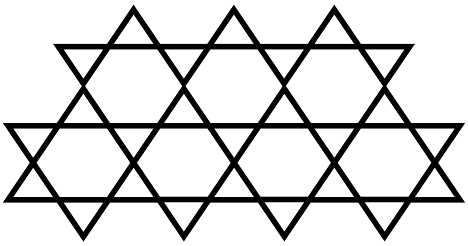
Large reduction of energy scale is due to GF?

PART A

Mott Transition in Kagomé Lattice Hubbard Model

[Ohashi, Kawakami, and Tsunetsugu, Phys. Rev. Lett. **97** ('06) 066401]

Kagomé Lattice Hubbard Model



$$H = -t \sum_{\langle i,j \rangle, \sigma} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

- 2D analog of pyrochlore lattice
- Effective model of $Na_xCoO_2 \cdot yH_2O$
  Koshibae & Maekawa PRL 91, 257003 (2003)
  Bulut, Koshibae, & Maekawa PRL 95, 37001 (2005)
- Spin systems on Kagomé lattice
  ⇒ unusual properties (gapped triplet, gapless singlet excitations)
  [today's morning sessions]

Relation btw charge fluctuations and spin correlations
Relation btw spin correlations and quasiparticle coherence
[fix density at half filling n=1]

Method

Metal-insulator transition in Kagomé lattice Hubbard model at half filling

- strong correlation
- geometrical frustration
- short-range quantum fluctuations ⇒ DMFT

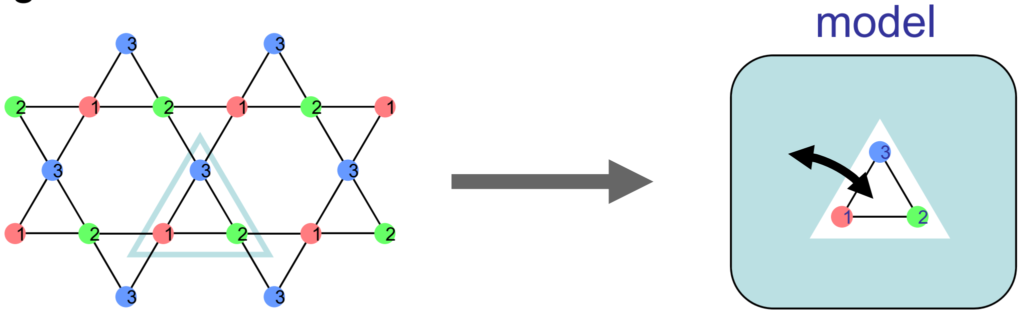
Cluster extension of DMFT:
Cellular dynamical mean field theory (CDMFT)

Kotliar, et al. PRL 87, (2001)
Lichtenstein & Katsnelson, PRB 62, (2000)
...

Cellular-DMFT

Kagomé lattice Hubbard model

Effective cluster model



$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

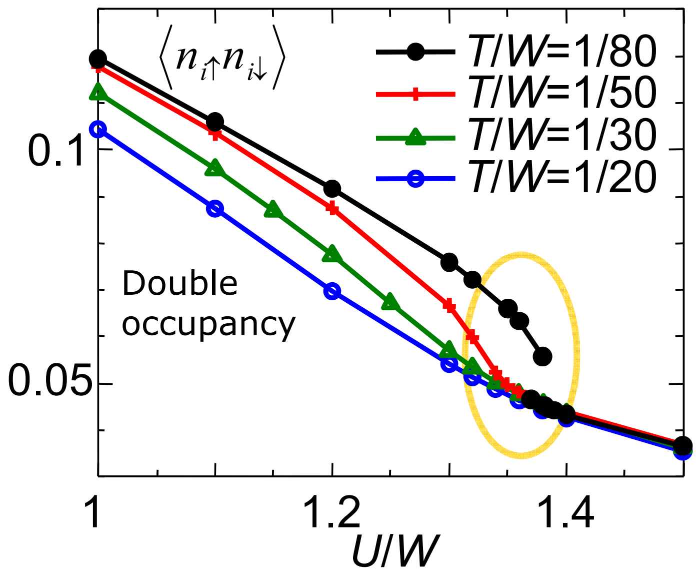
QMC
Hirsch & Fye,(1986)

Self-energy: 3x3 matrix $\Sigma_{ij}(\omega)$

- Spatially extended correlation
- Geometrical frustration

25000 k-points
L_β=12/T
10^6 QMC sweeps

Mott transition



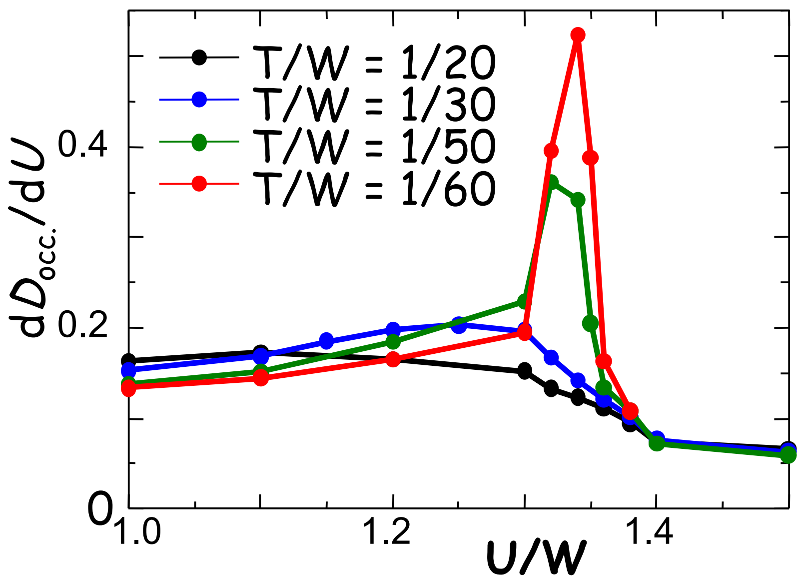
Band width: W=6t

- High temperature
  T/W>1/80
  crossover U^*∼1.35
- Low temperature
  T/W=1/80
  1st order transition
  with hysteresis:
  U_c∼1.37

