YKIS 07
Kyoto
November 14, 2007

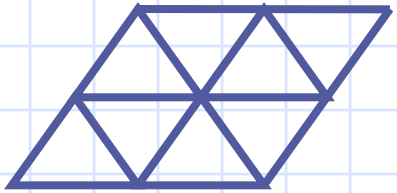
Finite-Temperature Mott Transition in 2D Frustrated Hubbard Models

Norio Kawakami
(Kyoto)

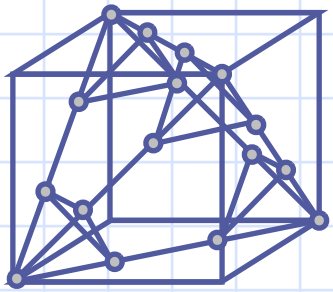
Collaborators

T. Ohashi (Osaka)
H.Tsunetsugu (Tokyo)
T. Momoi (Riken)

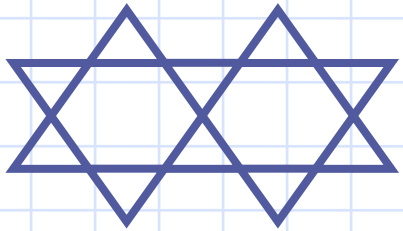
Electron Systems with Frustration



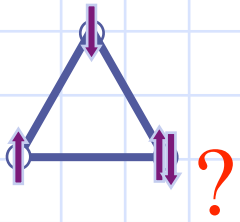
Triangular



Pyrochlore

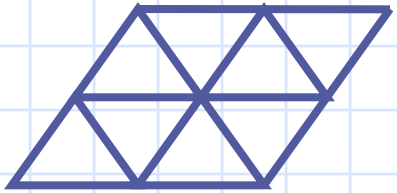


Kagomé



- **Heavy Fermion:** LiV_2O_4, etc
- **Superconductivity:** $Na_xCoO_2 \cdot yH_2O$, AOs_2O_6, etc
- **Quantum spin liquid:** κ-$(BEDT\text{-}TTF)_2$-X, etc

Electron Systems with Frustration



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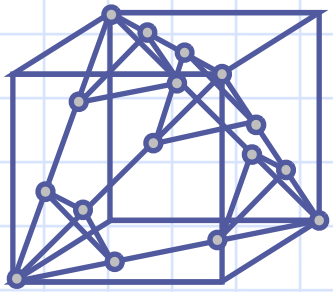

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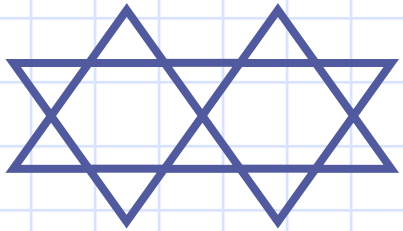

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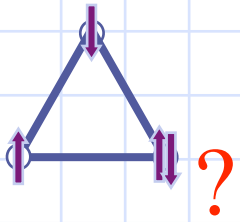

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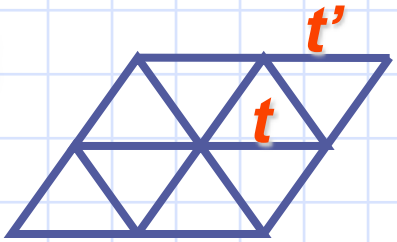
Mott Transitions
with Strong Frustration

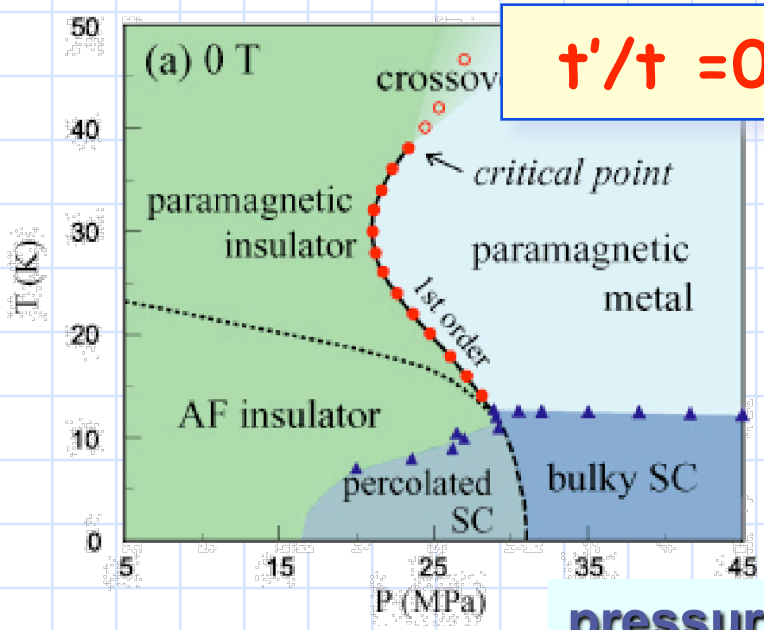
MIT in organic materials

Anisotropic triangular lattice



κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

F. Kagawa et al.(2004)

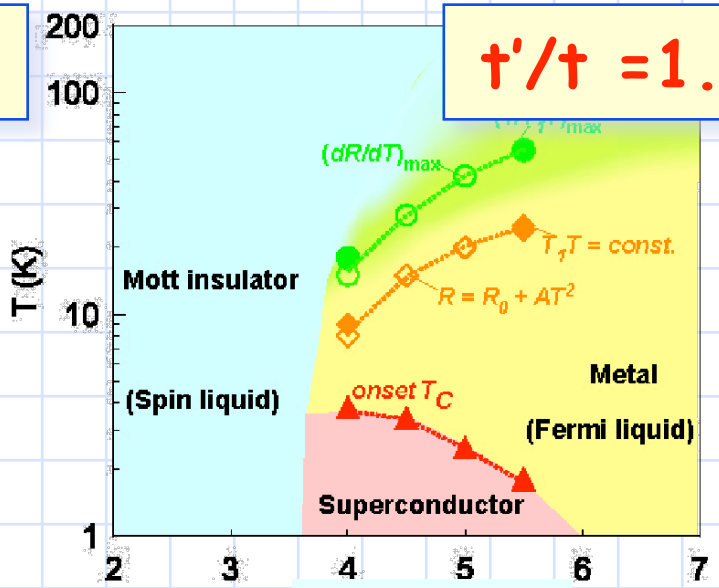


t'/t =0.75

pressure

κ-(BEDT-TTF)$_2$-Cu$_2$(CN)$_3$

Y. Kurosaki et al. (2005)

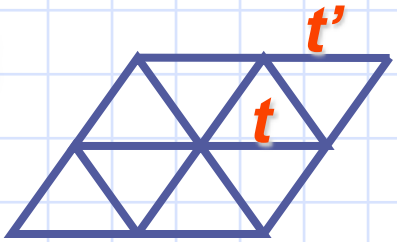


t'/t =1.06

pressure

MIT in organic materials

Anisotropic triangular lattice



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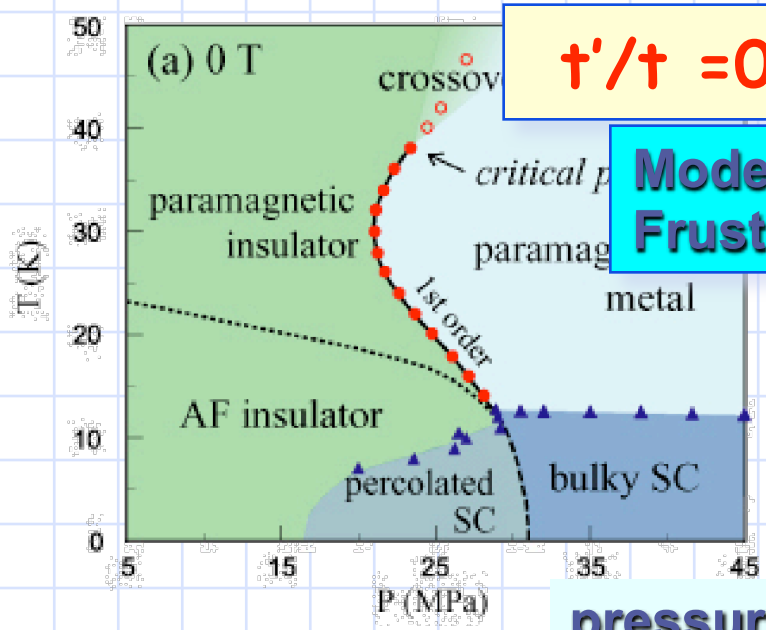

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Moderate Frustration

pressure

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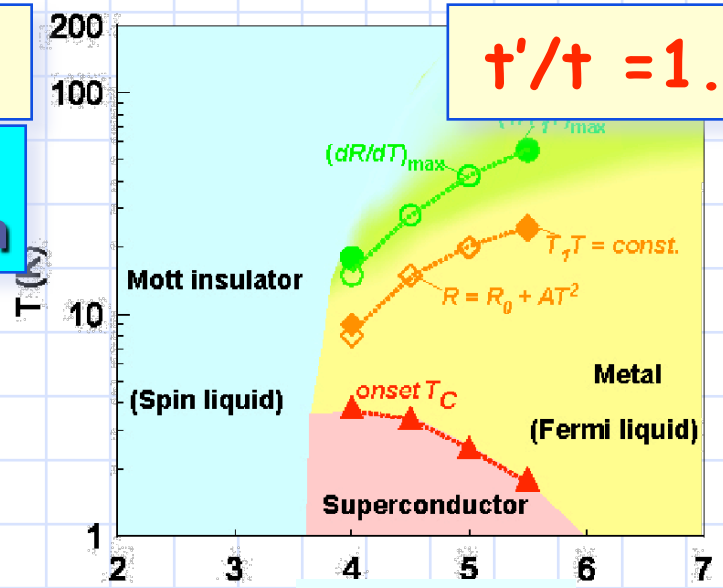

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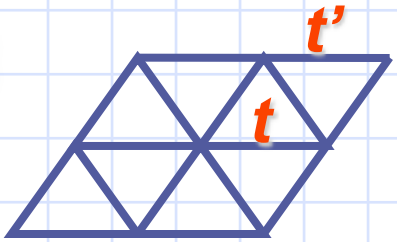
MIT in organic materials

Anisotropic triangular lattice



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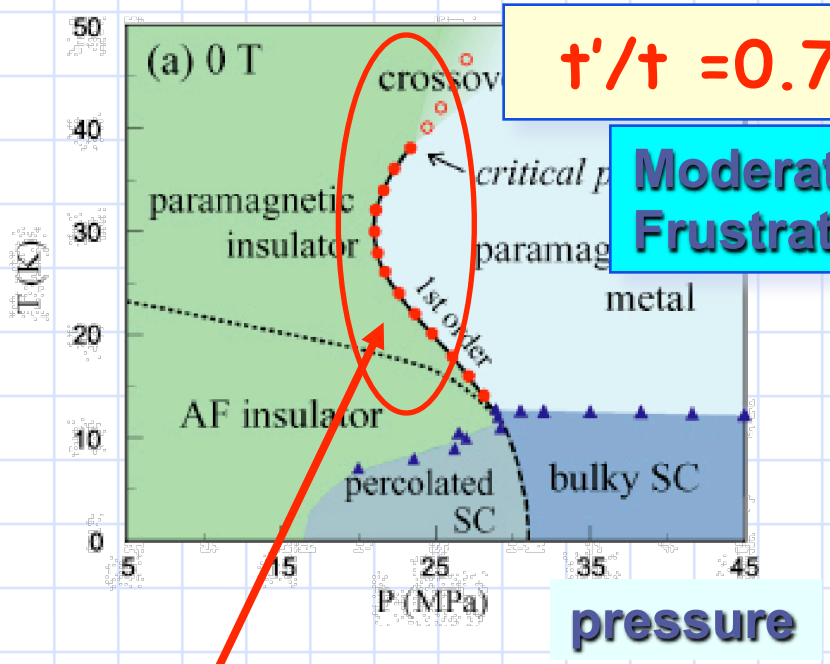

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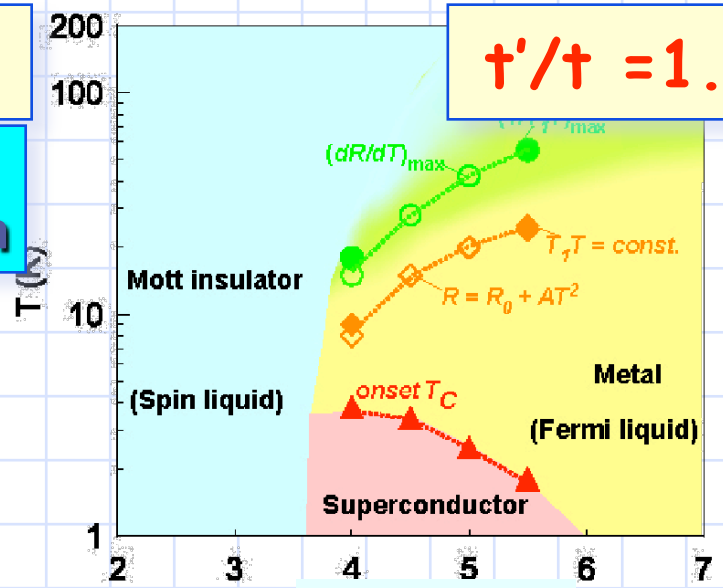

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Finite-T Mott transition

Reentrant behavior

MIT in organic materials

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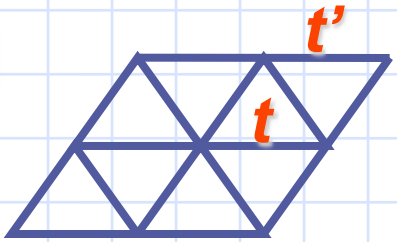

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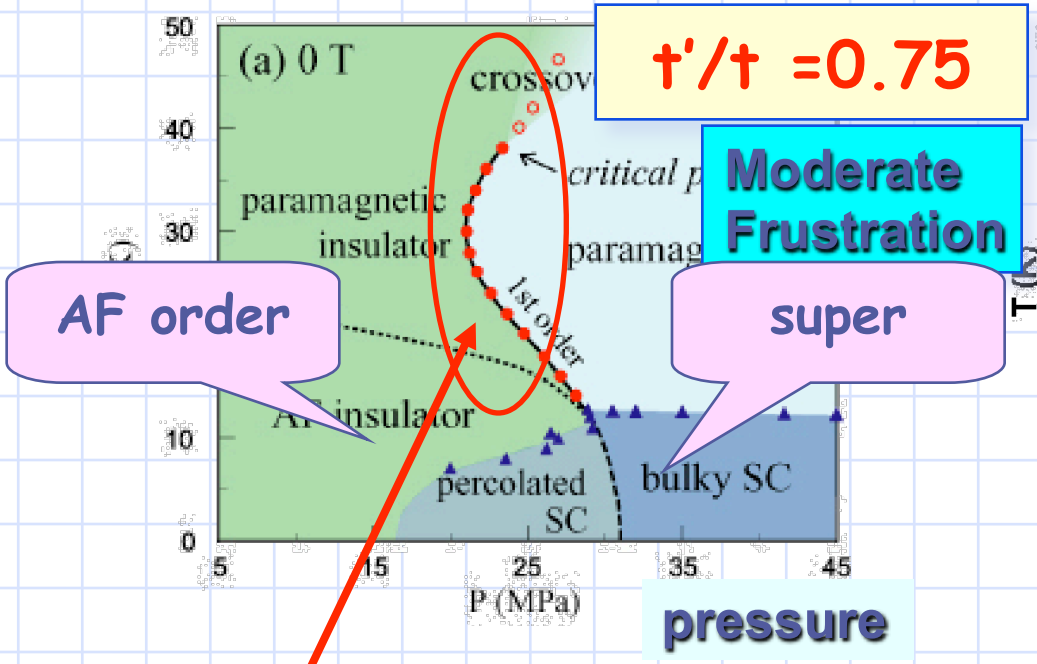

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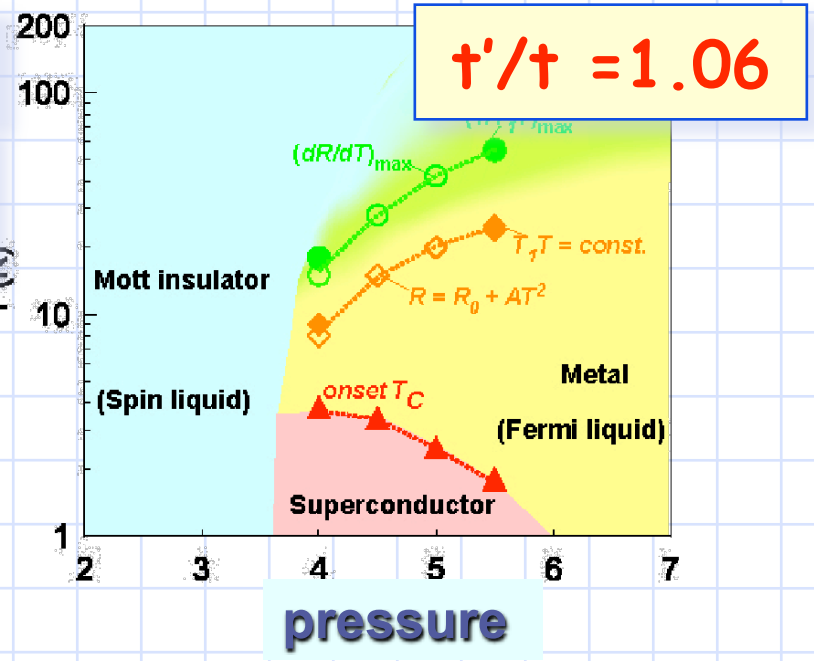
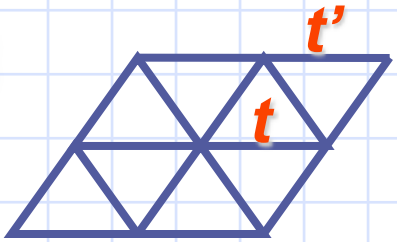


Finite-T Mott transition

Reentrant behavior

MIT in organic materials



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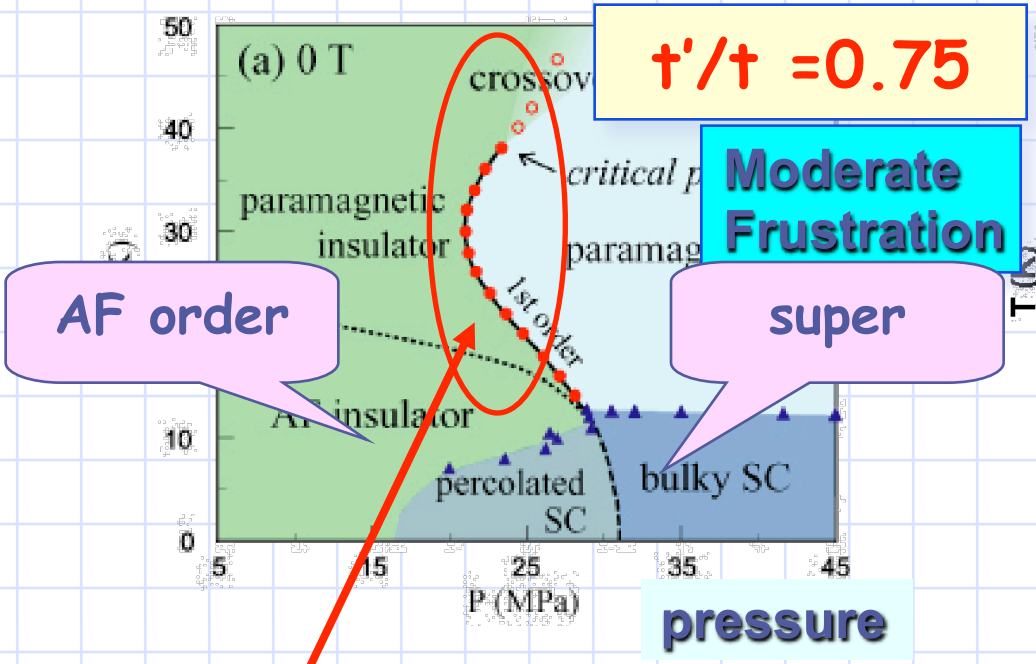