square lattice:
U_c∼0.5-1.0

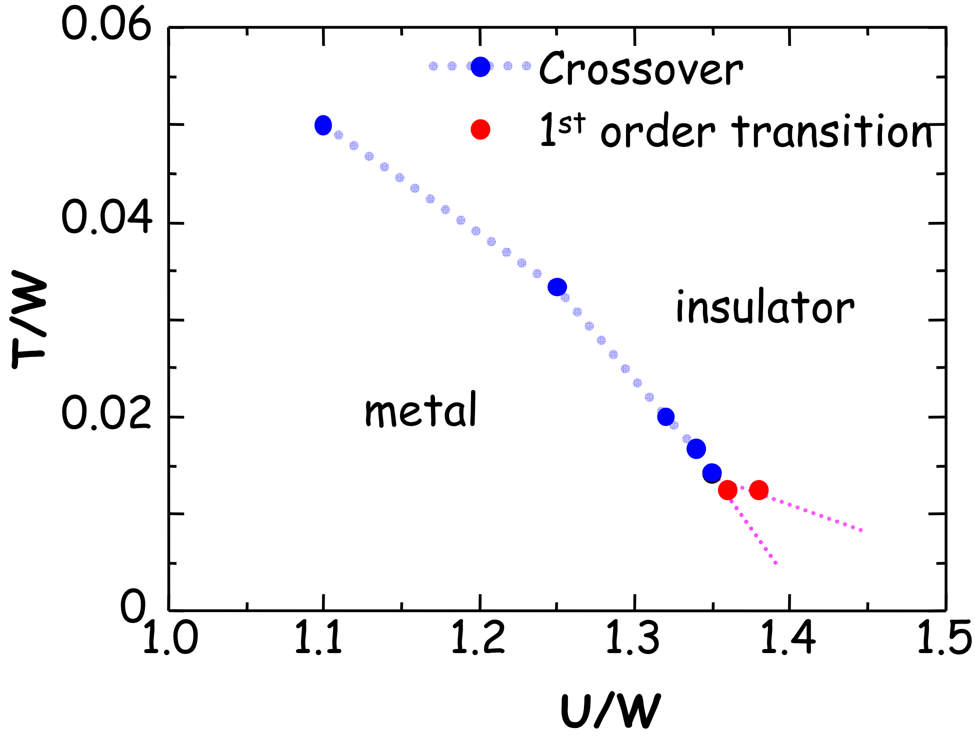
Larger critical value U_c

Crossover



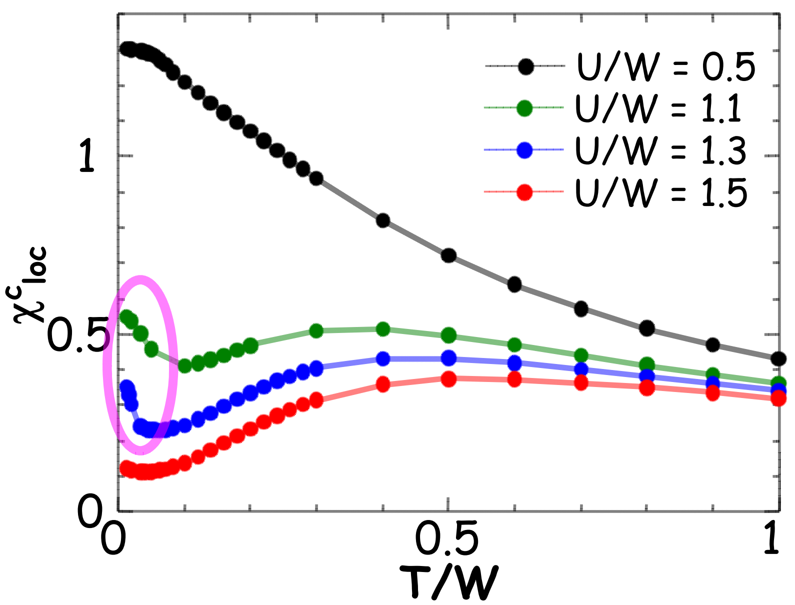
Define metal-insulator crossover points $U^*(T)$
by largest change in double occupancy