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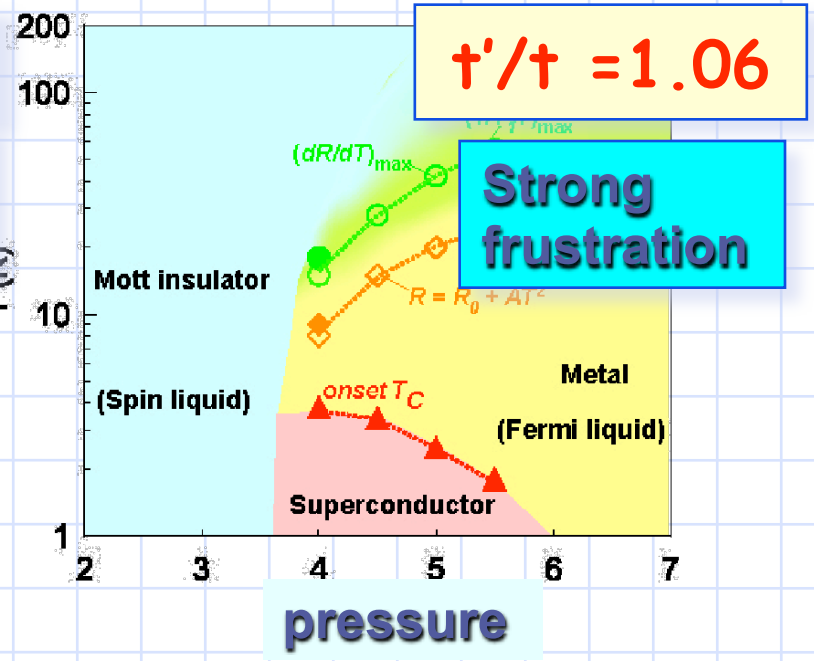

Finite-T Mott transition

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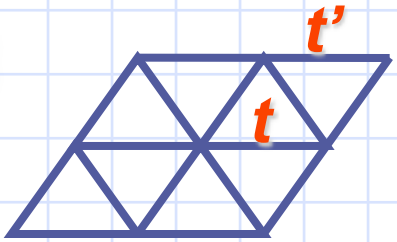

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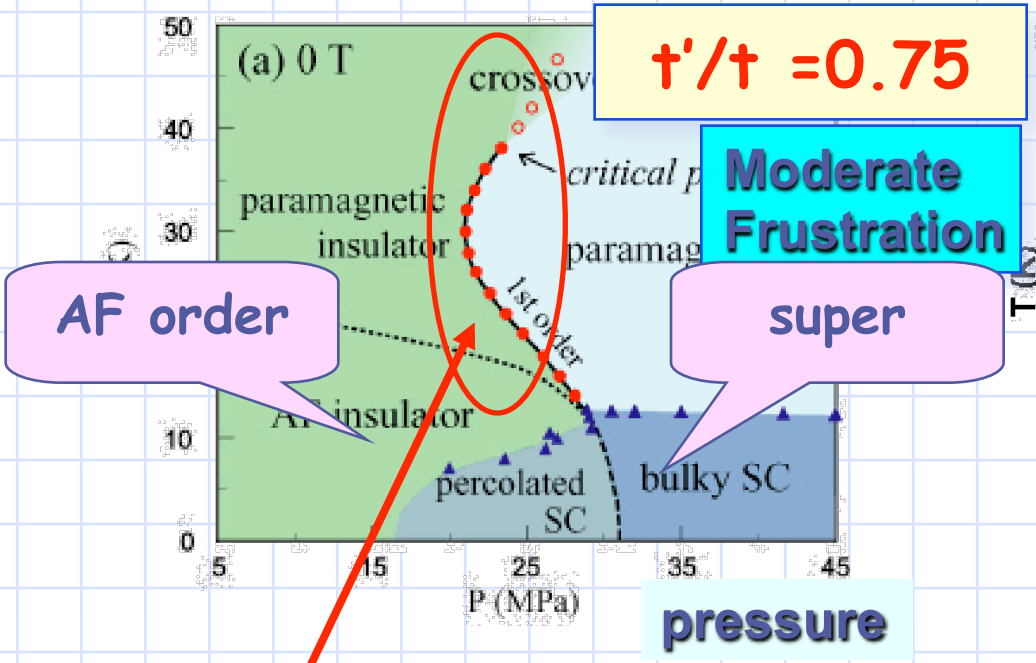

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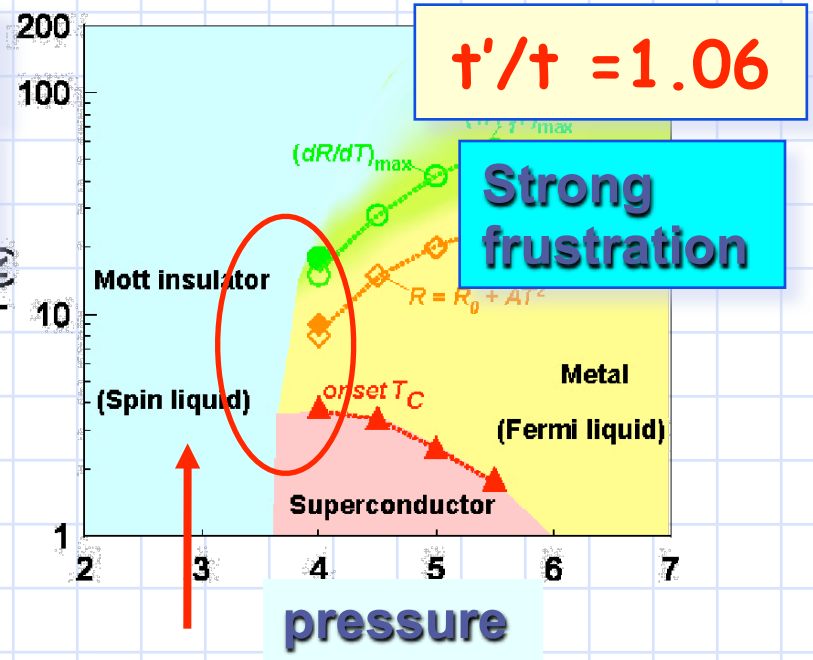


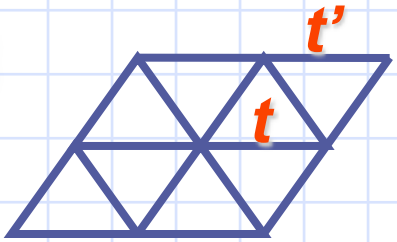
Finite-T Mott transition

Reentrant behavior

Spin liquid state

No Reentrant behavior

MIT in organic materials



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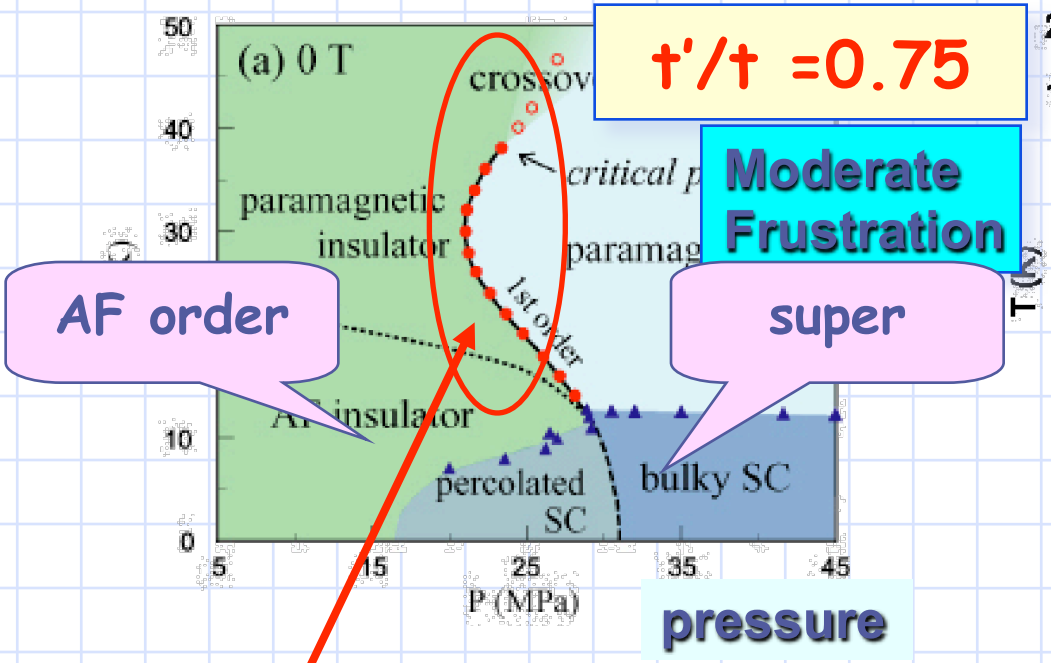

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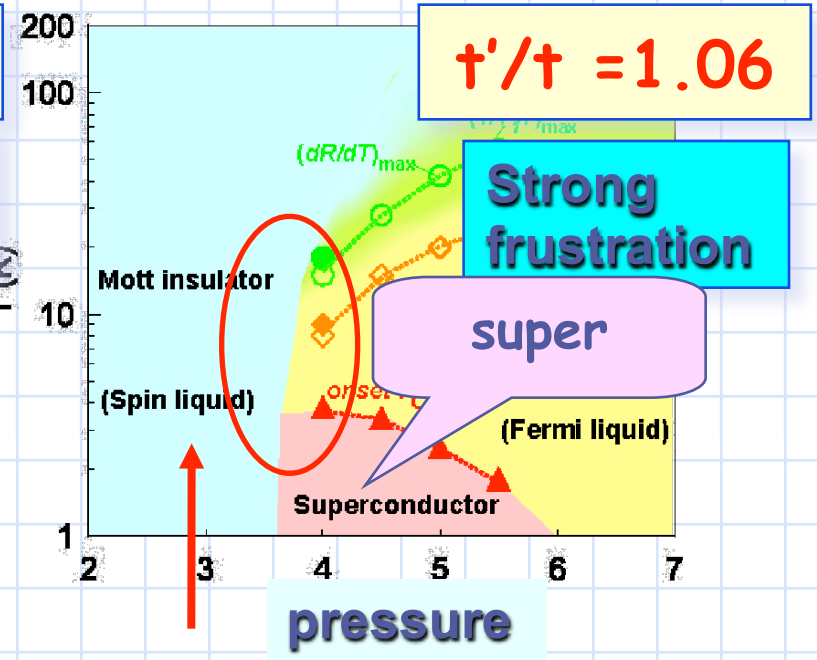


Finite-T Mott transition

Reentrant behavior

Spin liquid state

No Reentrant behavior

Outline

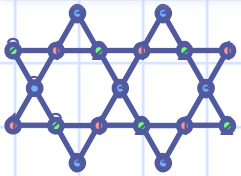
Frustrated Electron Systems in 2D

Mott transition with Frustration

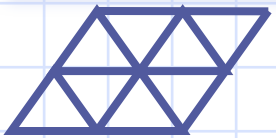
Hubbard Model

On-site repulsion

Kagome



Triangular



Common to Mott transition with frustration

Example

Reentrant behavior

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

Outline

Frustrated Electron Systems in 2D

Mott transition with Frustration

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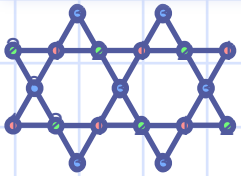

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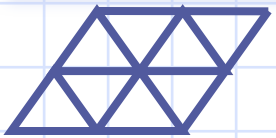

Itineracy **vs** Frustration

Anomalous properties near MIT

Common to Mott transition with frustration

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Reentrant behavior

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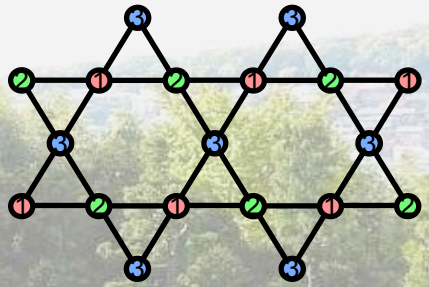

Ohashi et al. PRL (2006)

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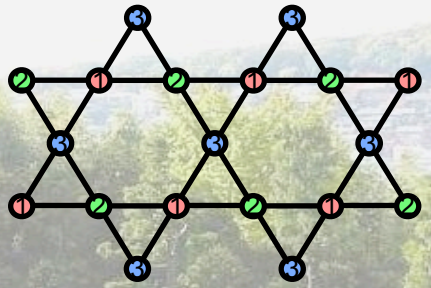
Kagome-lattice systems

Mott transition with Frustration



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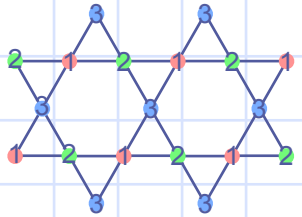
2D correlated systems

Frustration

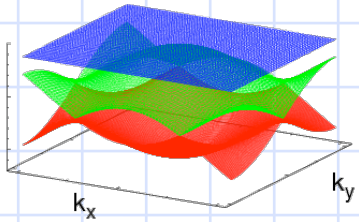


Kagome lattice Hubbard model

Imai, NK, Tsunetsugu(2003) FLEX
Koshibae - Maekawa (2003) Co superconductor
Bulut, Koshibae, Maekawa (2005) QMC

Co oxide
Supercoductor

3-band system



2D correlated systems

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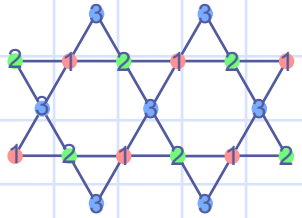

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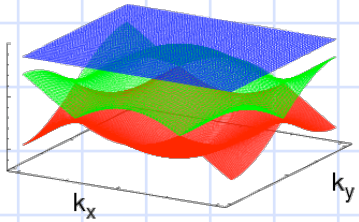


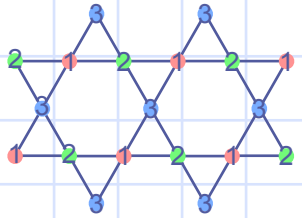
Metallic state near MIT ?

Ohashi et al. (2006) Cluster DMFT
Kuratani et al.(2006) Variational MC

2D correlated systems

Frustration

Kagome lattice Hubbard model



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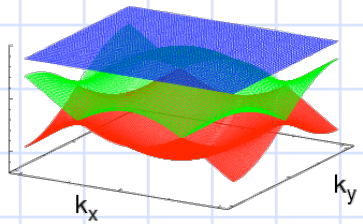

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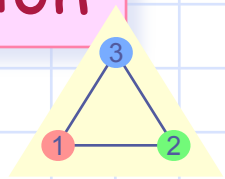
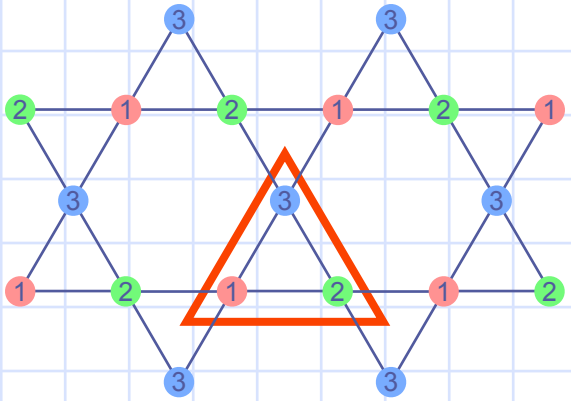


Cluster DMFT

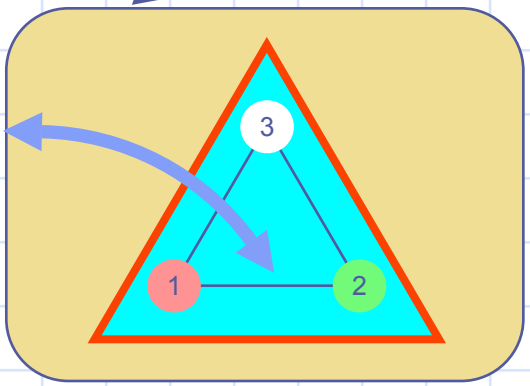
Cellular DMFT

Hubbard Model on Kagome lattice

Original Kagome lattice Hubbard model



Three sites cluster



Effective cluster model

- Strong correlation
- Frustration

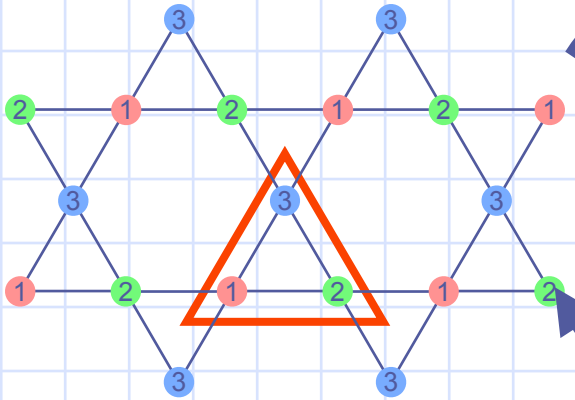
QMC method

(Hirsh-Fye algorism)

Cellular DMFT

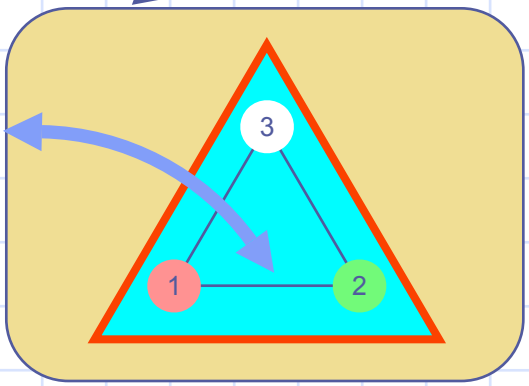
Hubbard Model on Kagome lattice

Original Kagome lattice Hubbard model



Self-consisten t

Three sites cluster



Effective cluster model

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- Frustration

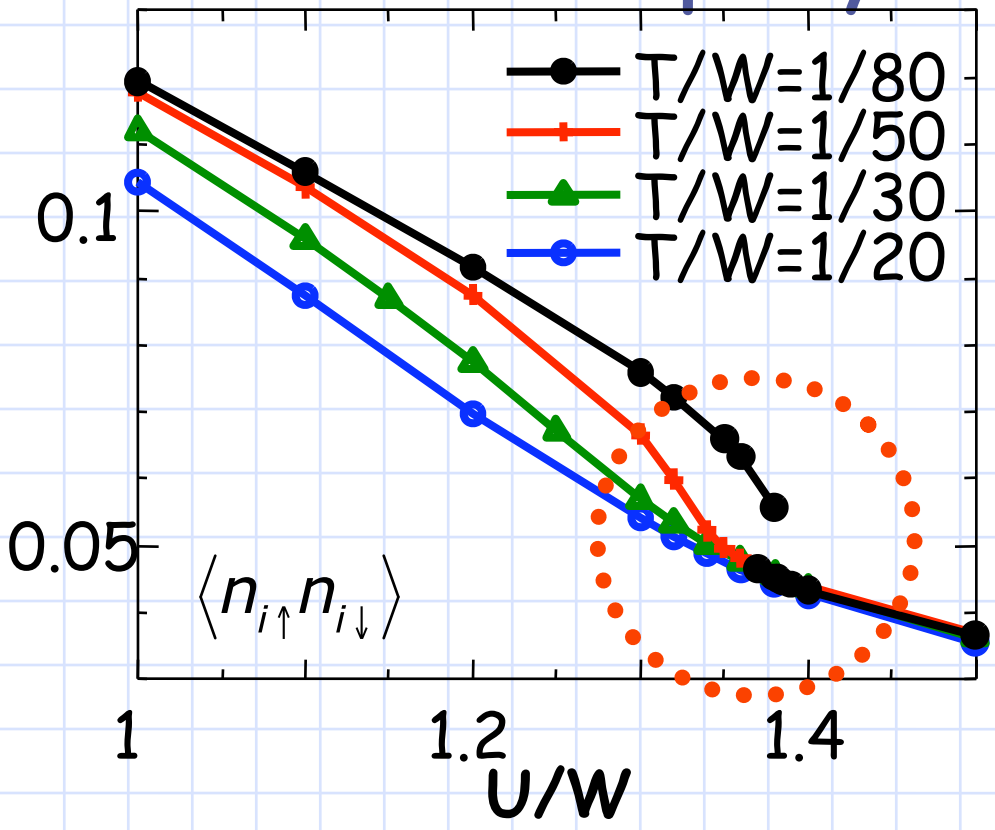
QMC method

(Hirsh-Fye algorism)