Phase diagram



Mott transition in Kagome Hubbard model

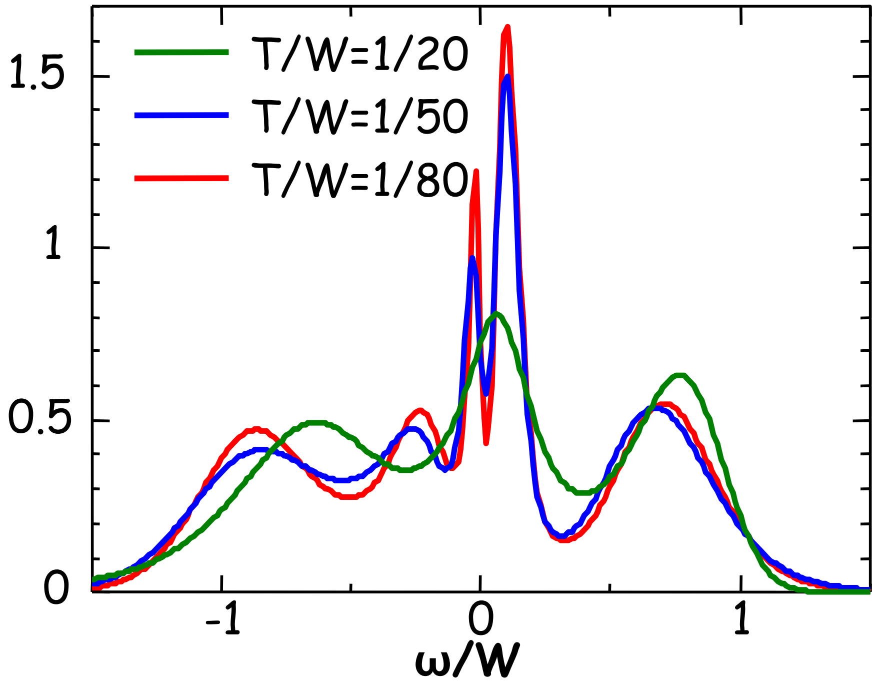
Local charge susceptibility



Charge response grows once again
in low-T metallic region

Density of States: U/W=1.1

Evolution of heavy quasiparticles at low temperatures

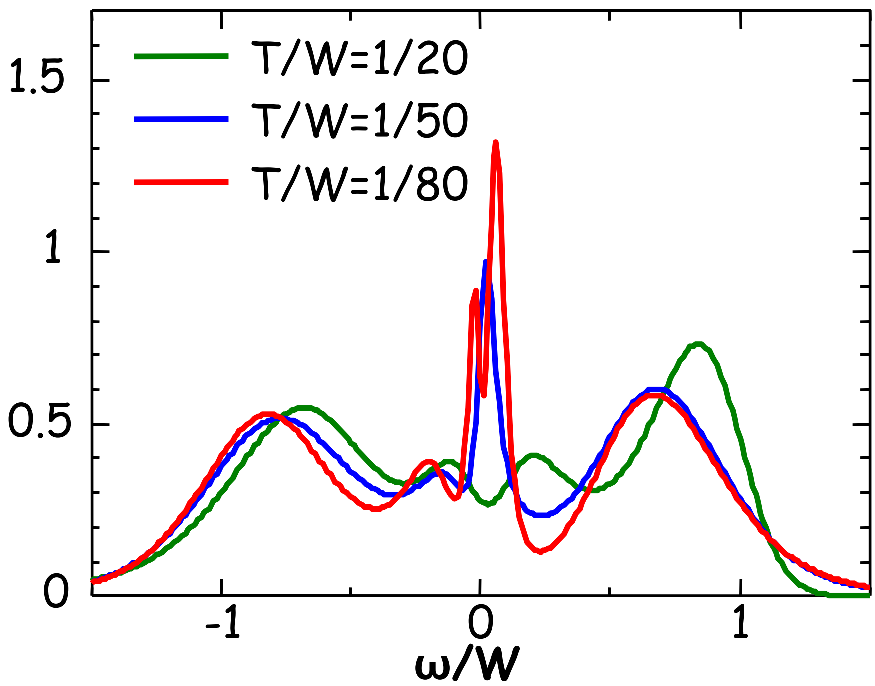


Density of States: U/W=1.3

Precursor of insulating behavior

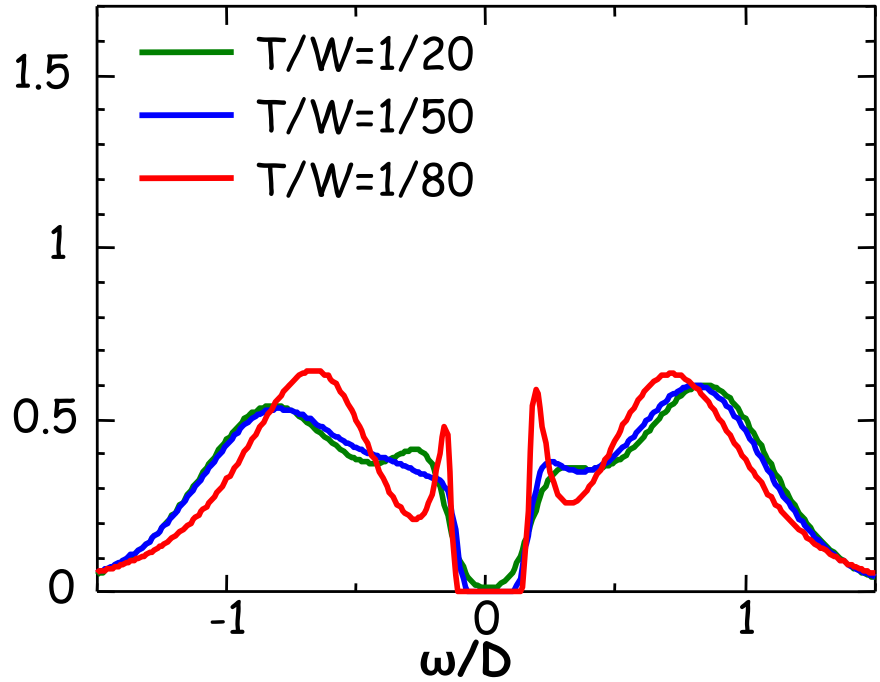
+

Evolution of heavy quasiparticles at low temperatures



Density of States: *U*/*W*=1.5

Clear formation of Mott gap



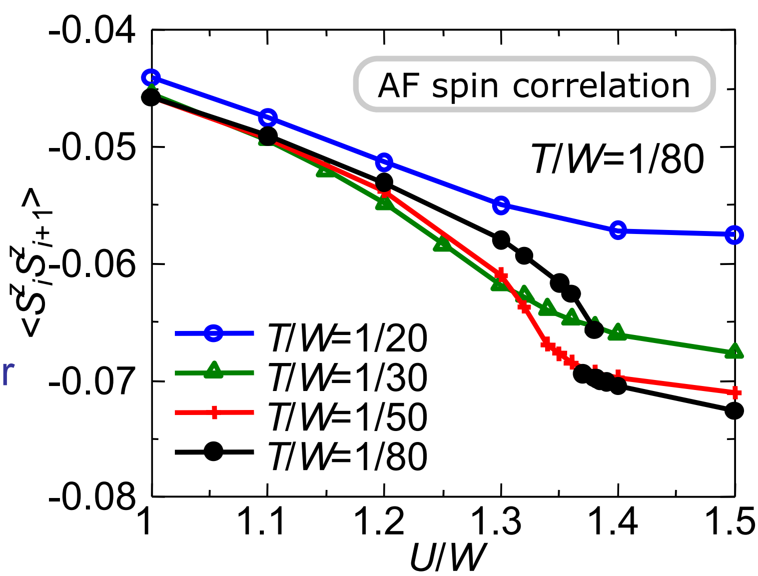
Spin correlation function

Nearest-neighbor spin correlation $\langle S_i^z S_{i+1}^z \rangle$

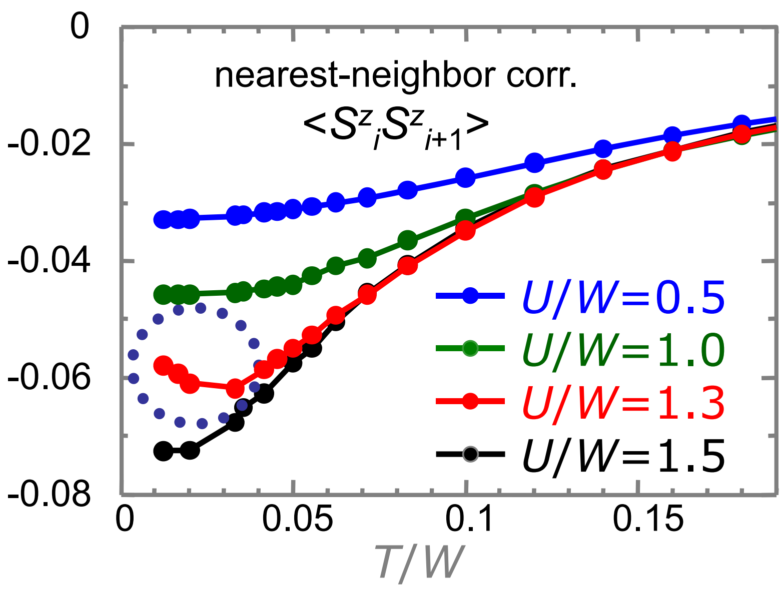
Insulating phase:
AF correlation ⇒ monotonic enhancement

Metallic phase:
Nonmonotnic behavior

Recover of itinerancy



Temperature Dependence of Spin Correlations



- Antiferromag.
- **insulator:** Monotonic growth of AF correlation
- **correlated metal:** Nonmonotonic T-dep

Suppressed AF correlation at low-T

↓

Characteristic for frustrated systems near MIT

- recovery of coherence
- relax frustration

Dynamical Susceptibility near Mott Transition

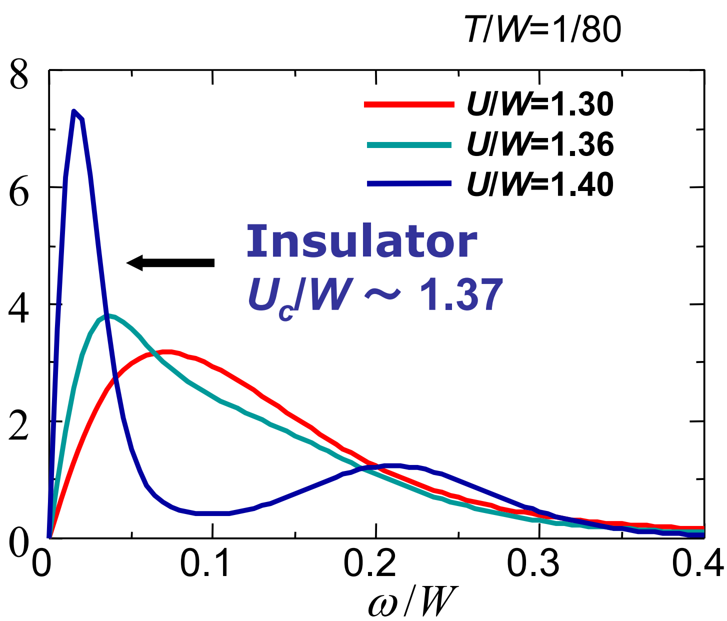
Imaginary part of local susceptibility

$$\chi_{loc}(\omega) = -i \int \left\langle \left[S_i^z(t), S_i^z(0) \right] \right\rangle e^{-it\omega} dt$$

metal ⇒ insulator

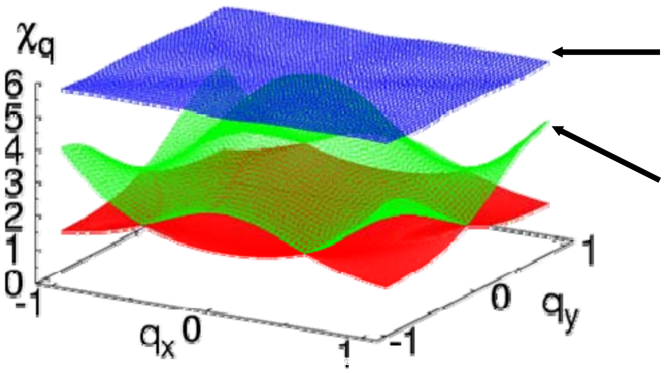
Double peak

Metallic phase:
Renormalized single peak



Magnetic instabilities

Static susceptibility $\chi_m(\boldsymbol{q})$: 3 magnetic modes

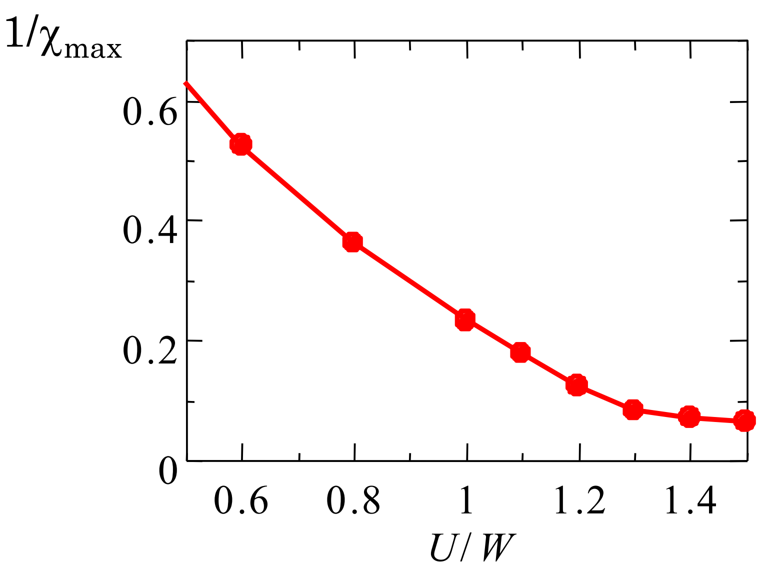


- maximum mode: weak q-dependence <- *geometrical frustration*
- second largest mode: maximum at q=(0,0)

Consistent with previous studies

- FLEX approximation
  Imai, et al., PRB 68, 195103 (2003)
- QMC simulation
  Bulut, et al. PRL 95, 37001 (2005)