Mott transition

Hubbard
half-filling

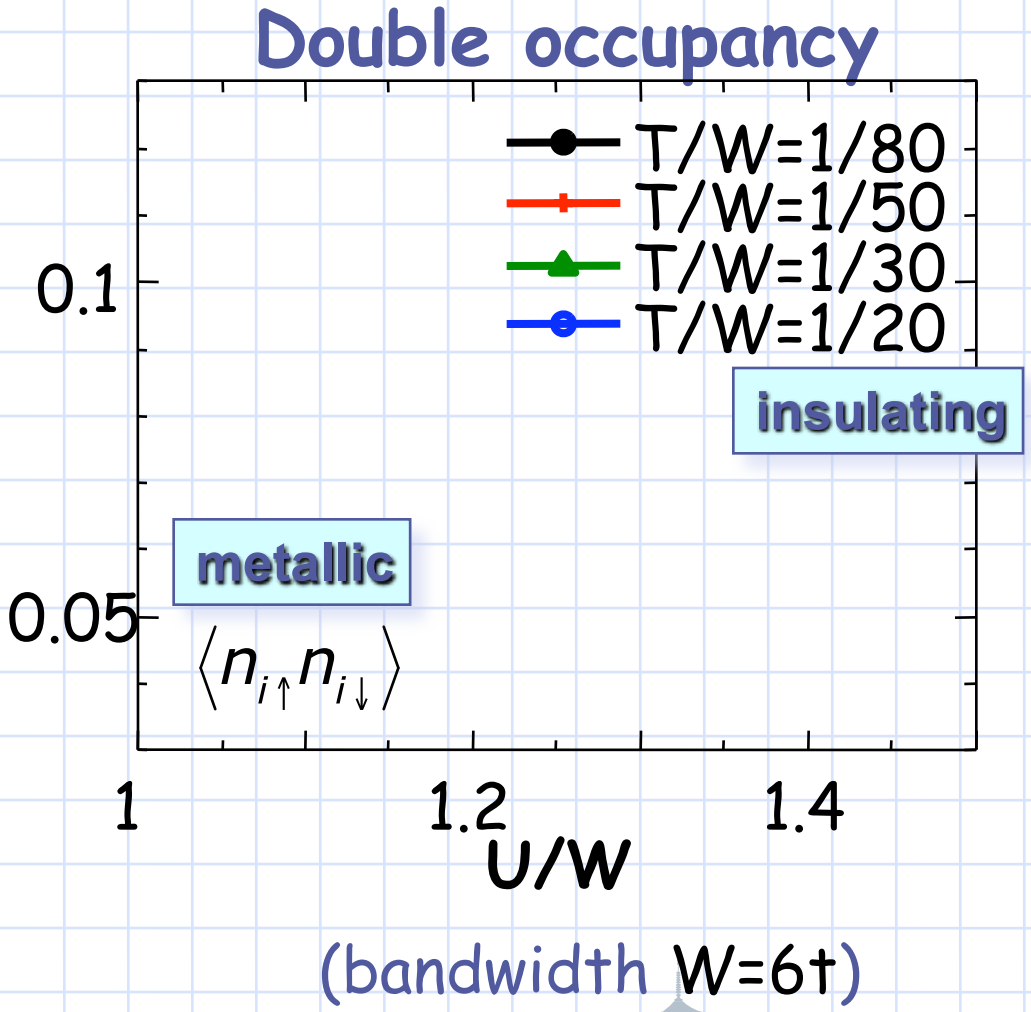
Double occupancy



(bandwidth W=6t)

Mott transition

Hubbard
half-filling



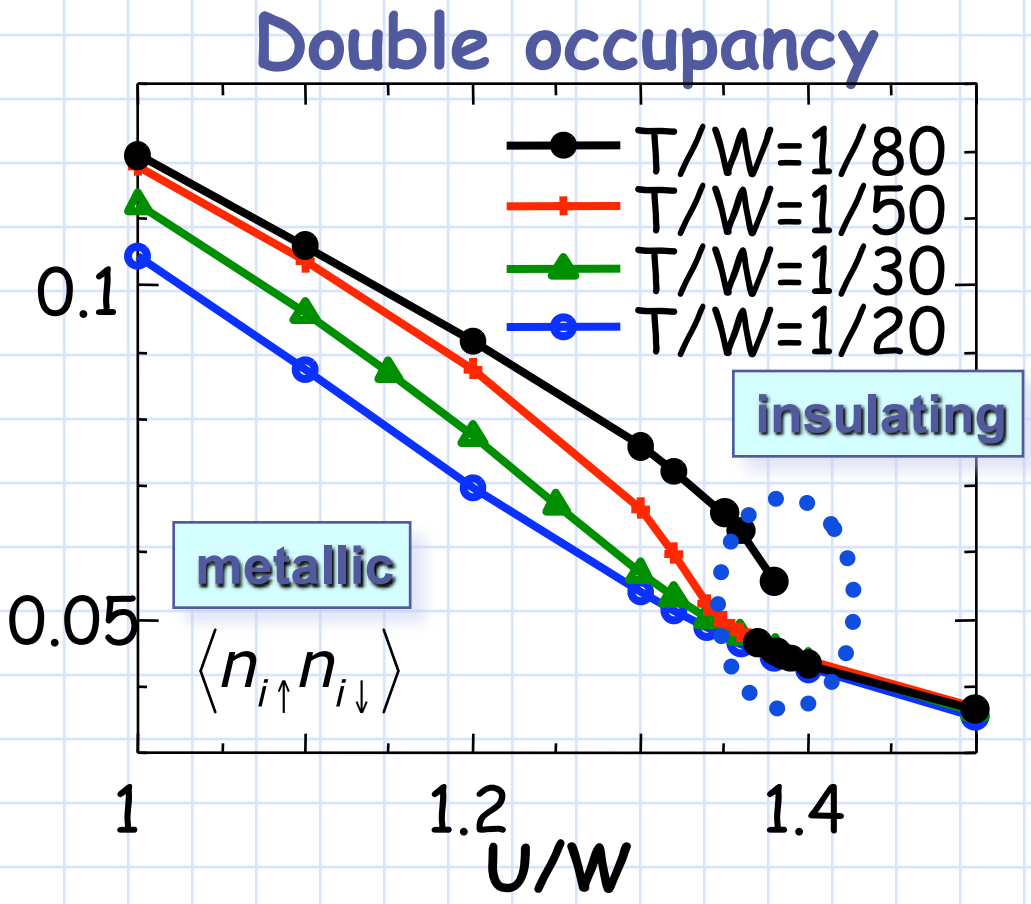
(bandwidth W=6t)

High temperature
T/W > 1/80

Crossover: $U_c/W \sim 1.35$

Mott transition

Hubbard
half-filling



(bandwidth W=6t)

High temperature
T/W > 1/80

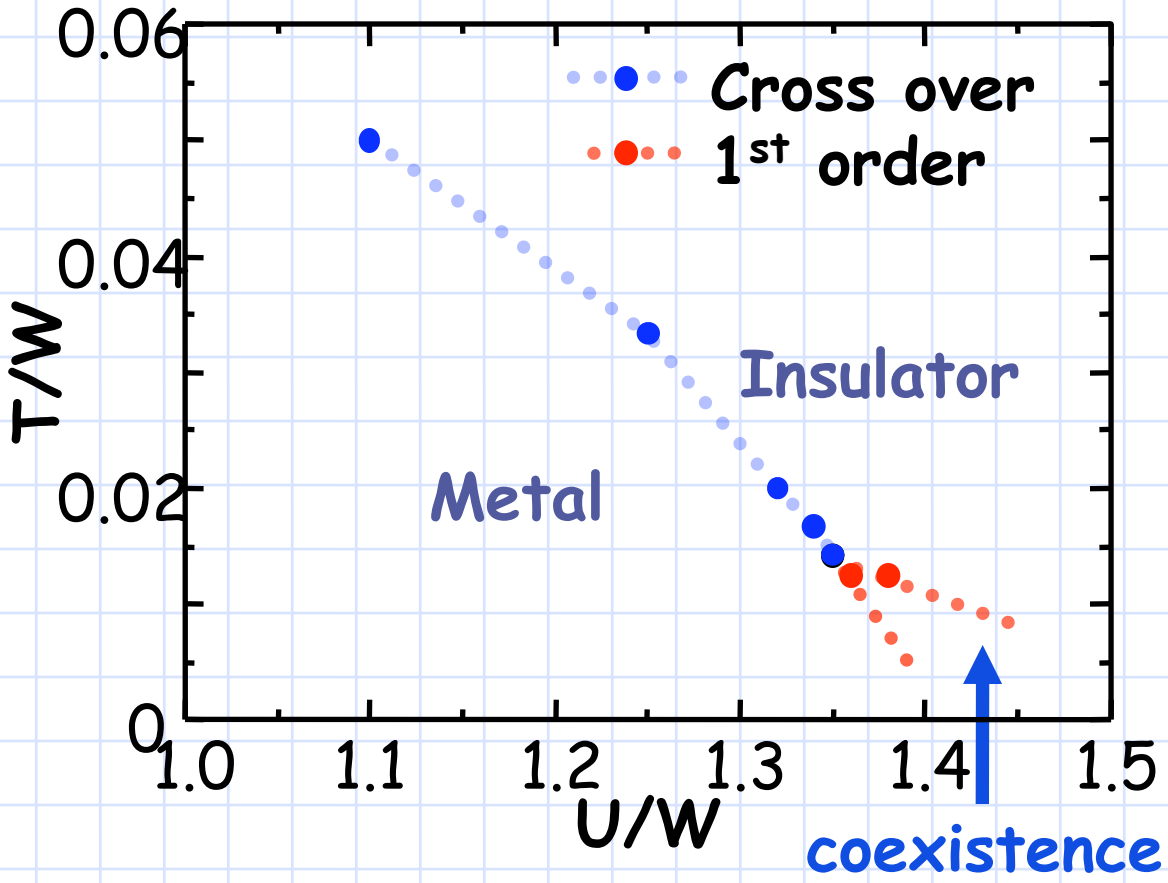
Crossover: $U_c/W \sim 1.35$

Low temperature
T/W = 1/80

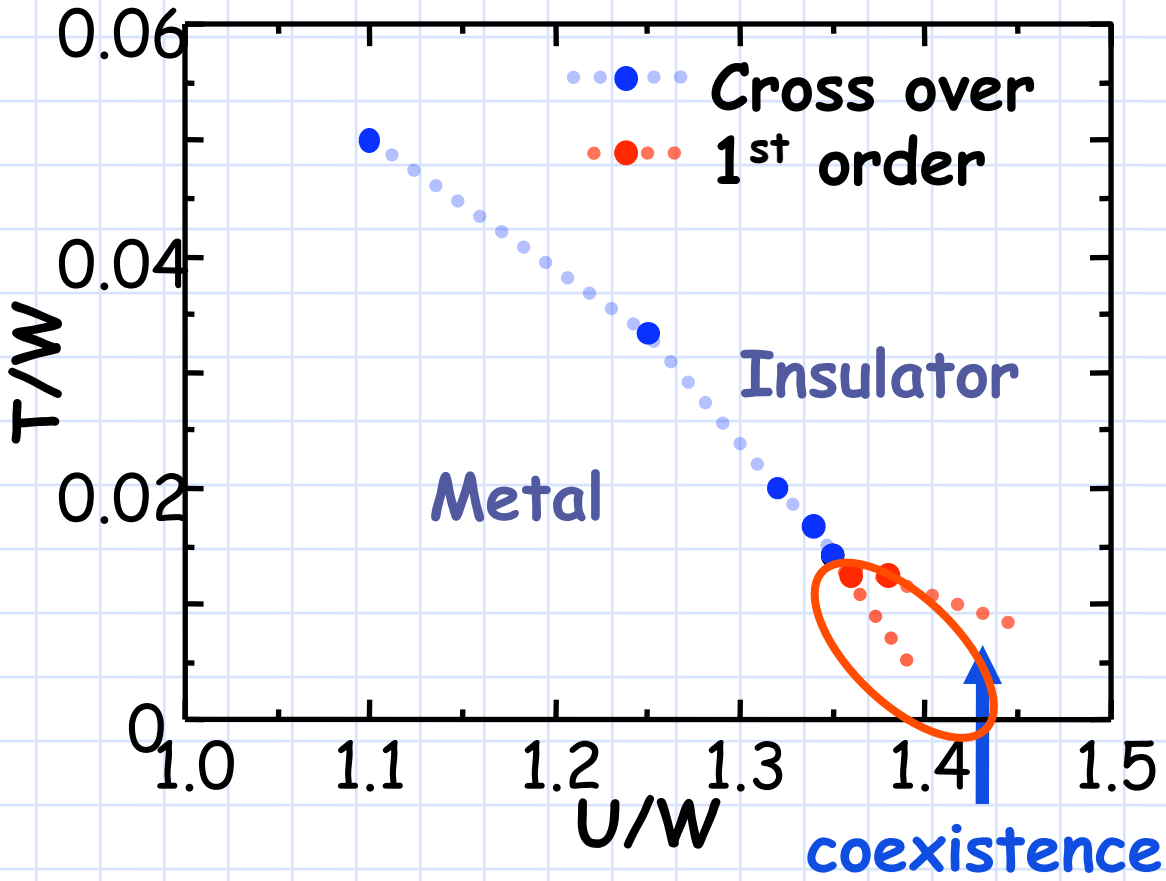
1st order transition with hysteresis

$U_c/W \sim 1.37$

Phase diagram of MIT



Phase diagram of MIT



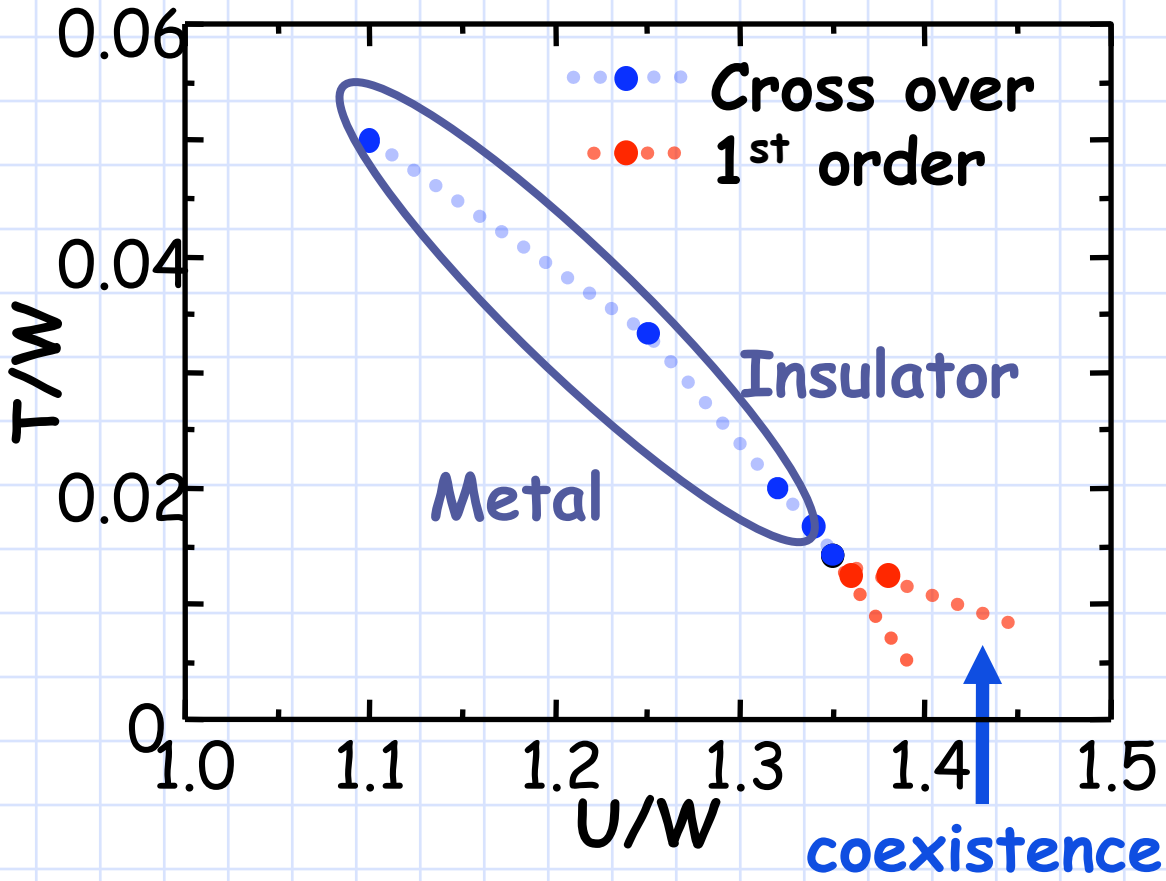
- Mott transition:
  $U_c/W \sim 1.4$
  Large U_c
- Square lattice
  (Cross over)
  $U_c/W < 0.5$

Moukouri & Jarrell (2001).

- triangular lattice
  $U_c/W \sim 1.04$

Parcollet & Kotliar (2003).

Phase diagram of MIT



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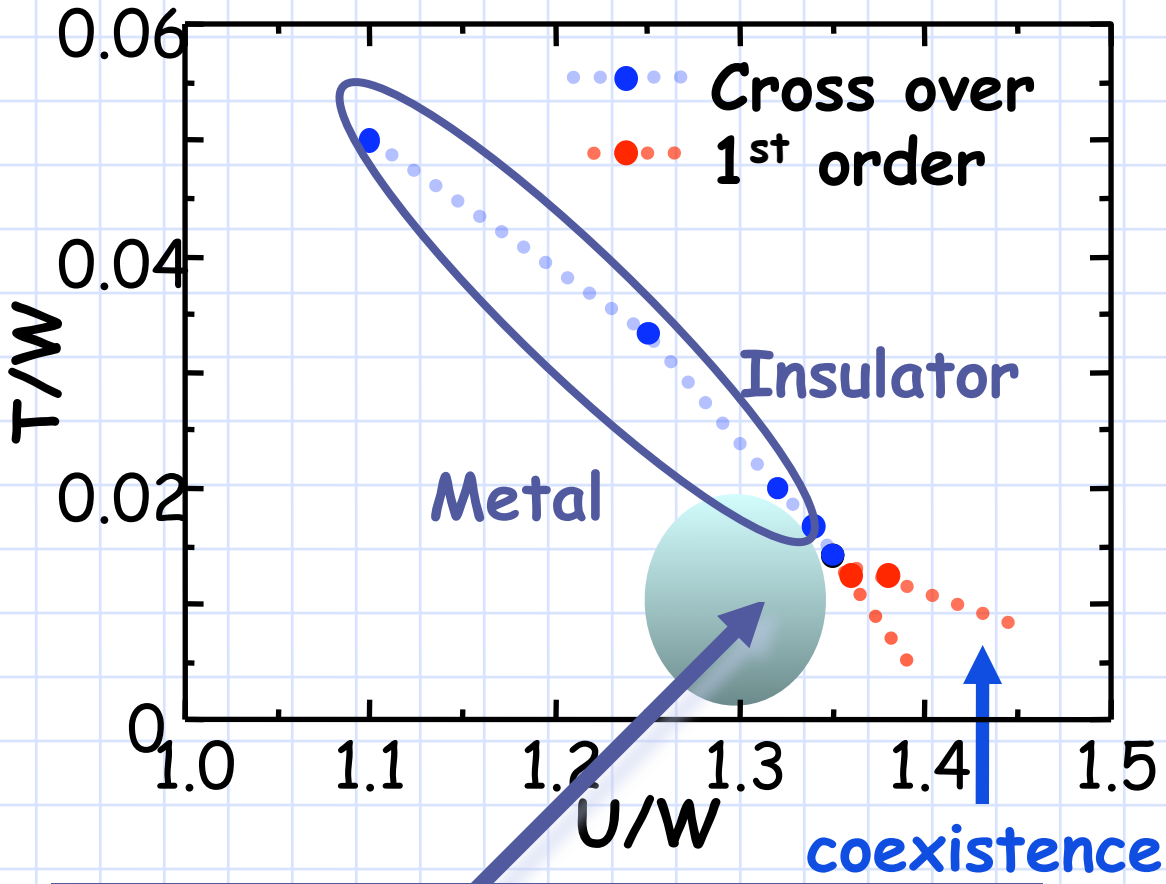
Phase diagram of MIT



- Mott transition:
  $U_c/W \sim 1.4$
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  (Cross over)
  $U_c/W < 0.5$

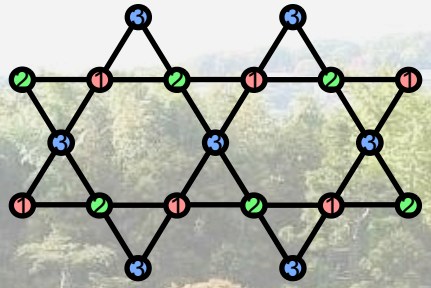
Moukouri & Jarrell (2001).

- triangular lattice
  $U_c/W \sim 1.04$

Parcollet & Kotliar (2003).