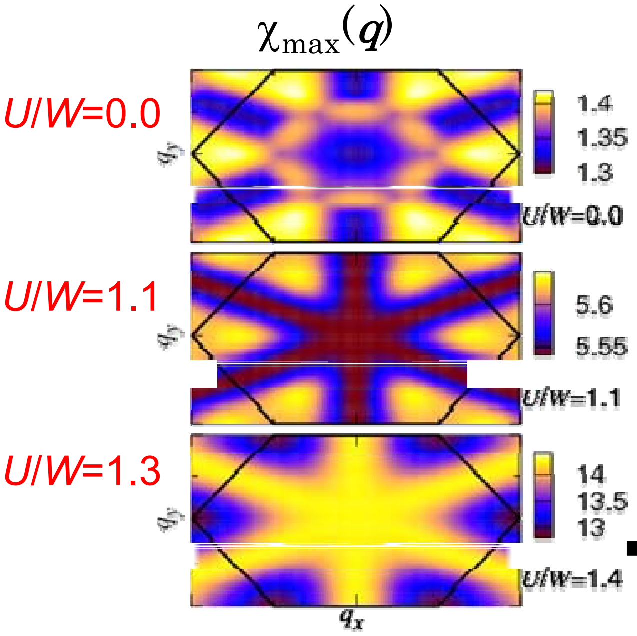
Suppressed Magnetic Instability



T/W=1/30

Mott transition : $U_c/W \sim 1.35$

Wavevector dependence of dominant mode



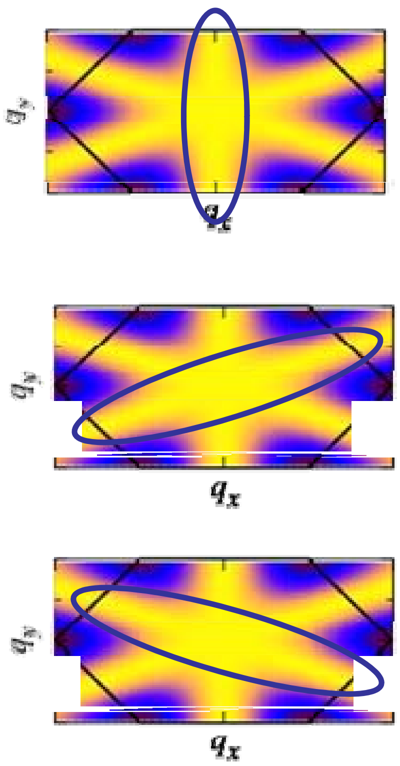
Metallic phase

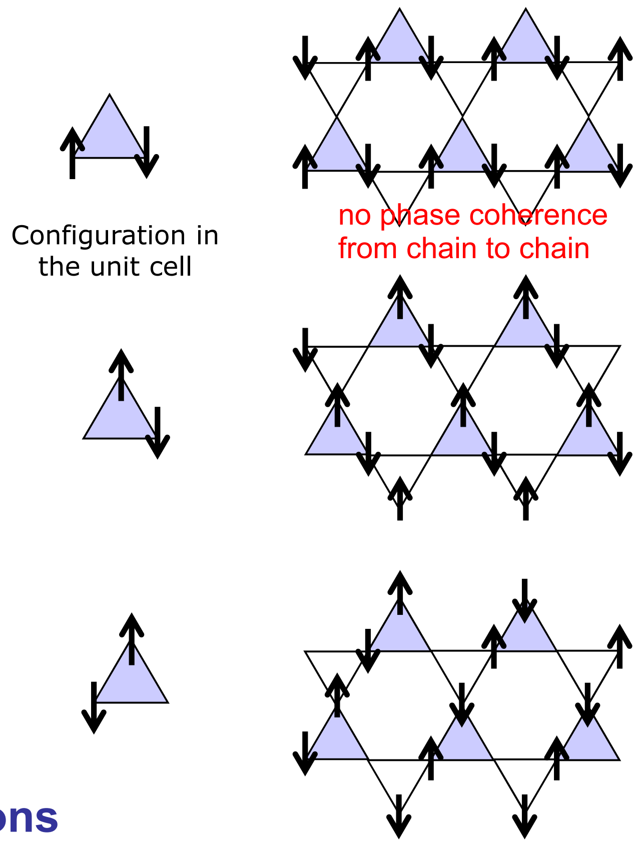
Leading magnetic mode:
6 points ⇒ nesting

Insulating phase
Leading magnetic mode:
Three lines in the B.Z. ⇒
1-dimensional order

temperature: T/W=1/30

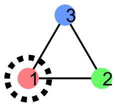
Spin correlations in the real space





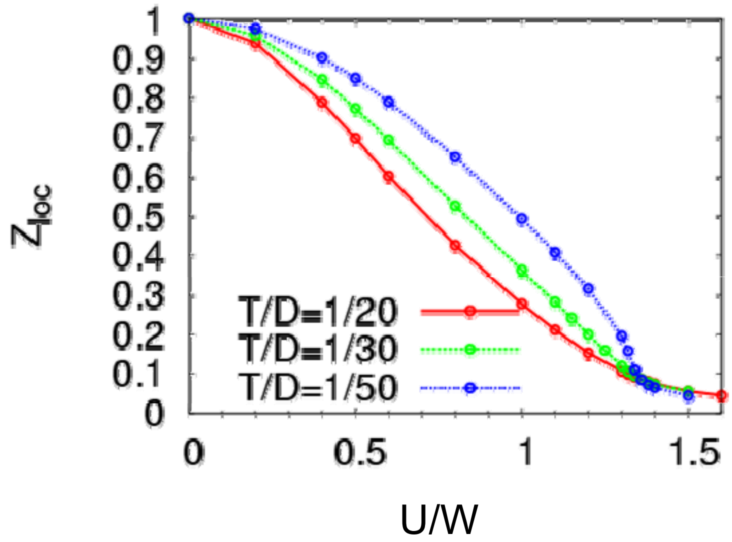
1-dim. spin correlations

Quasiparticle Renormalization Factor



self energy $\Sigma_{11}(i\omega_n)$ → Renormalization factor Z_{loc}

Mass enhancement
～ 10-20
near Mott transition



PART B
Mott Transition in Anisotropic Triangular-Lattice Hubbard Model

- Phase Boundary Topology
- Heavy Quasiparticles

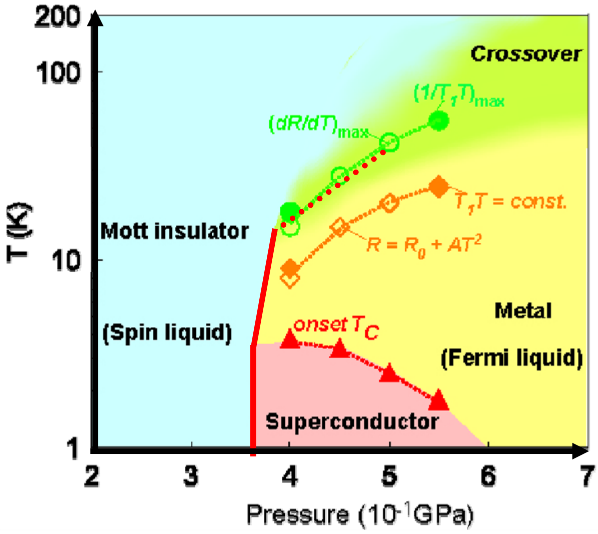
[Ohashi, Momoi, Tsunetsugu, and Kawakami, in preparation]