Close to MIT:
anomalous metallic properties

YKIS 07
Kyoto
November 14, 2007

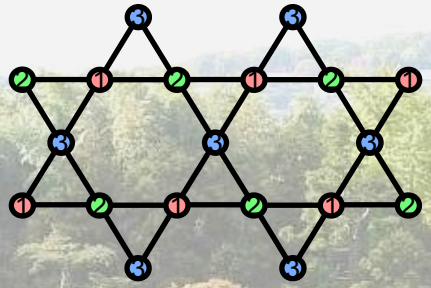


Ohashi et al. PRL (2006)

YKIS 07
Kyoto
November 14, 2007

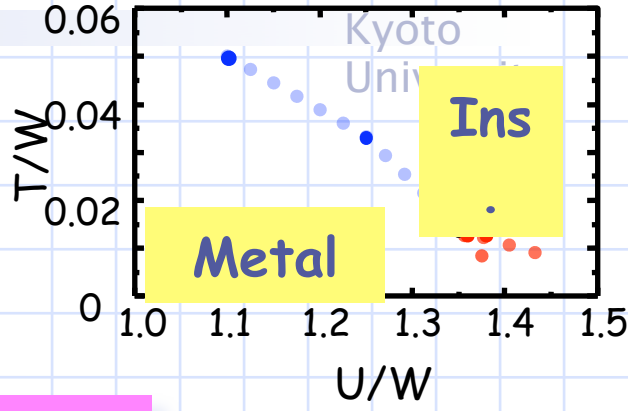
Anomalous metallic properties

Near Mott phase

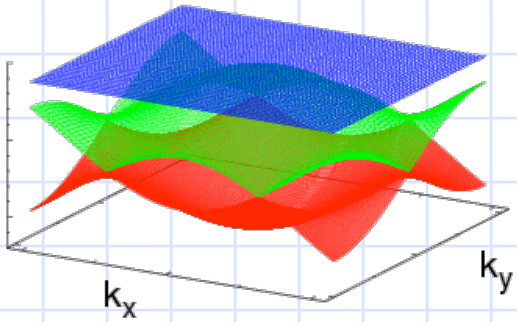


Ohashi et al. PRL (2006)

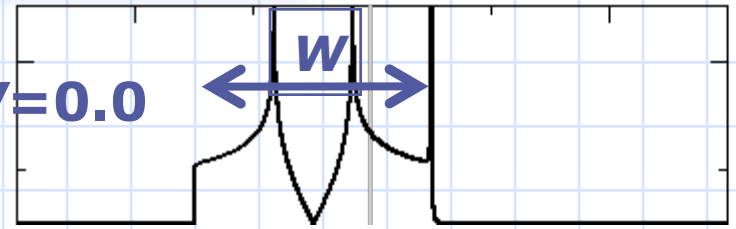
Hubbard (half-filling)



dispersion: U=0



DOS (T/W=1/80)



Bandwidth
: $W=6t$

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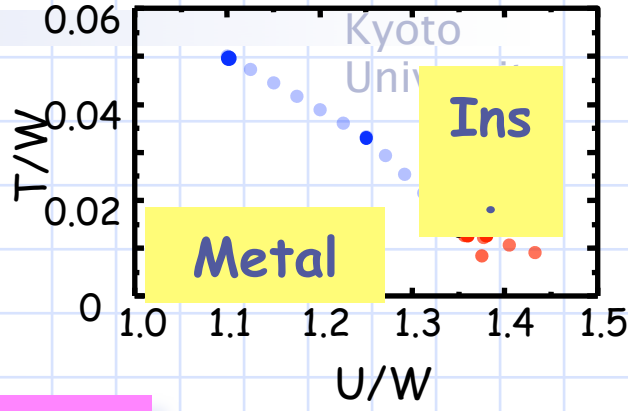
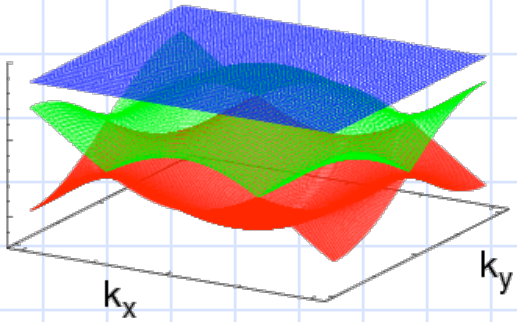
Density of states

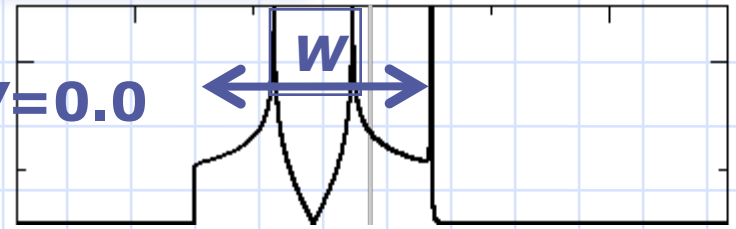
Hubbard (half-filling)



dispersion: U=0



DOS (T/W=1/80)



Bandwidth
: $W=6t$

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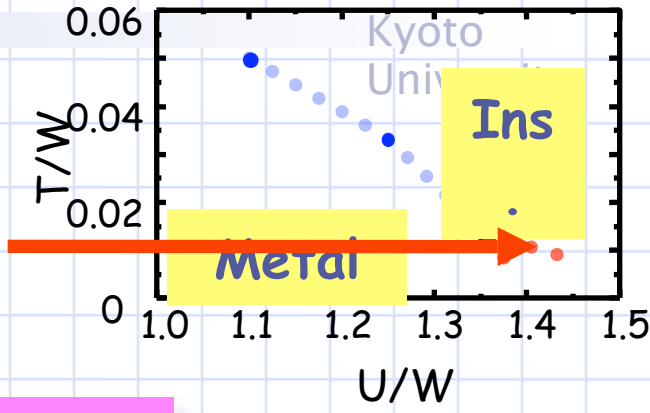
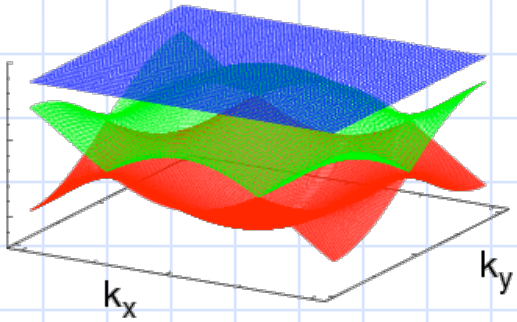
Density of states

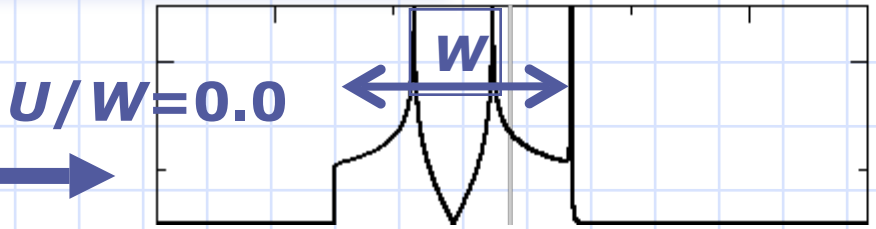
Hubbard (half-filling)



dispersion: U=0



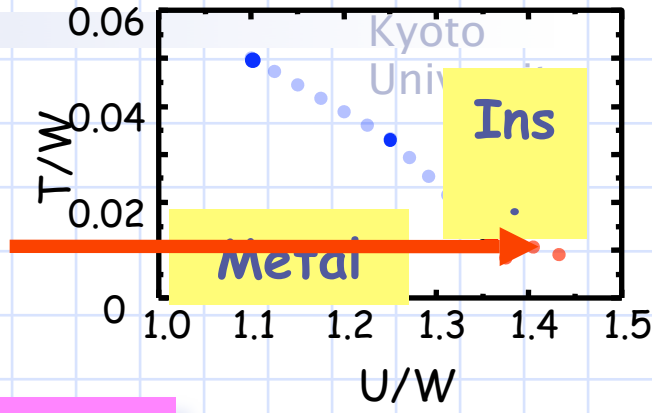
DOS (T/W=1/80)



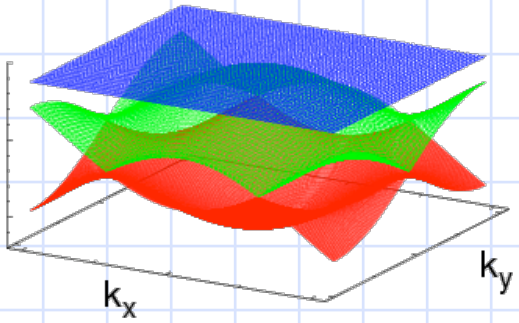
Bandwidth
: $W=6t$

Density of states

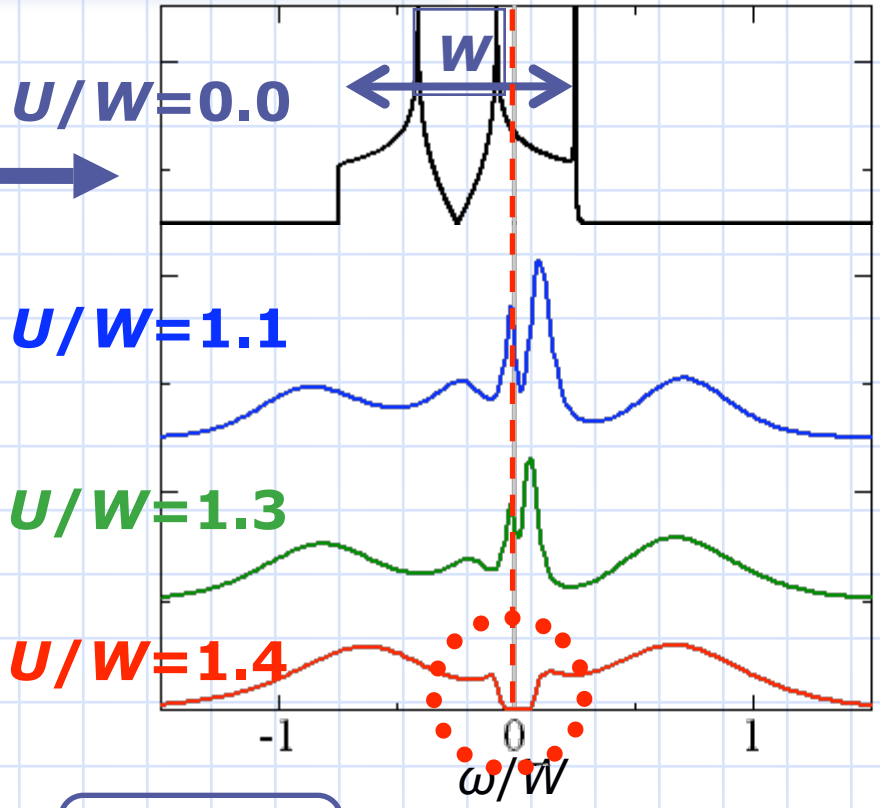
Hubbard (half-filling)



dispersion: U=0



DOS (T/W=1/80)



Bandwidth
: W=6t

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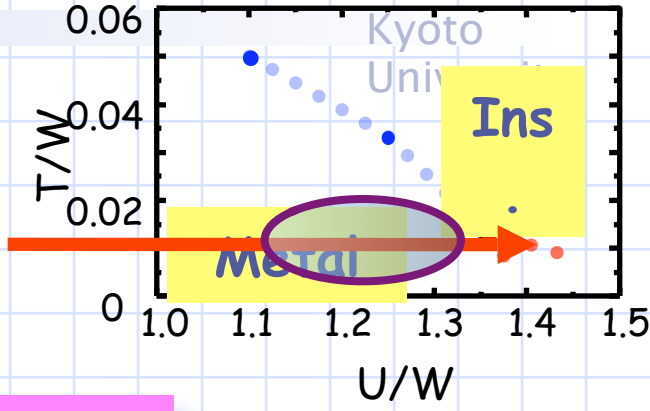
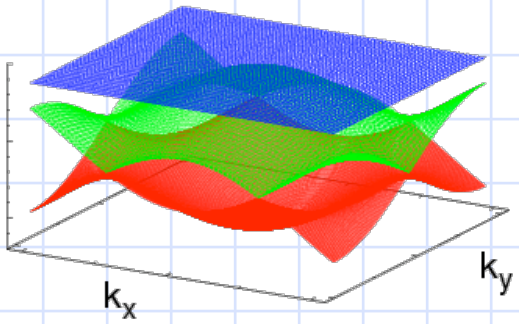
Density of states

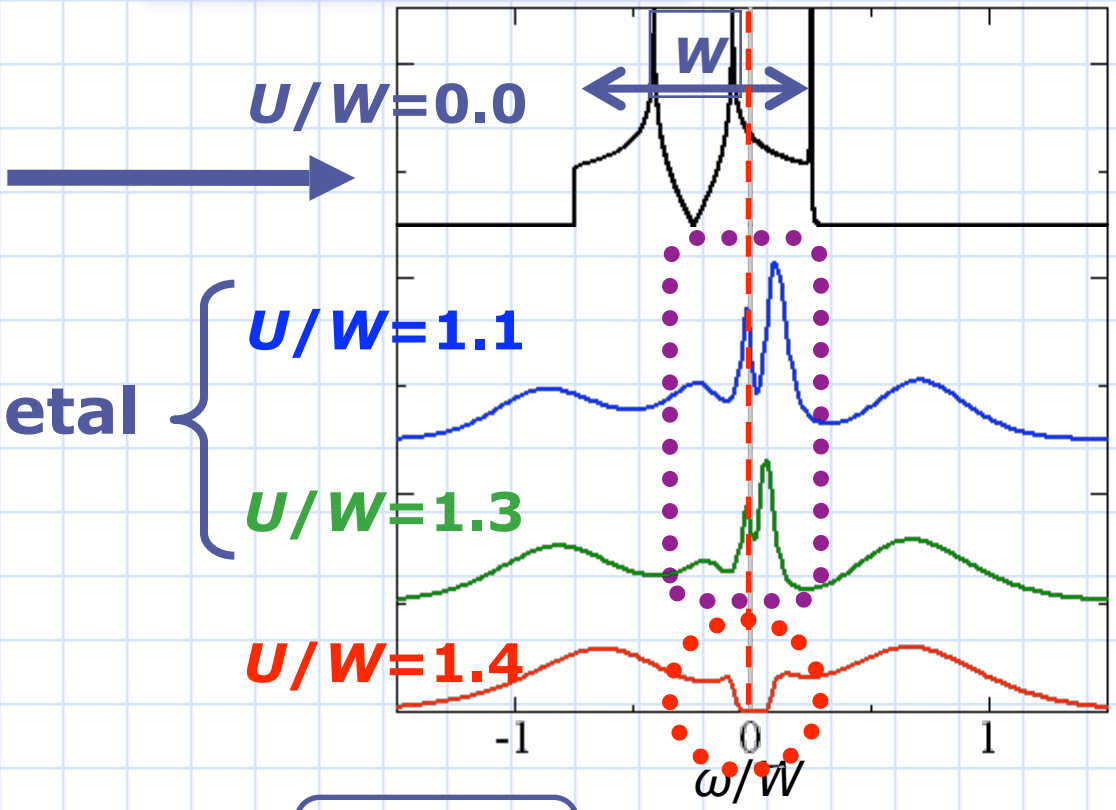
Hubbard (half-filling)



dispersion: U=0



DOS (T/W=1/80)



Bandwidth : $W=6t$

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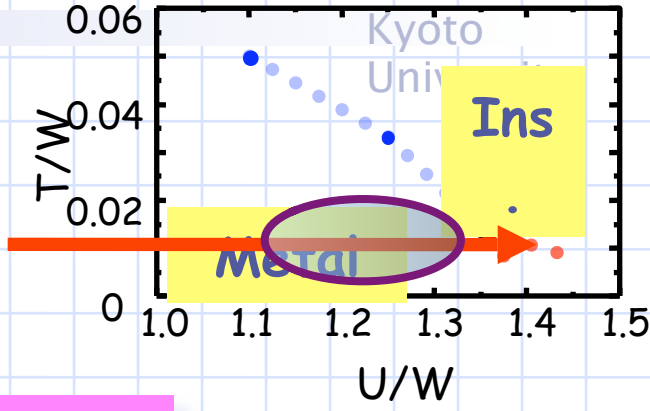
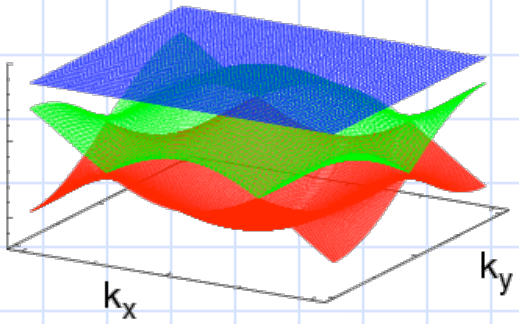
Density of states

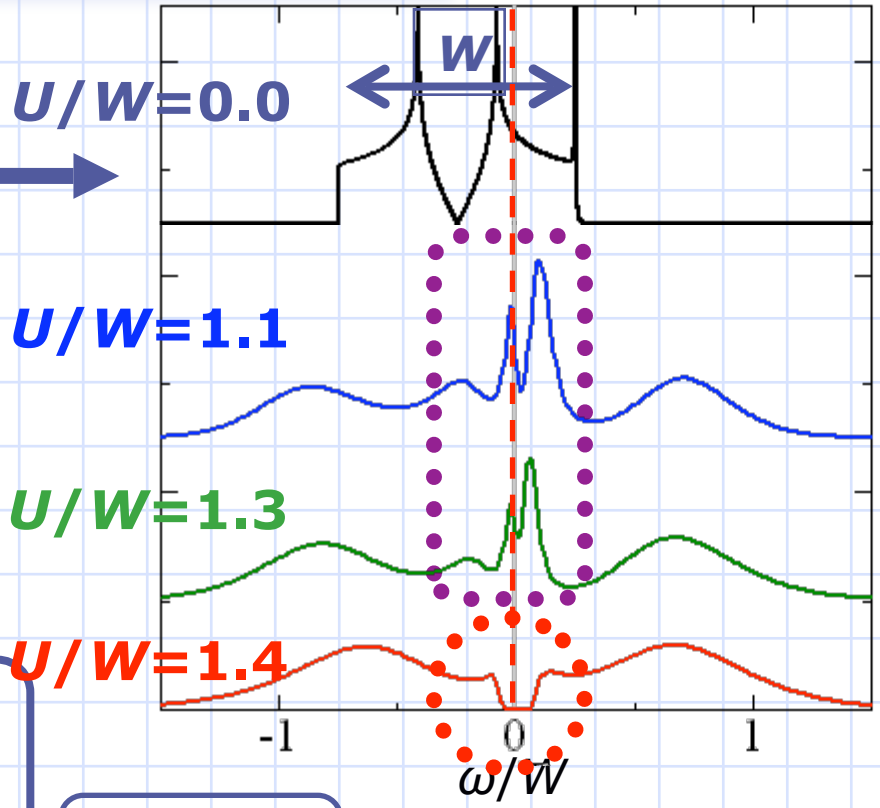
Hubbard (half-filling)



dispersion: U=0



DOS (T/W=1/80)



metal

- **all bands renormalized**
- **multi-band heavy fermions**

Bandwidth : $W=6t$

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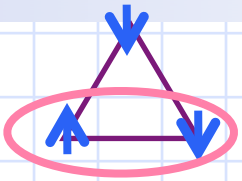
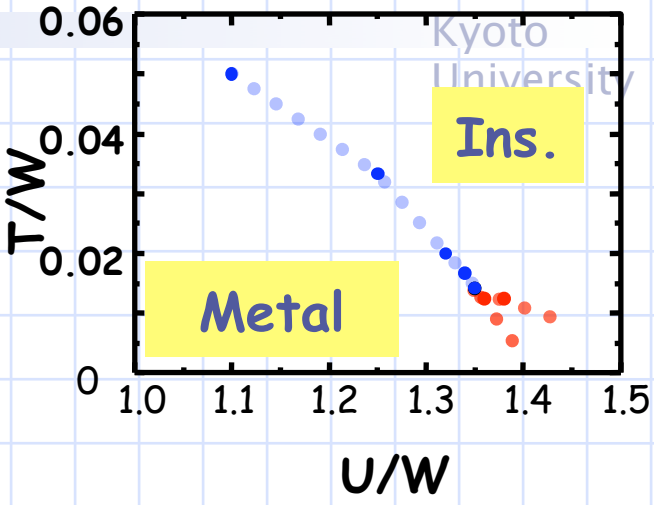
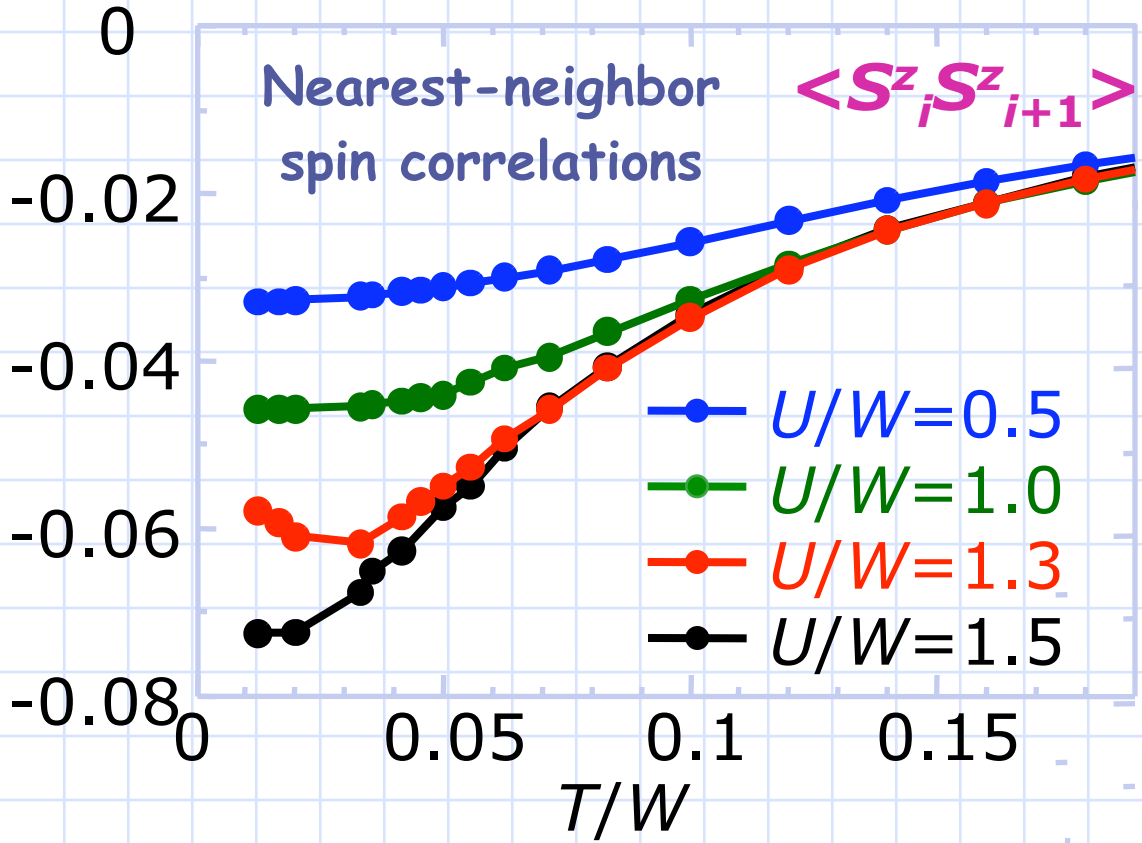
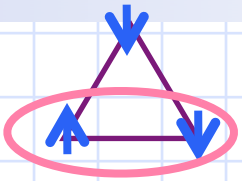
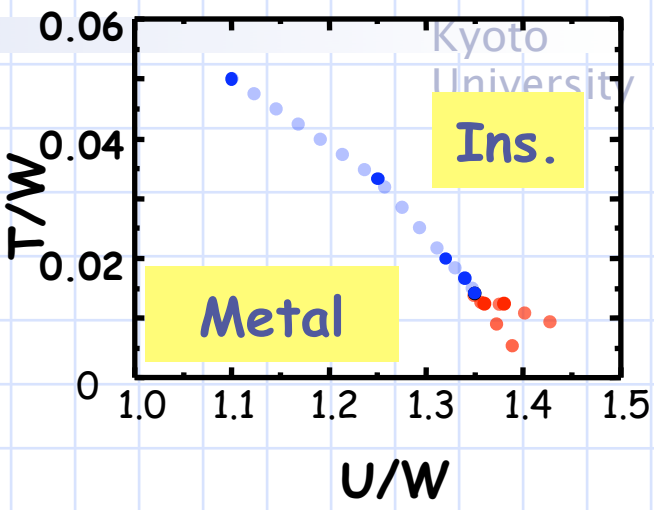


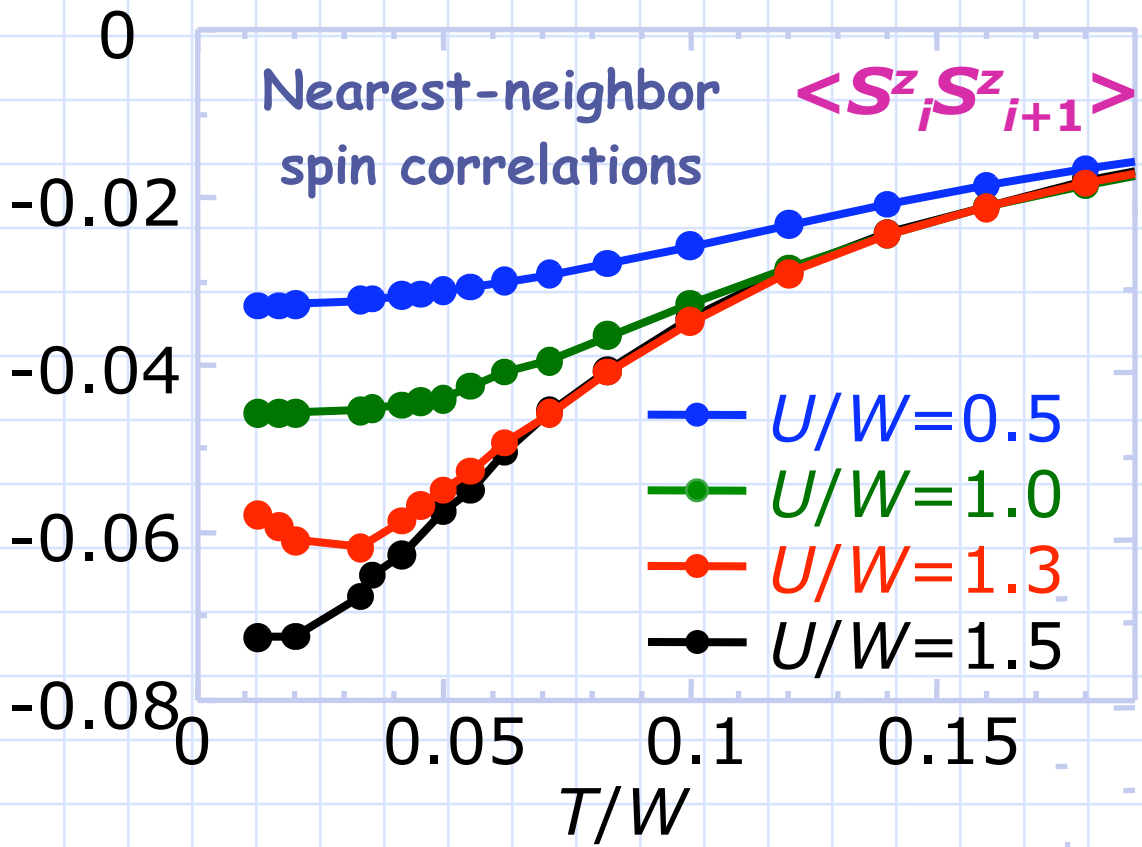

0.06
0.04
0.02
0
T/W
Ins.
Metal
1.0
1.1
1.2
1.3
1.4
1.5
U/W


Nearest-neighbor
spin correlations
<SzᵢSzᵢ₊₁>
U/W=0.5
U/W=1.0
U/W=1.3
U/W=1.5
0
-0.02
-0.04
-0.06
-0.08
0
0.05
0.1
0.15
T/W

Unusual behavior in spin correlations







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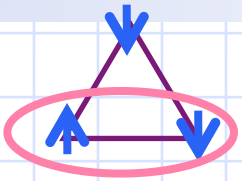
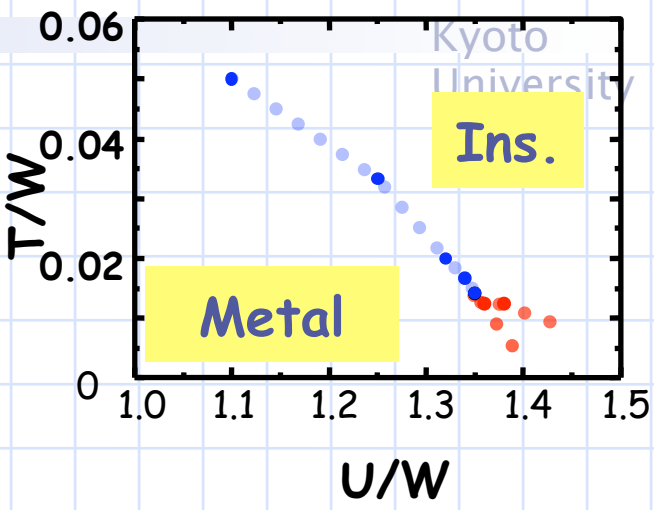
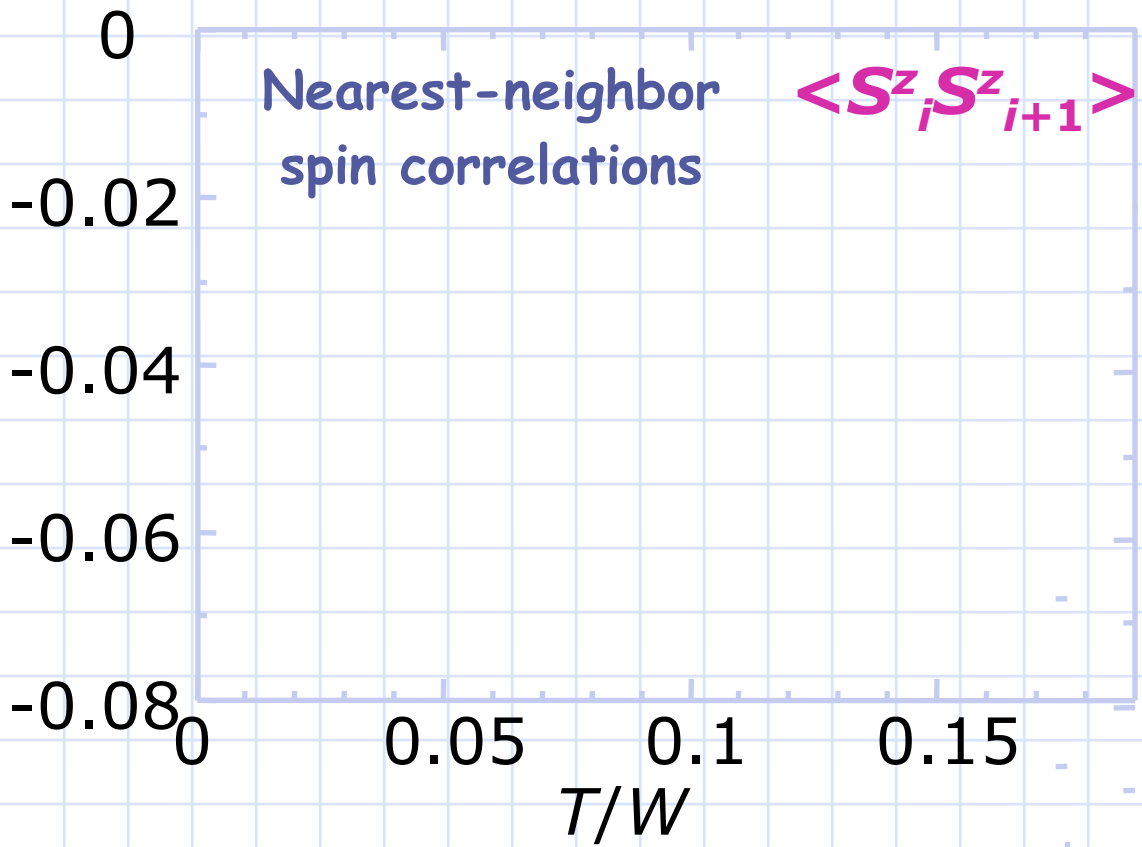
Unusual behavior in spin correlations

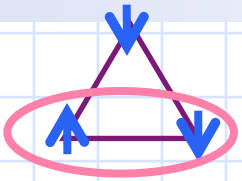


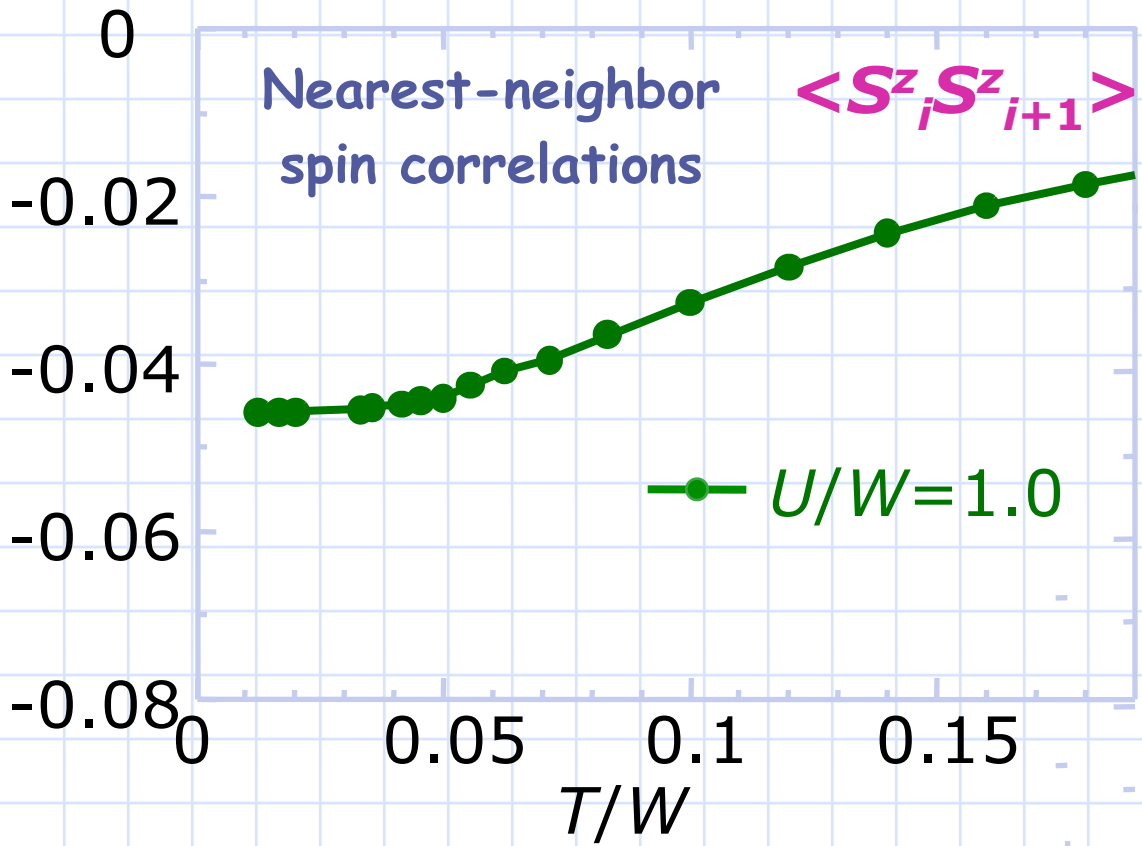


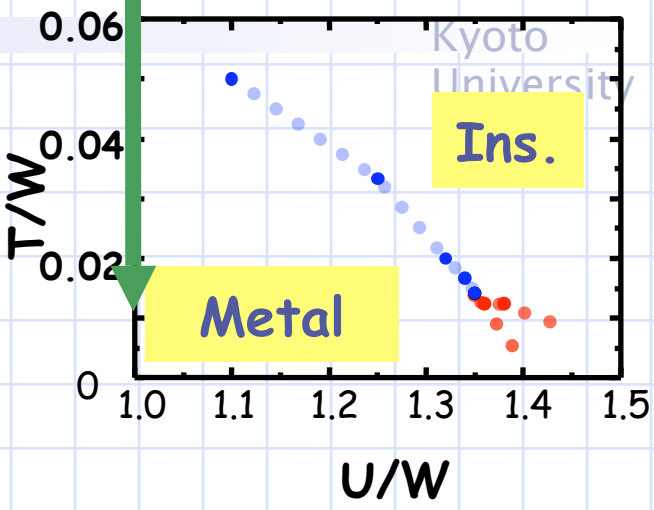


Kyoto University

Unusual behavior in spin correlations







Metallic phase
⇒ weak AF correlations

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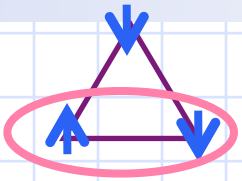
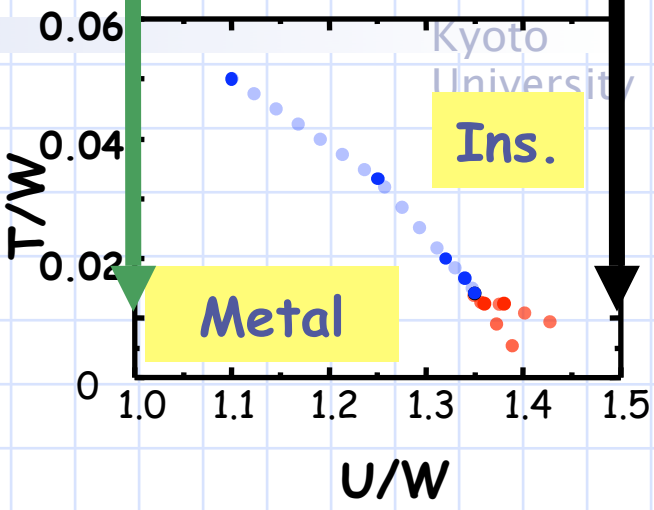
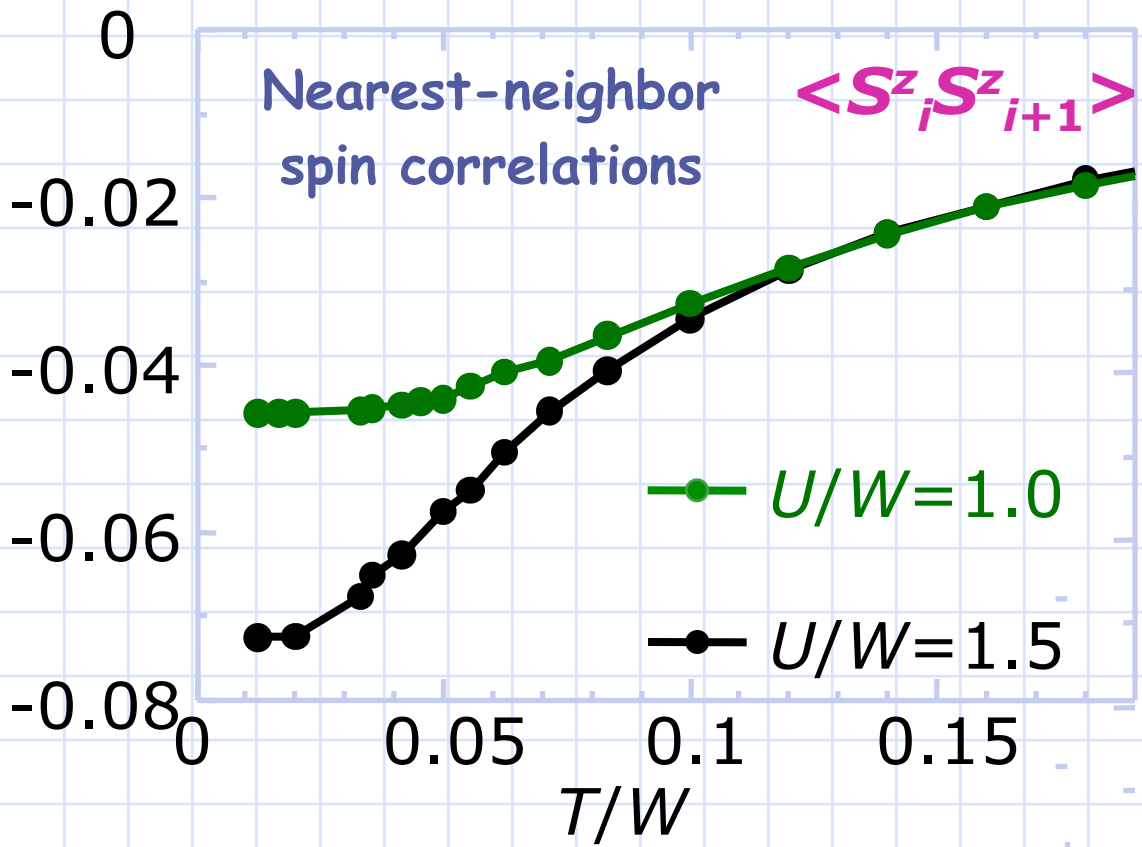
Unusual behavior in spin correlations