Mott transition in κ-type organic materials

STRONG frustration

κ–(BEDT-TTF)$_2$-Cu$_2$(CN)$_3$

Y. Kurosaki et al., PRL 95, 177001 (2005)

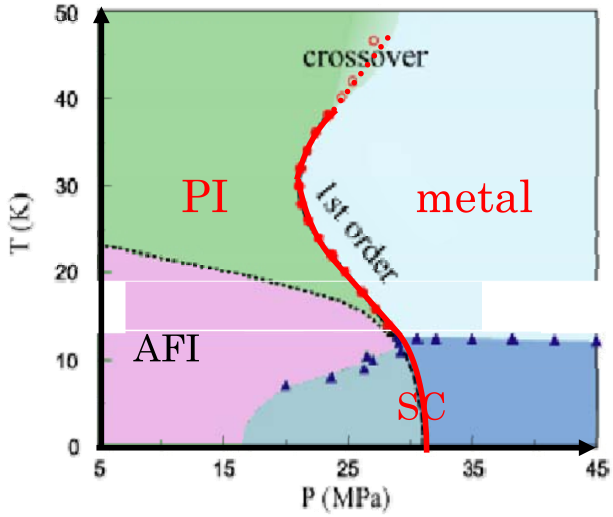


[talk by Kanoda, Aug. 8]

INTERMED. frustration

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

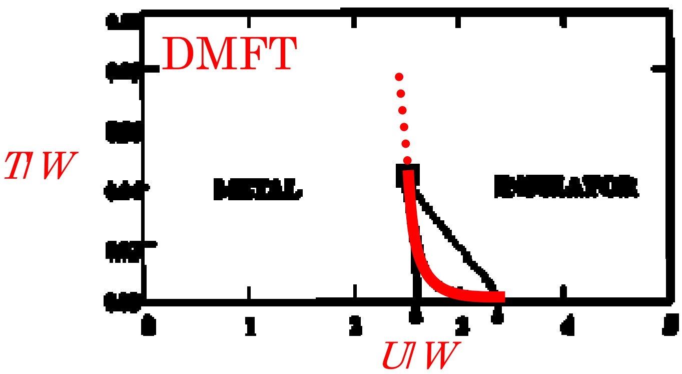
F. Kagawa et al., PRB 69, 064511 (2004)



Reentrant !!

Mott transition line in Phase Diagram

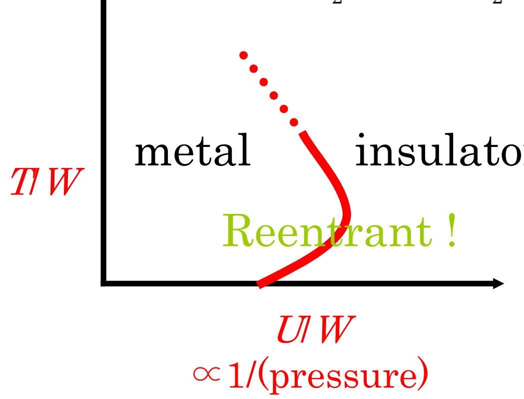
d=∞ Hubbard model



Georges et al., RMP, 68, 13 (1996)

organic conductor

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

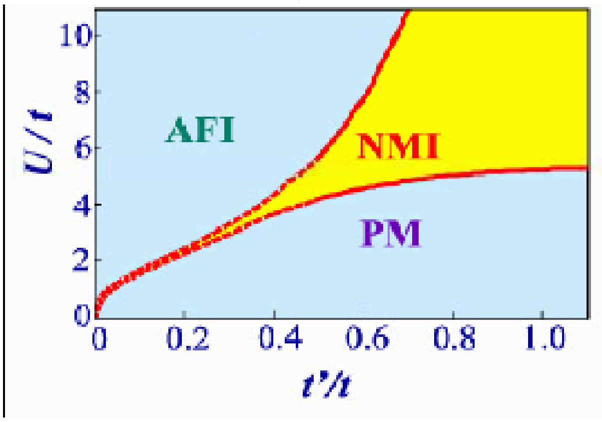


Anisotropic Hubbard model → Cellular-DMFT

effects of 1-site approx. or frustration?

Previous studies

PIRG results



Ground state

- PIRG
  Kashima & Imada, JPSJ 70, 3052 (2001).
- Cellular-DMFT + ED
  Kyung & Tremblay, PRL 97, 046402 (2006).
- Variational Monte Carlo
  Watanabe et al., JPSJ 75, 074707 (2006).
- Exact Diagonalization
  Koretsune, Motome, & Furusaki, cond-mat/0703111.

Finite temperature

Cellular-DMFT + QMC
Parcollet et al., PRL 92, 226402 (2004)

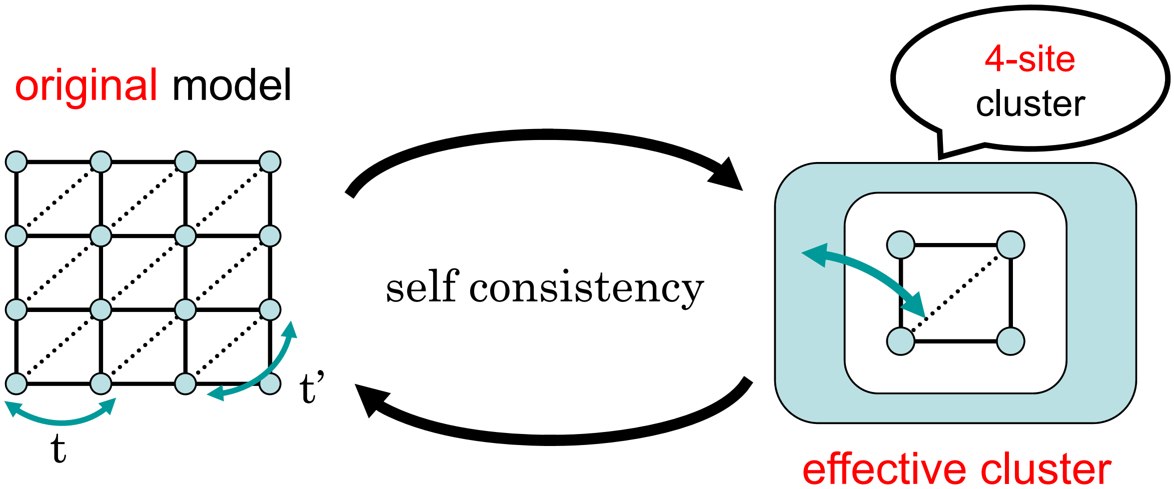
Correlator Projection method
Onoda & Imada, PRB 67, 161102 (2003).

Finite-T Mott transition

RG & MF
Onoda & Nagaosa, JPSJ 72, 2445 (2003).