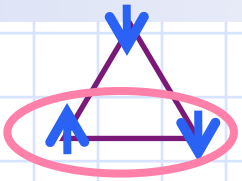


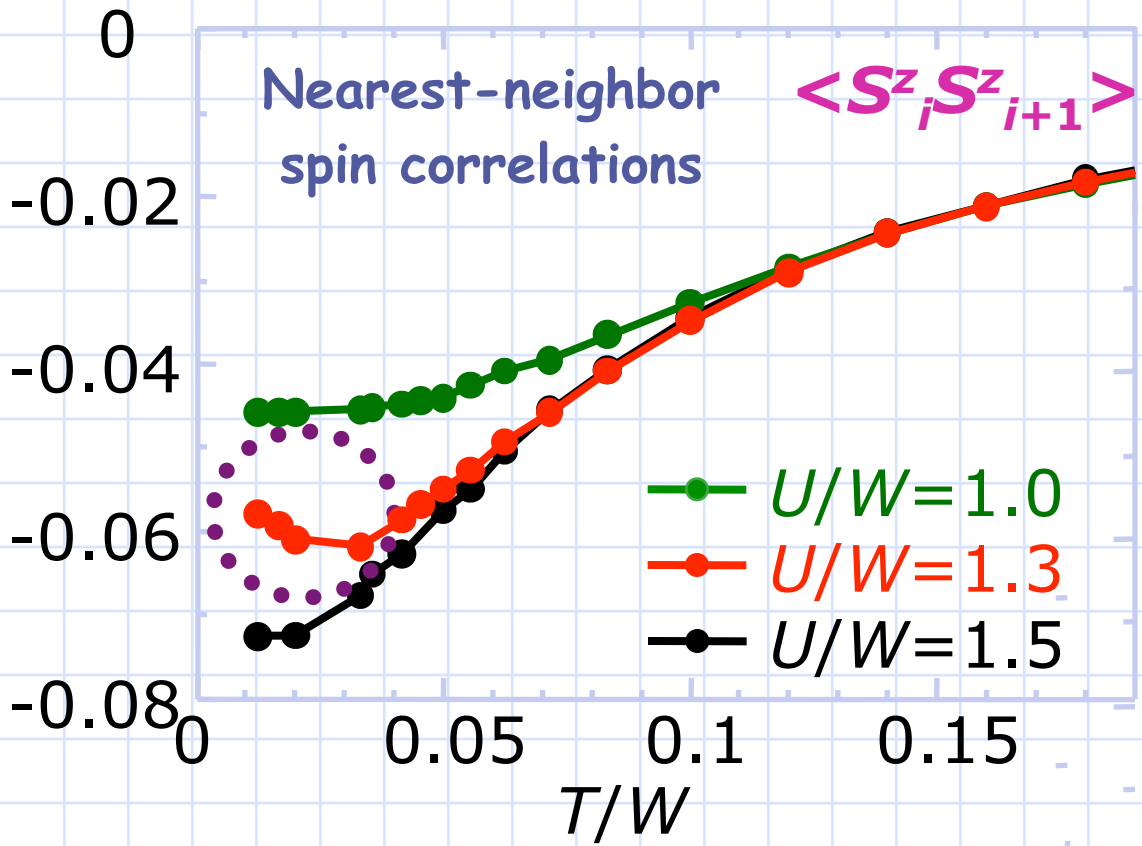
Metallic phase
⇒ weak AF correlations

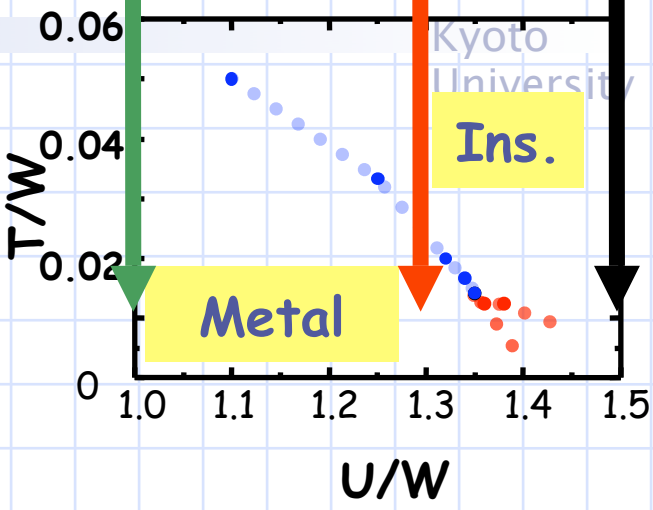
Insulating phase
⇒ Strong frustration
RVB-like insulator

Kyoto University

Unusual behavior in spin correlations







Metallic phase
⇒ weak AF correlations

Insulating phase
⇒ Strong frustration
RVB-like insulator

Metallic phase near MIT
Non-monotonic behavior

⇒ AF correlations
suppressed at low T !

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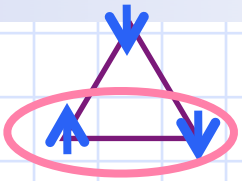
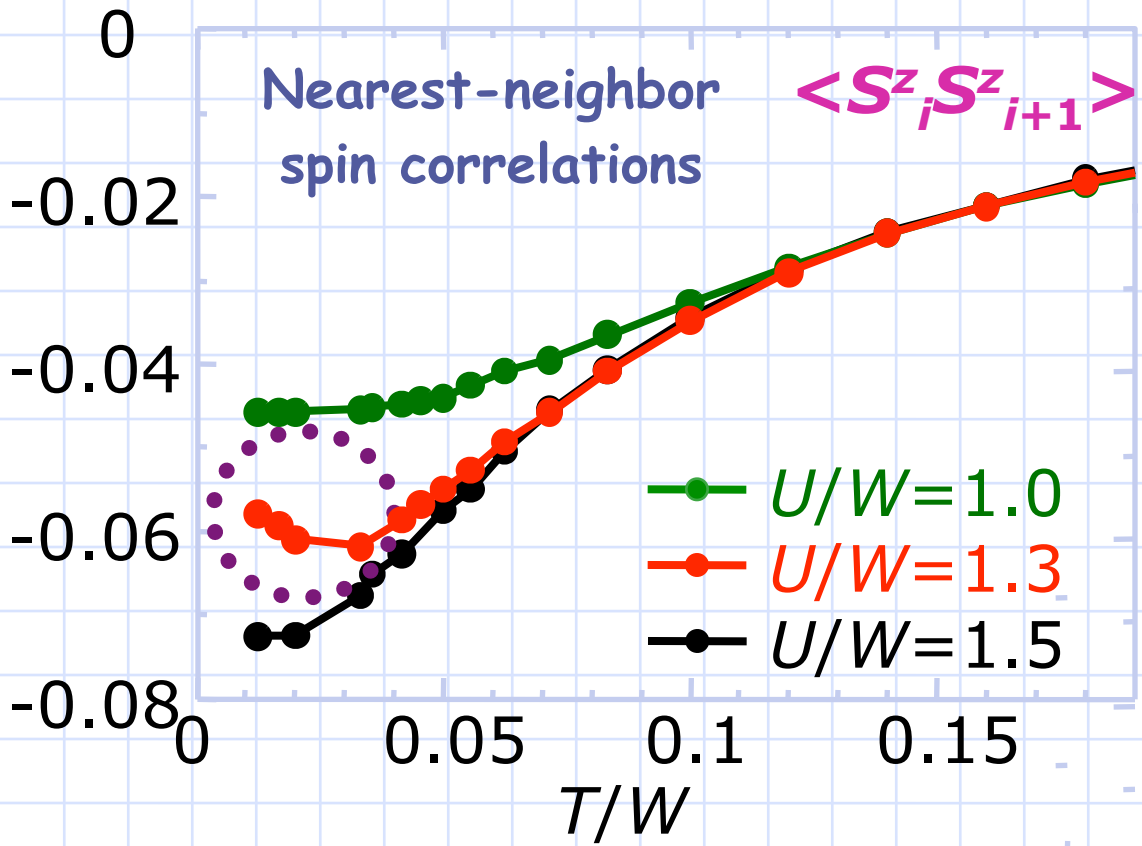
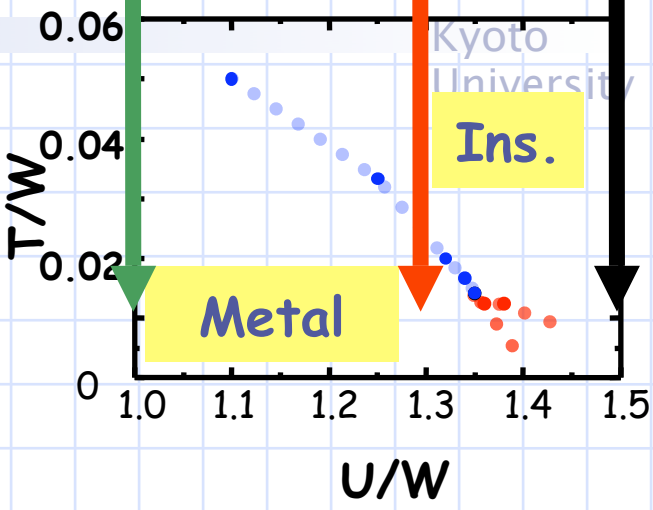
Unusual behavior in spin correlations







Metallic phase
⇒ weak AF correlations

Insulating phase
⇒ Strong frustration
RVB-like insulator

Metallic phase near MIT
Non-monotonic behavior
⇒ AF correlations
suppressed at low T !

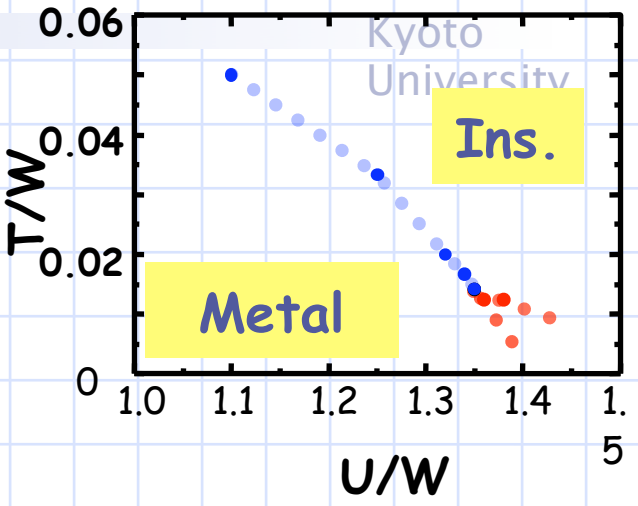
Recovery of coherence
Relaxation of frustration

Dynamical spin susceptibility

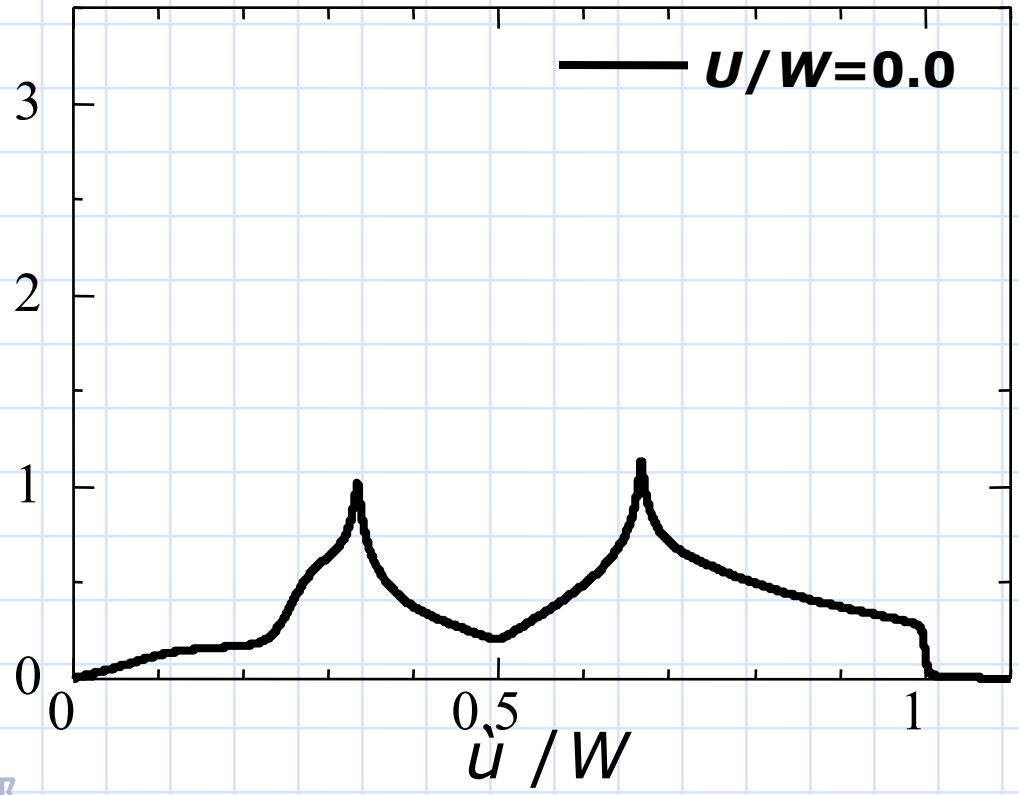
Loca
l

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

Metallic phase



Temp: $T/W=1/80$



Dynamical spin susceptibility

Loca
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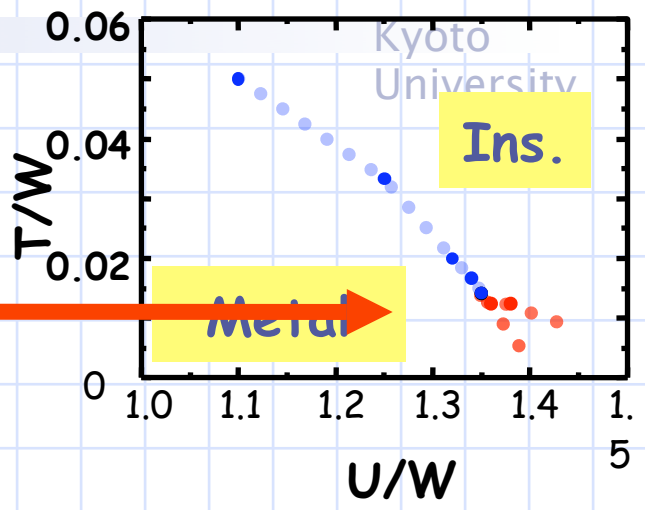
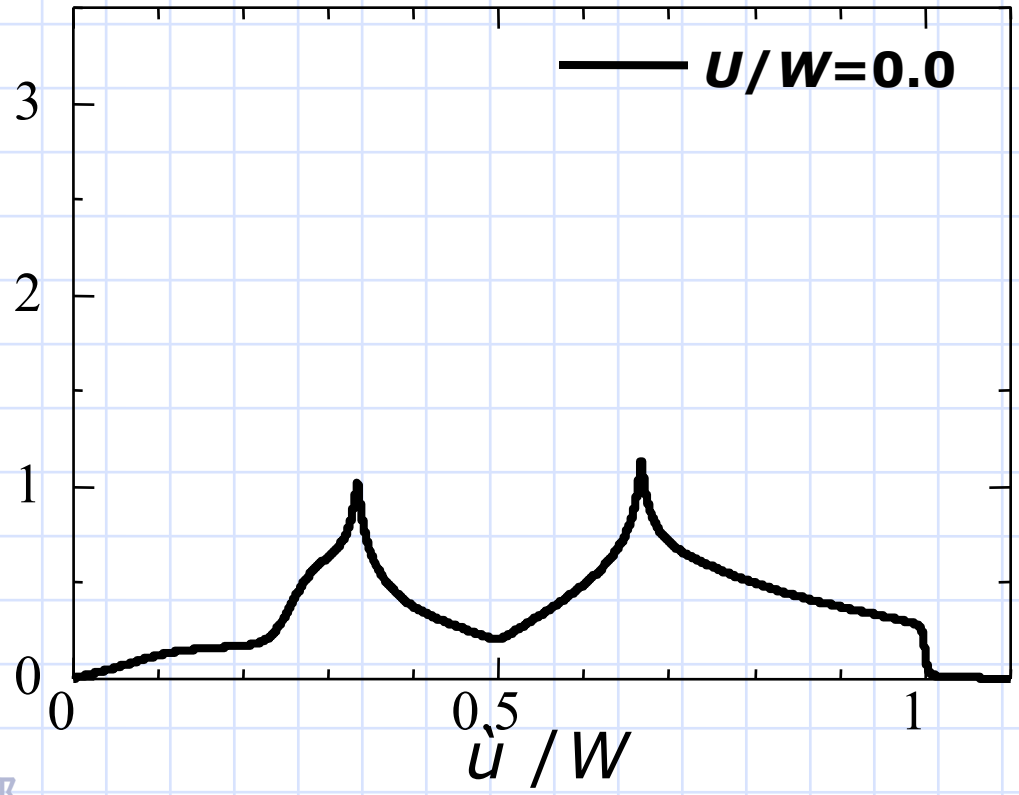
Metallic phase



Temp: $T/W=1/80$



Dynamical spin susceptibility

Loca
l

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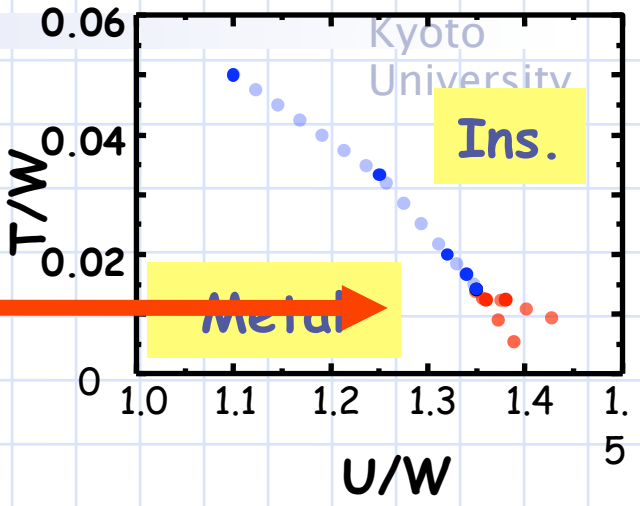
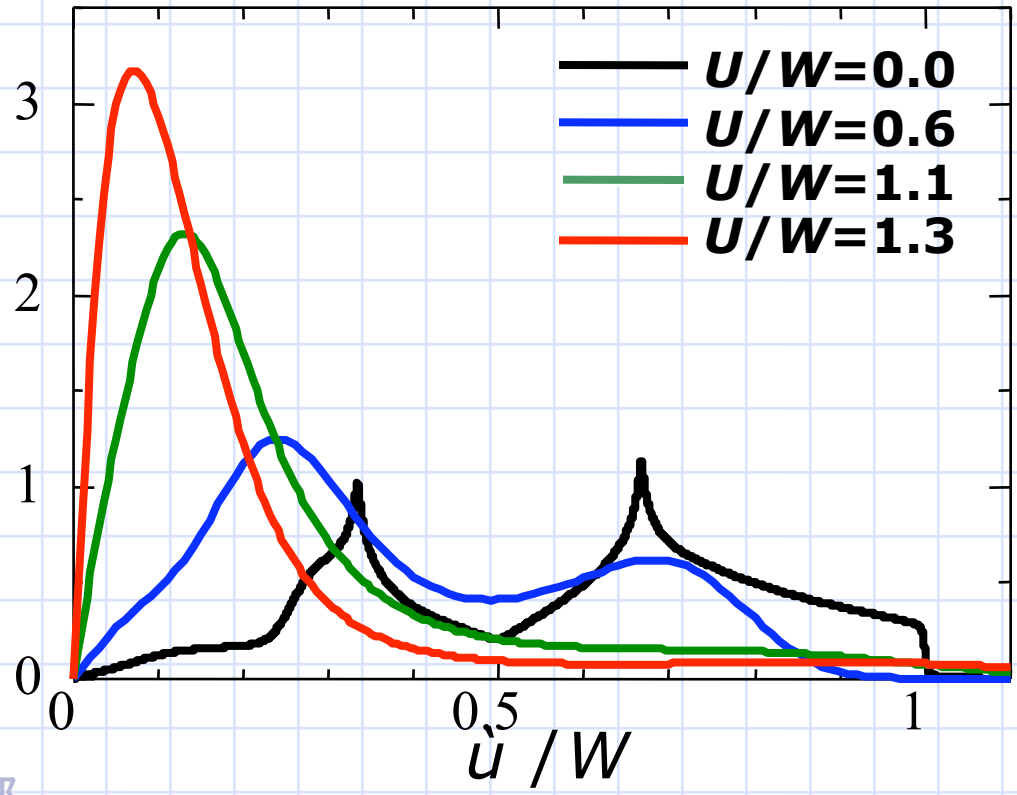
Metallic phase



Temp: $T/W=1/80$



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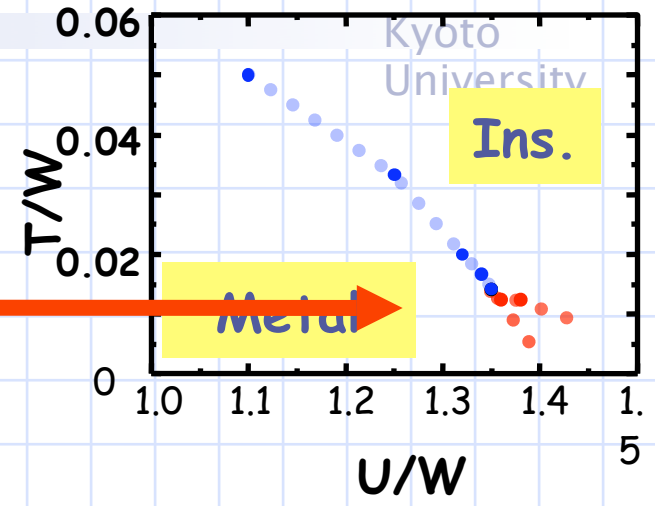
Dynamical spin susceptibility

Loca
l

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

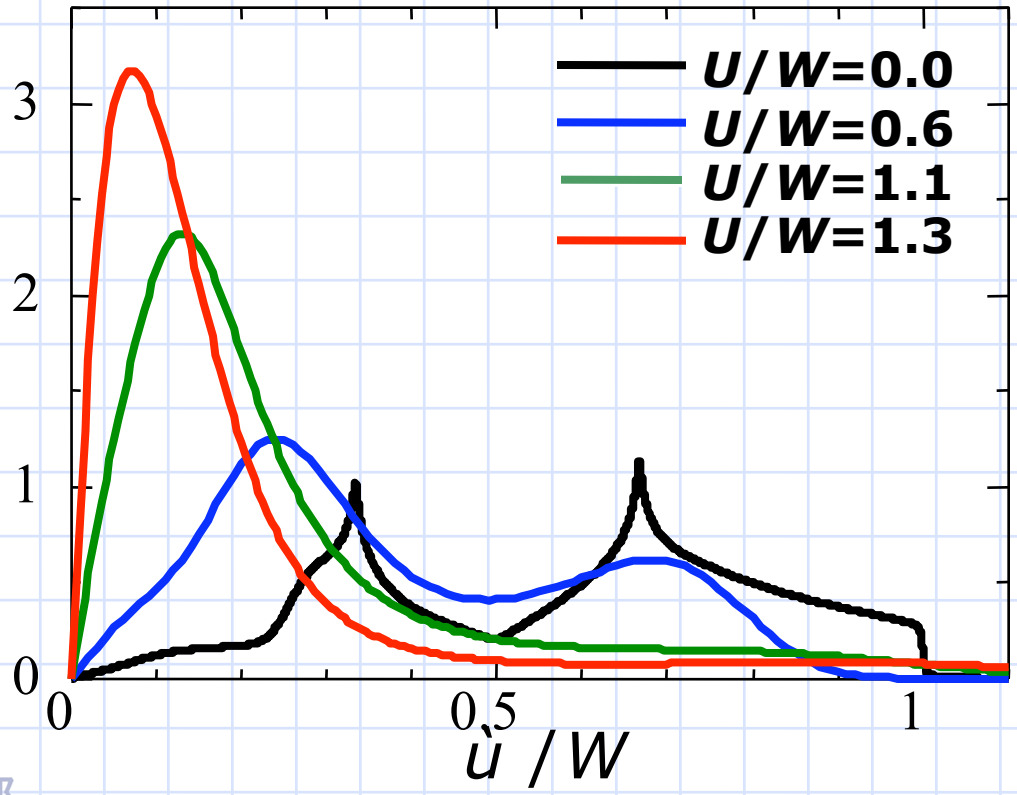


Metallic phase

U ⇒ large

- shift
- peak enhanced

Temp: $T/W=1/80$



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Dynamical spin susceptibility

Local

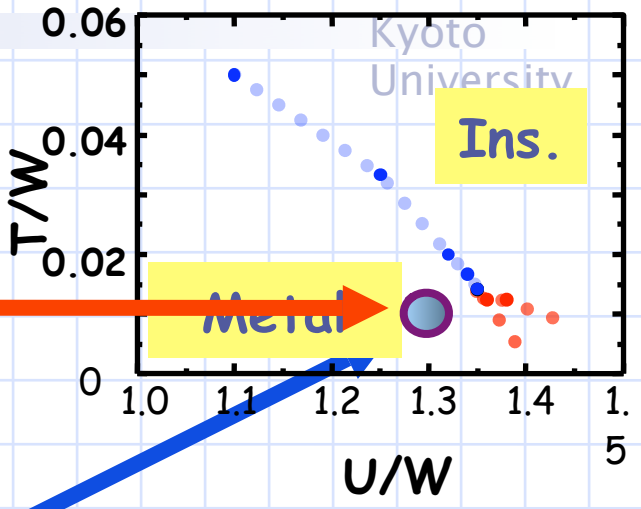
$$\chi_{loc}(\omega) = -i\int \left\langle \left[S_i^z(t), S_i^z(0) \right] \right\rangle e^{-i\omega t}\, dt$$

Metallic phase

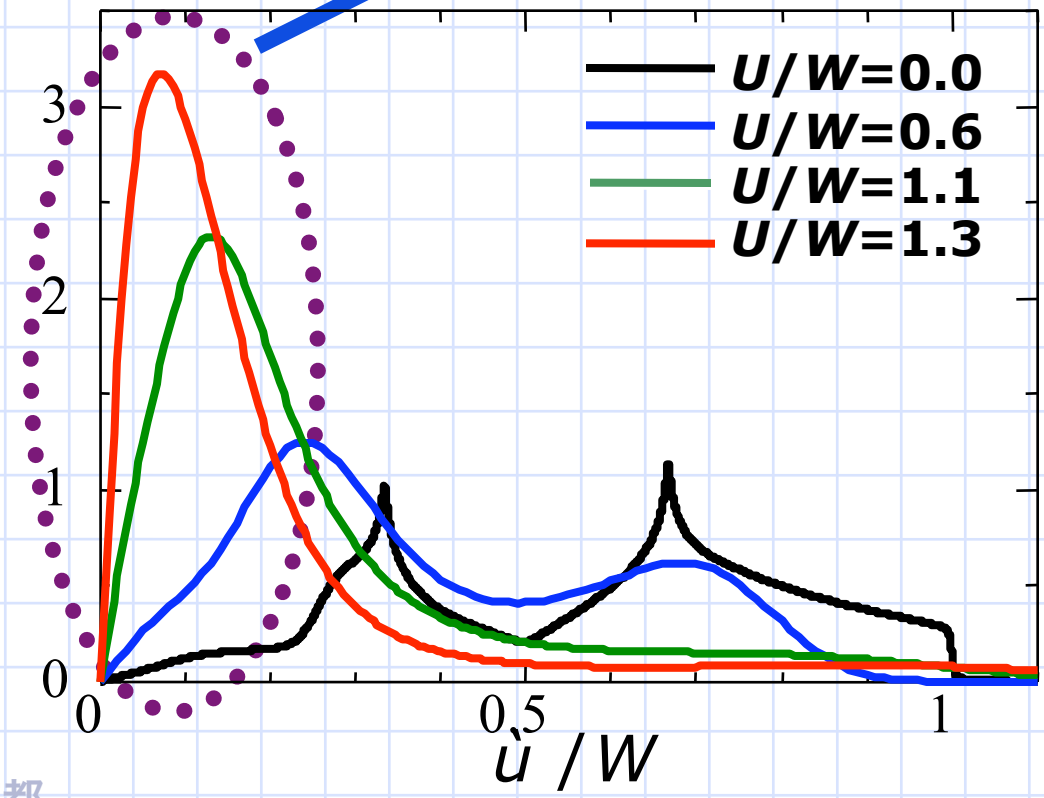
U ⇒ large

- shift
- peak enhanced

Heavy fermions



Temp: $T/W=1/80$



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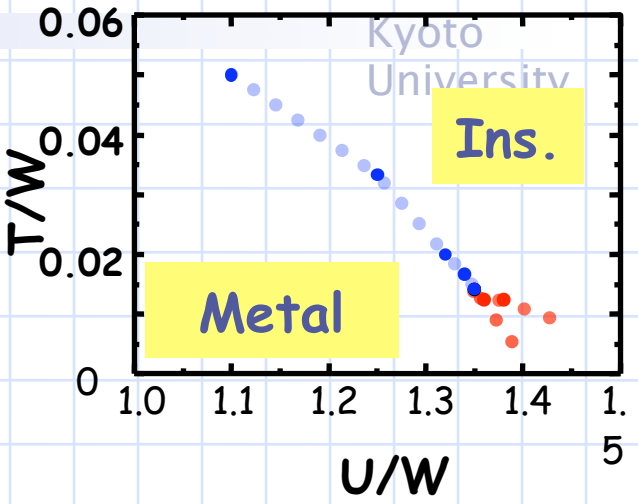
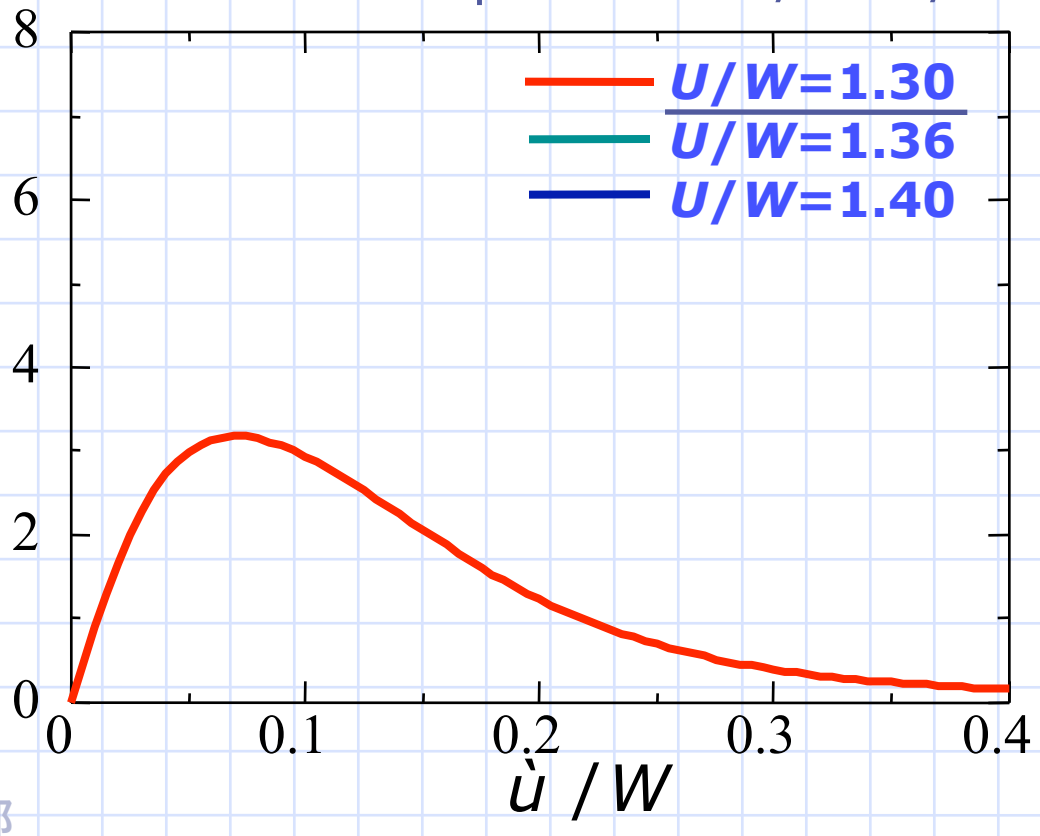
Dynamical spin susceptibility

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



temperature: $T/W=1/80$



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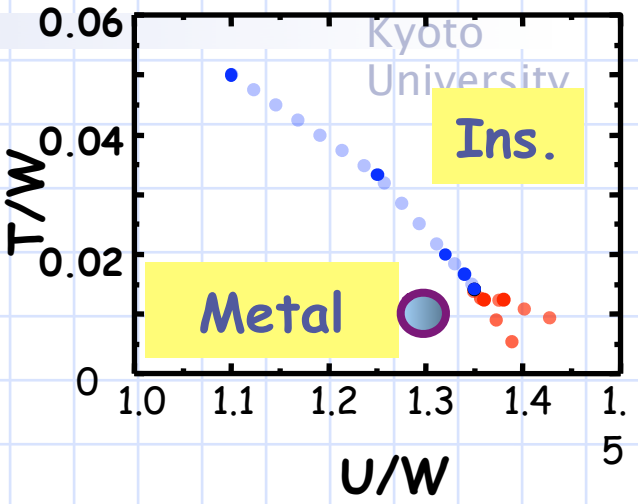
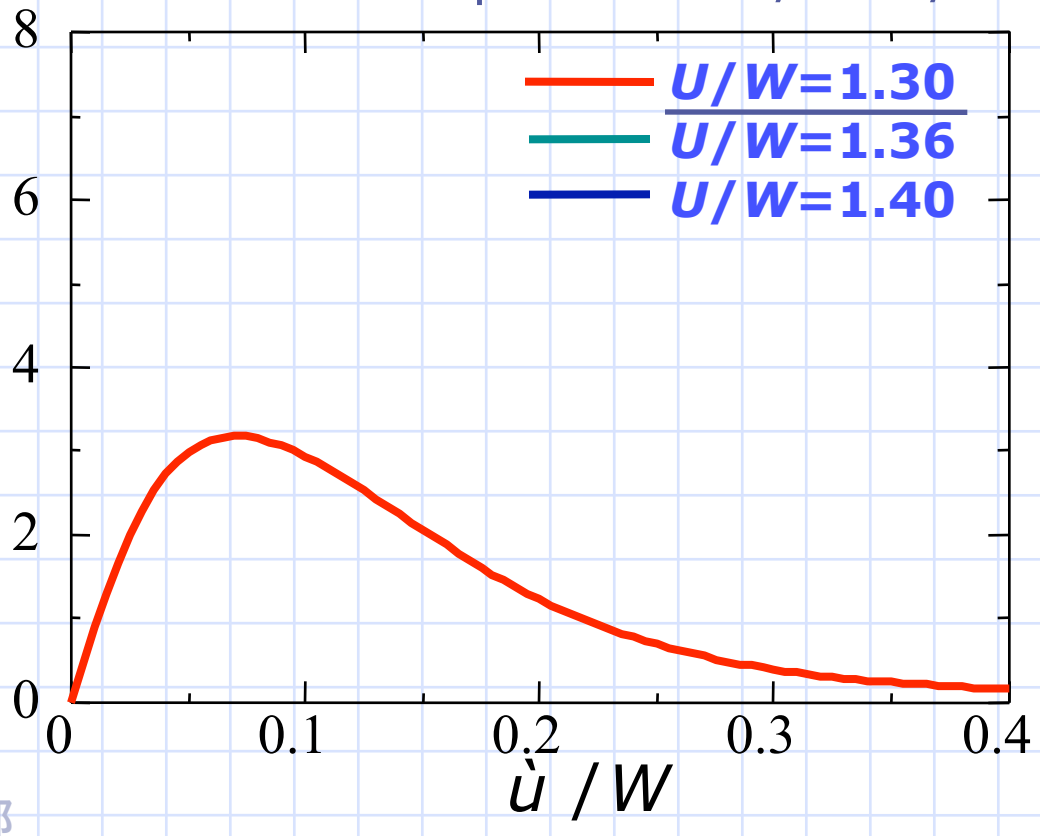
Dynamical spin susceptibility

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



temperature: $T/W=1/80$



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Dynamical spin susceptibility

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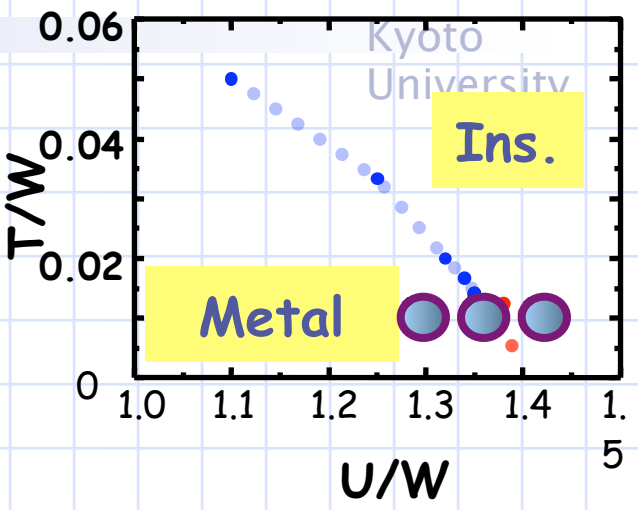
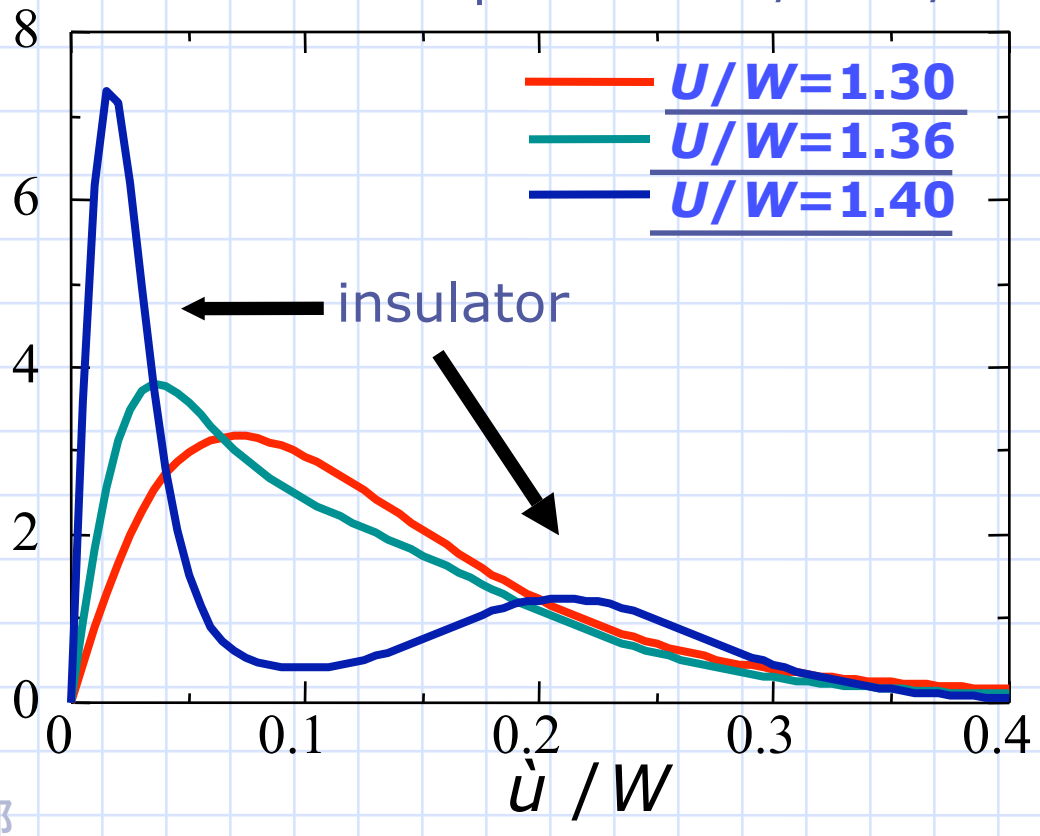


Mott transition ($U_c/W \sim 1.37$)

temperature: $T/W=1/80$



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Dynamical spin susceptibility