Cellular-DMFT for Anisotropic Triangular Lattice Model

original model



effective cluster model

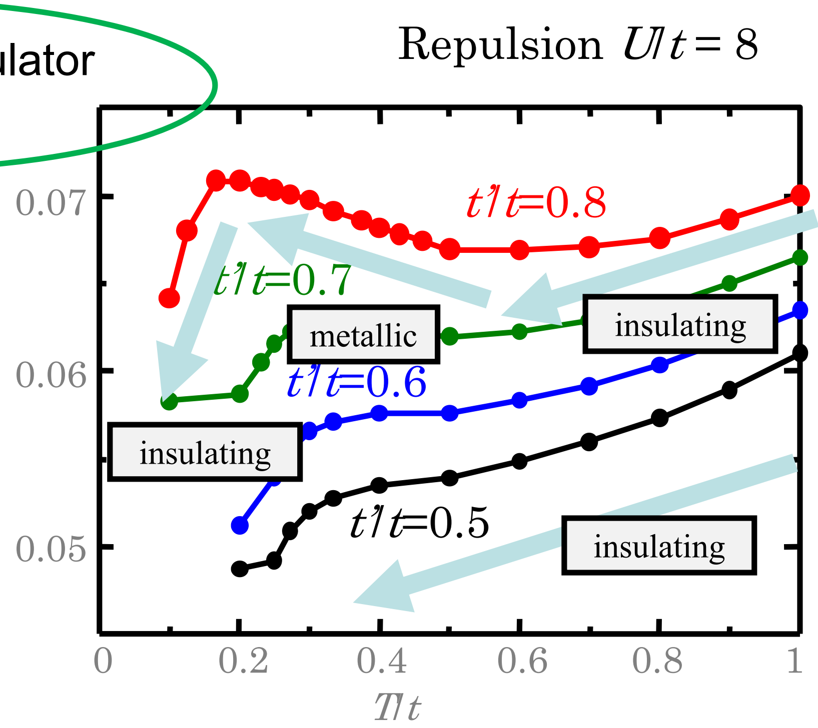
anisotropic triangular lattice
- t'/t=0: regular square
- t'/t=1: regular triangular

Quantum Monte Carlo Simulation (Hirsh-Fye algorism)

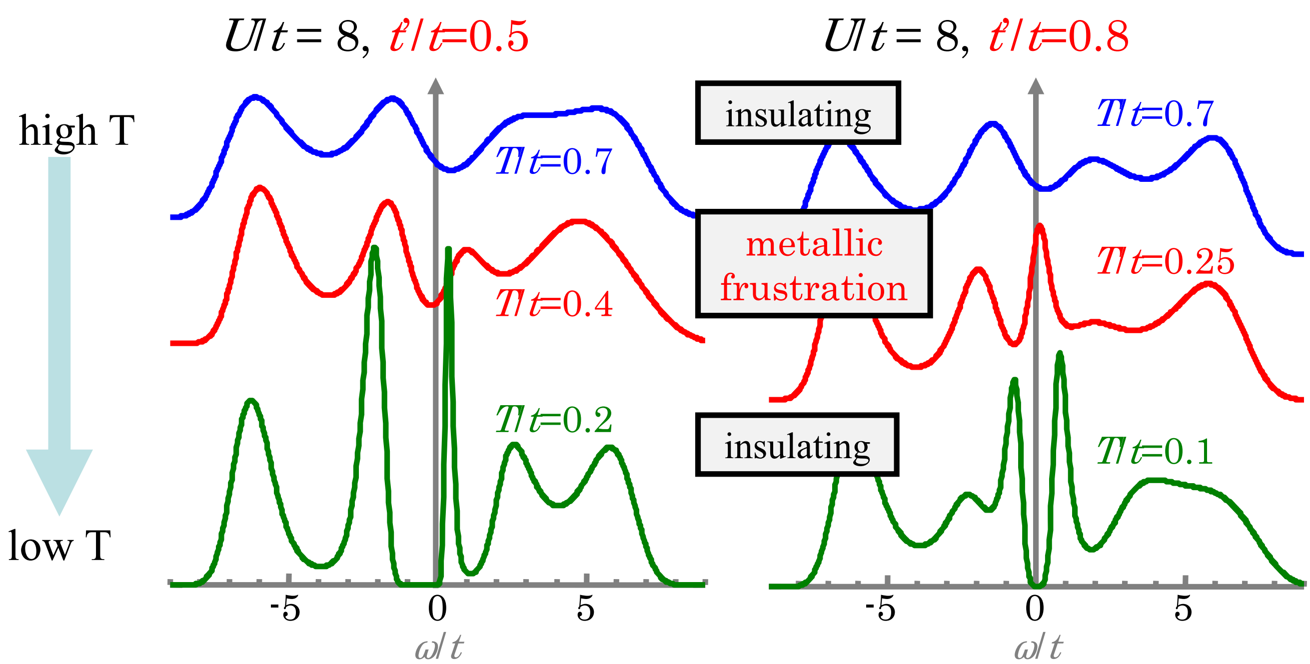
T-Dependence of Double Occupancy

Insulator-Metal-Insulator Transition?

- large t'-strong GF: nonmonotonic T-dep.
- small t'-weak GF: almost monotonic insulating



Electron Spectral Function

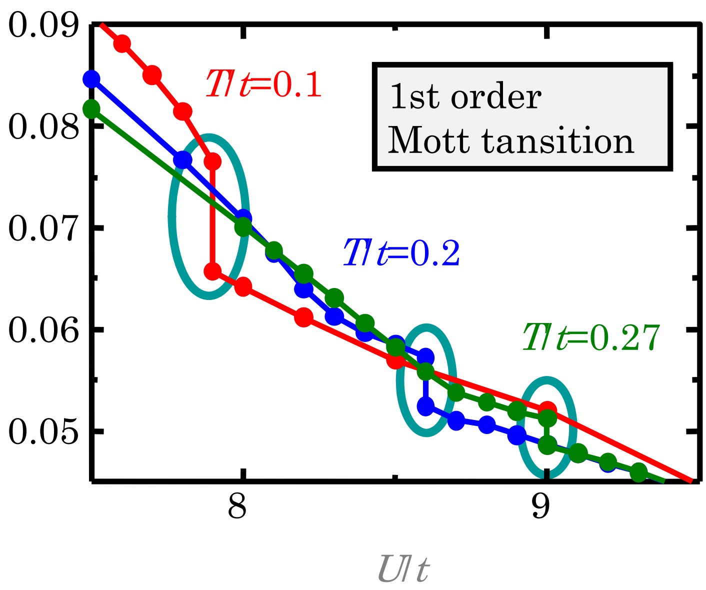


gap emerges :insulating

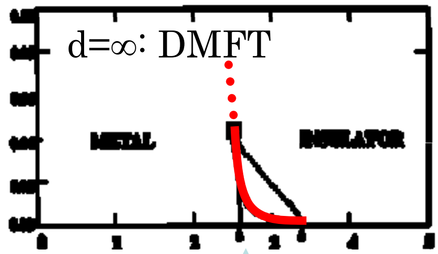
Reentrant: I→M → I

Mott Transition

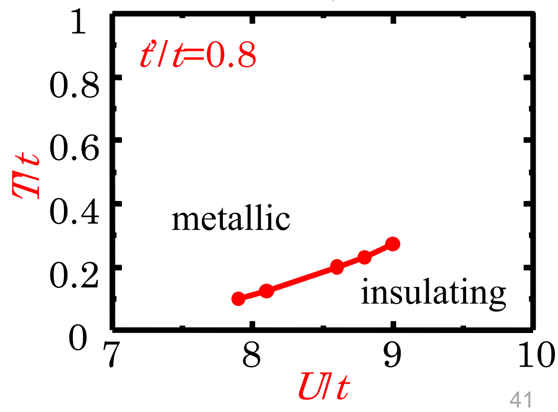
U-dep of double occupancy



higher T ⇒ larger U_c

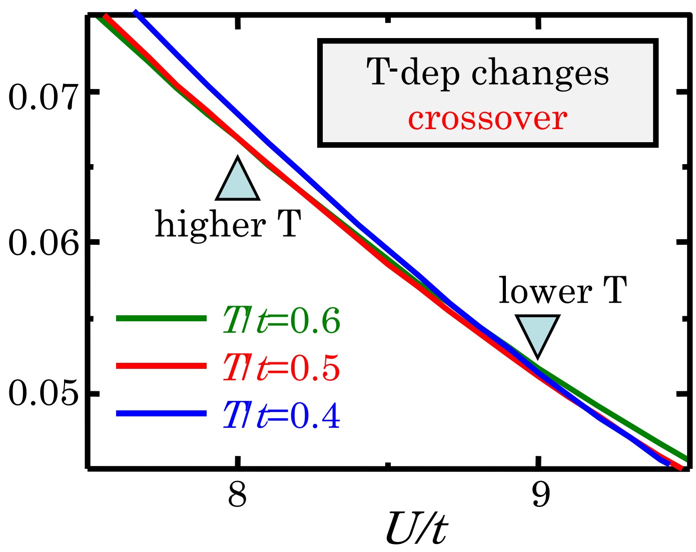


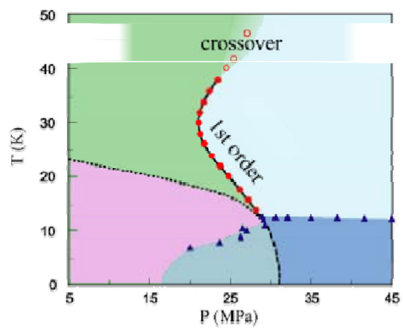
T-dep reversed

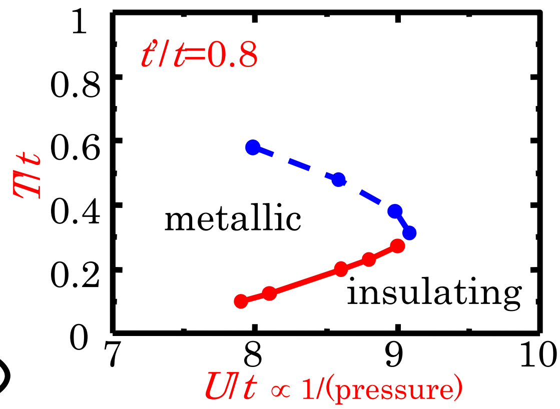


Crossover at a higher temperature

U-dep of double occupancy





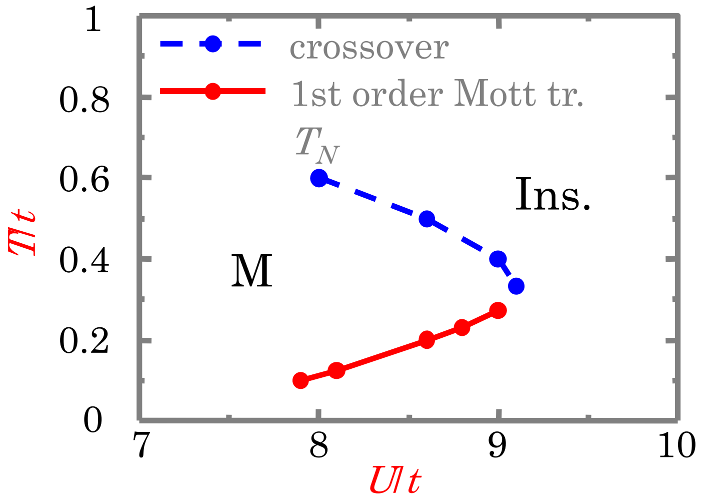


Reentrant !!

Comparison with Organic Materials

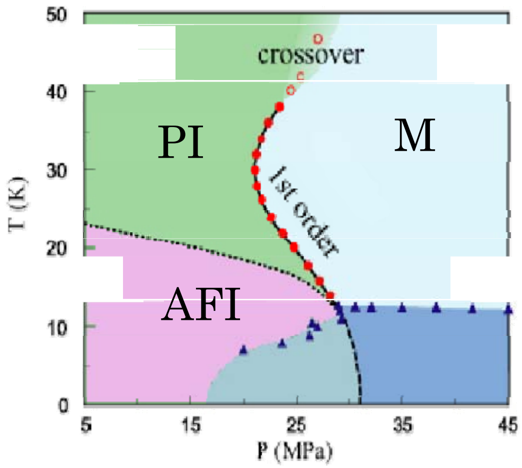
consistent with experiments

anisotropy: $t'/t=0.8$



Maier et al., PRL 85, 1524 (2000)

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



$\propto 1/U$

Summary (1)

Kagome lattice Hubbard model

Cellular dynamical mean field theory

- Metal-insulator transition
  - 1st order transition :$U_c/W\sim 1.37$
- Strongly correlated metal
  - Whole bands are renormalized
  - large mass enhancement
  - nonmonotonic temperature dependence of spin correlation functions
- Magnetic instability
  - one-dimensional spin correlations

Summary (2)

Anisotropic Triangular Lattice Hubbard model (mainly t'/t=0.8)

Cellular dynamical mean field theory

- Metal-insulator transition
  - different shape of transition line from unfrustrated systems – entropy effects
- Intermediate Correlation Regime:
  - "reentrant" insulator → metal → insulator transition
  - heavy quasiparticle formation in the intermediate metallic phase
  - gap formation inside heavy qp band
- Magnetic instability
  - transition to paramagnetic insulator phase