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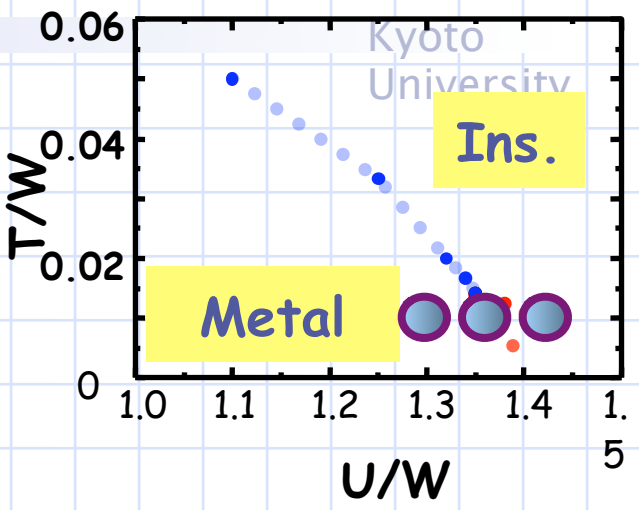
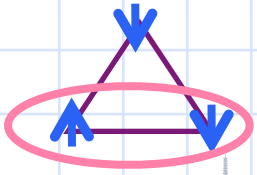


Mott transition ($U_c/W \sim 1.37$)

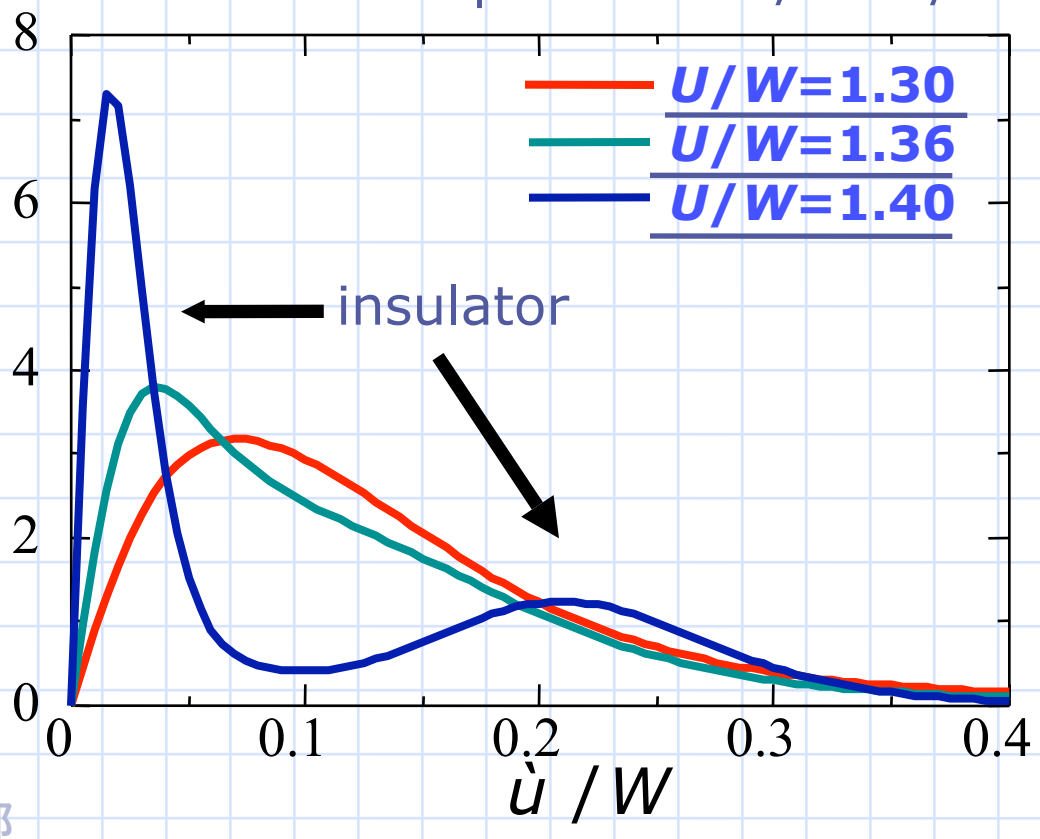
metal ⇒ insulator

Peak: splitting

Pair correlations revived



temperature: $T/W=1/80$



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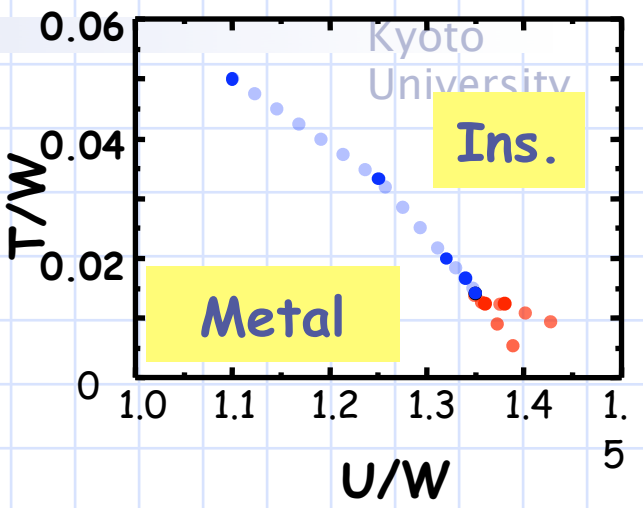

Low T

Very low T

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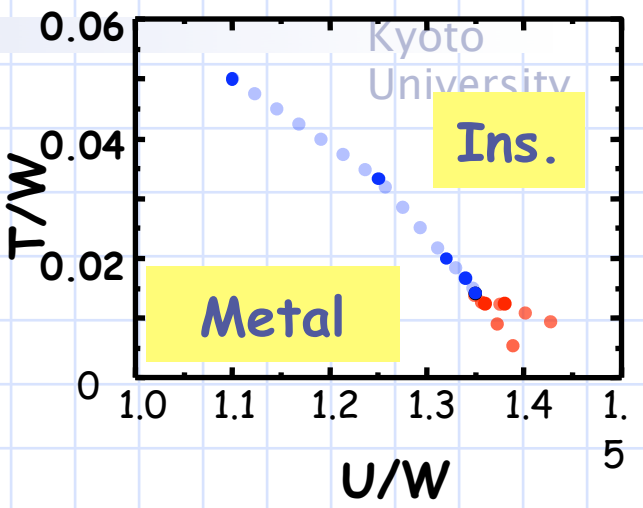
Near Mott transitions



Low T

Very low T

Kyoto University

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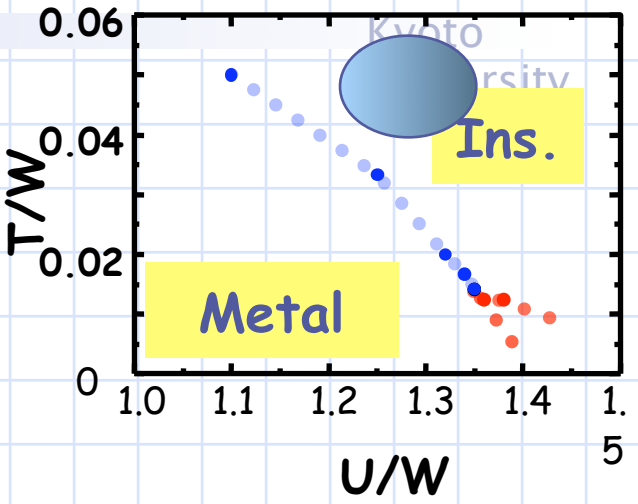
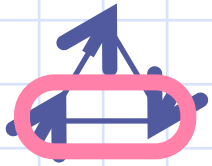


Low T

Pair correlations developed

Very low T



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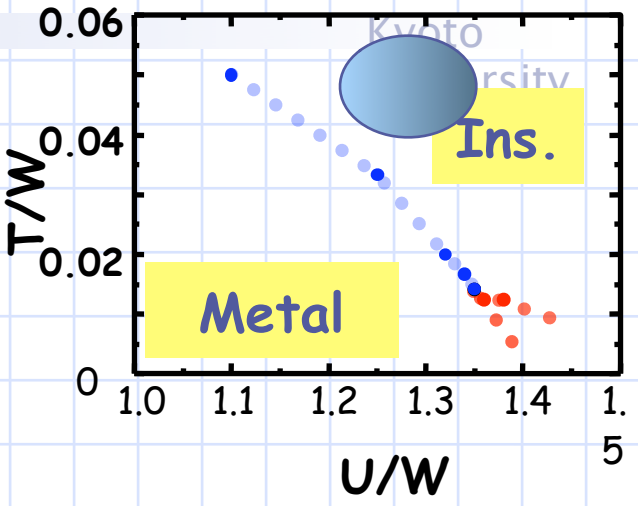
Near Mott transitions

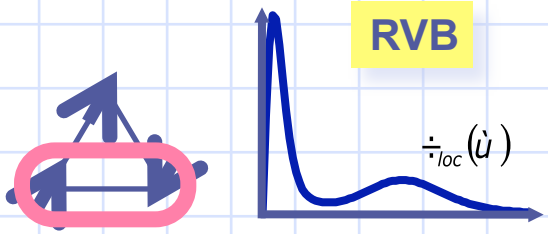


Low T

Pair correlations developed

Causes frustration

Very low T



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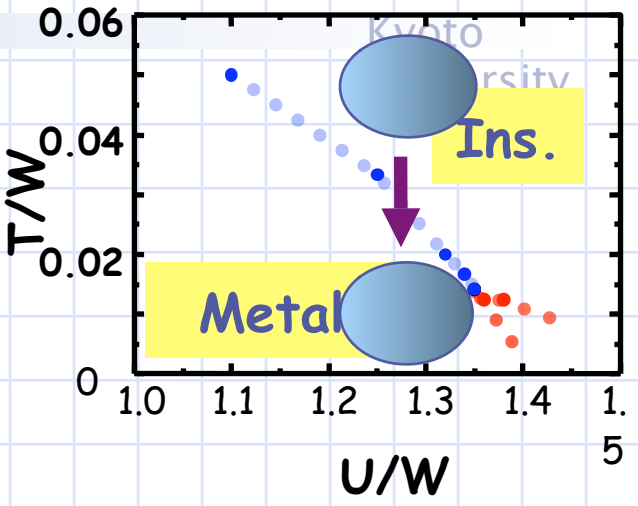
Near Mott transitions



Low T

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Causes frustration

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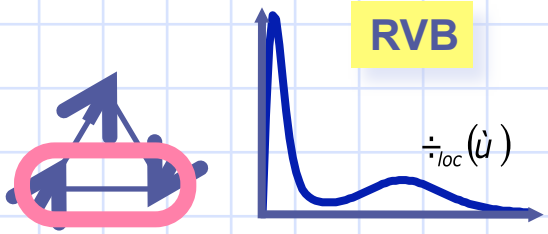

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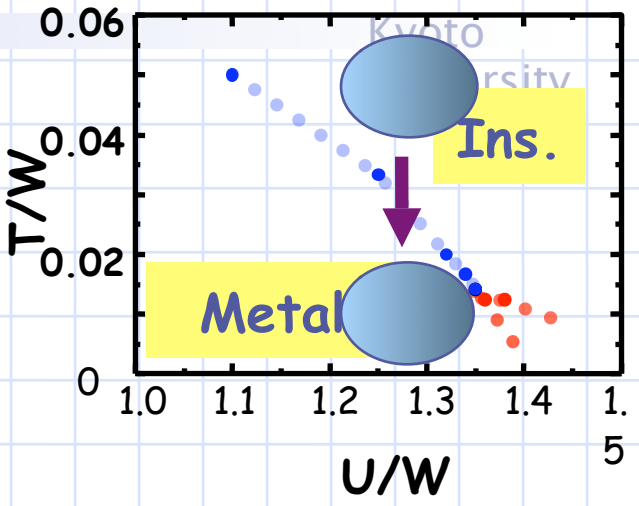
Near Mott transitions



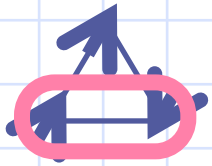
Low T

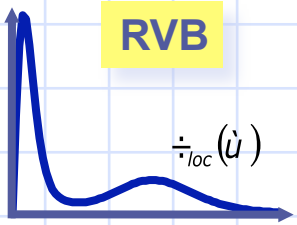
Pair correlations developed

Causes frustration

Very low T

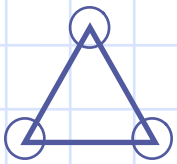
reduce frustration





Itineracy induced

Suppresses pair correlations



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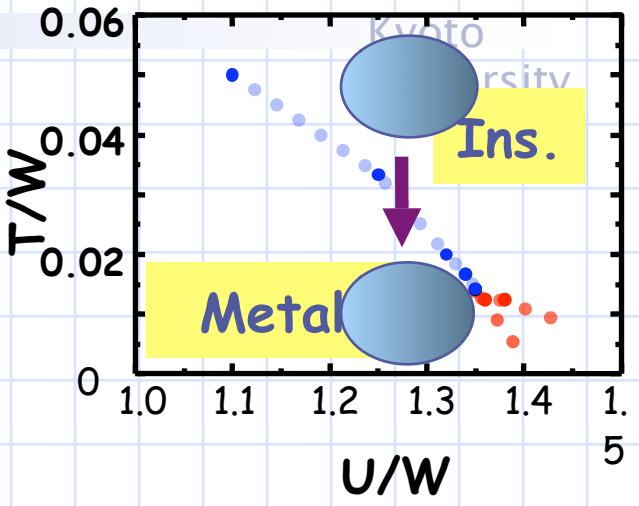
Near Mott transitions



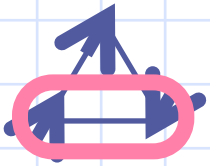
Low T

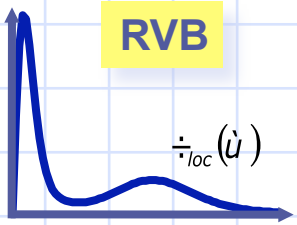
Pair correlations developed

Causes frustration

Very low T

reduce frustration

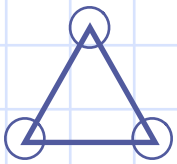


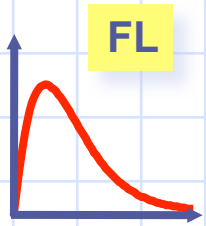


Itineracy induced

Suppresses pair correlations

Heavy fermions





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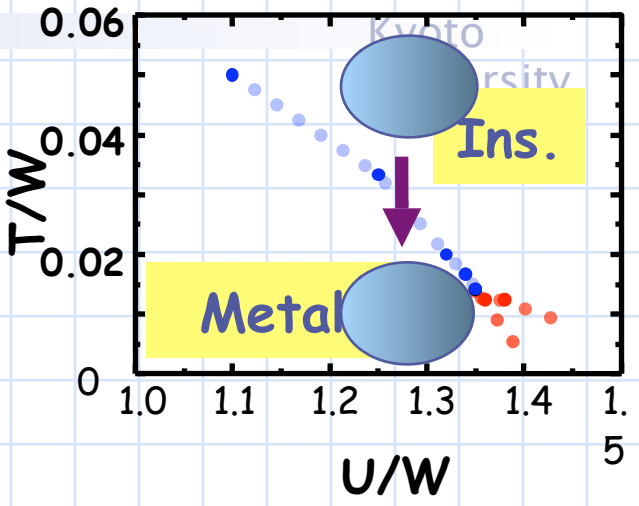
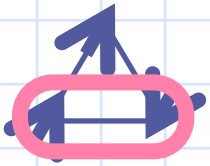
Near Mott transitions



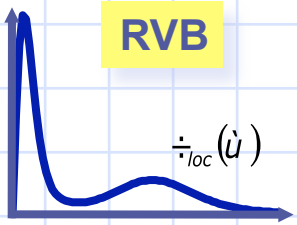
Low T

Pair correlations developed

Causes frustration



reduce frustration

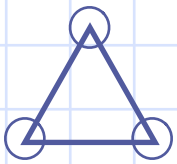


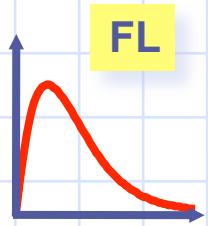
Very low T

Itineracy induced

Suppresses pair correlations

Heavy fermions





Anomalous metallic behavior

Frustration induced

Crossover: RVB-Fermi liquid

Enhanced pair correlations

Masked by itineracy

Very low energy scale

To avoid strong frustration

What is expected ?

Enhanced pair correlations

Masked by itineracy

Very low energy scale

To avoid strong frustration

What is expected ?

Enhanced pair correlations

hidden

Masked by itineracy

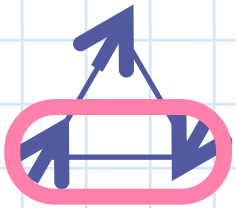
Very low energy scale

To avoid strong frustration

Slight deviations

Filling control

Temperature, etc



Revive pair correlations

What is expected ?

Enhanced pair correlations

hidden

Masked by itineracy

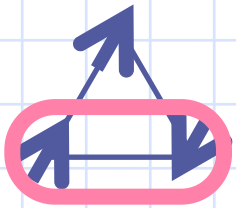
Very low energy scale

To avoid strong frustration

Slight deviations

Filling control

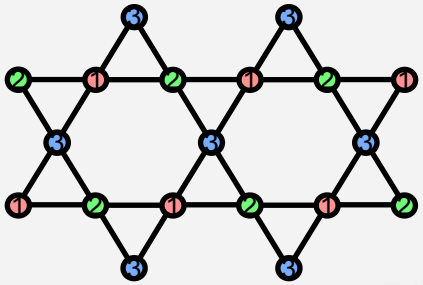
Temperature, etc

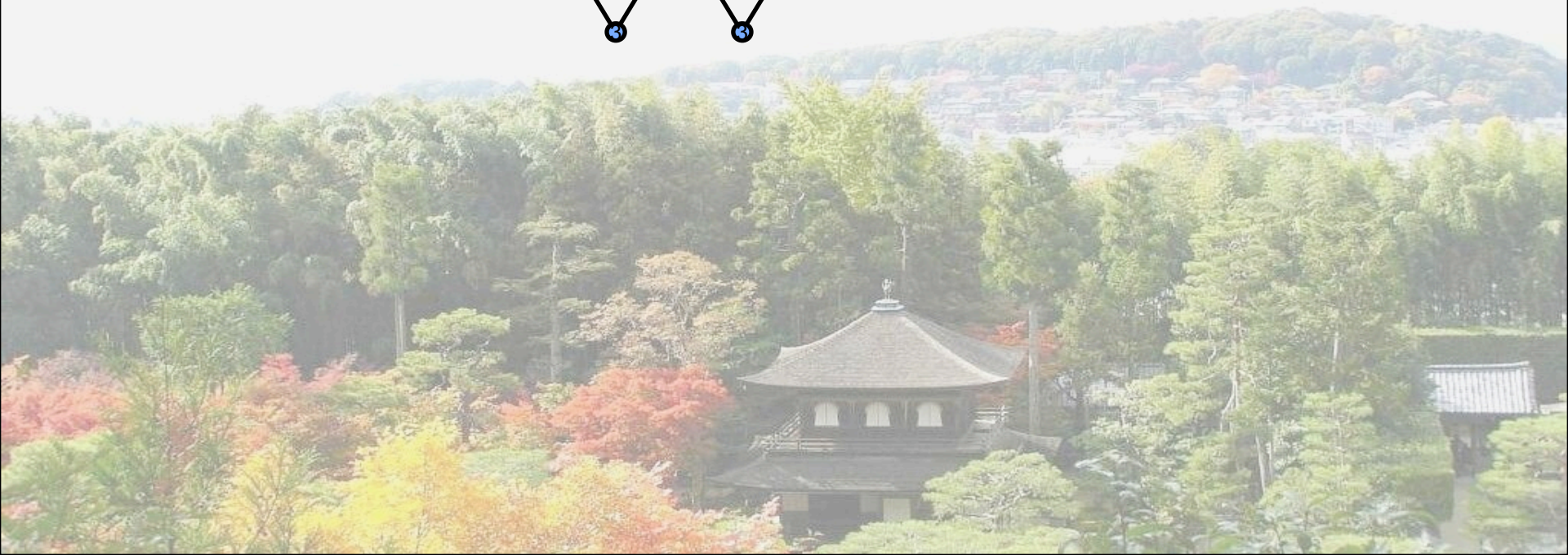


Revive pair correlations

Unusual phenomena ?

YKIS 07
Kyoto
November 14, 2007





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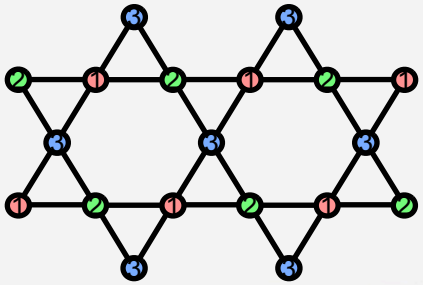
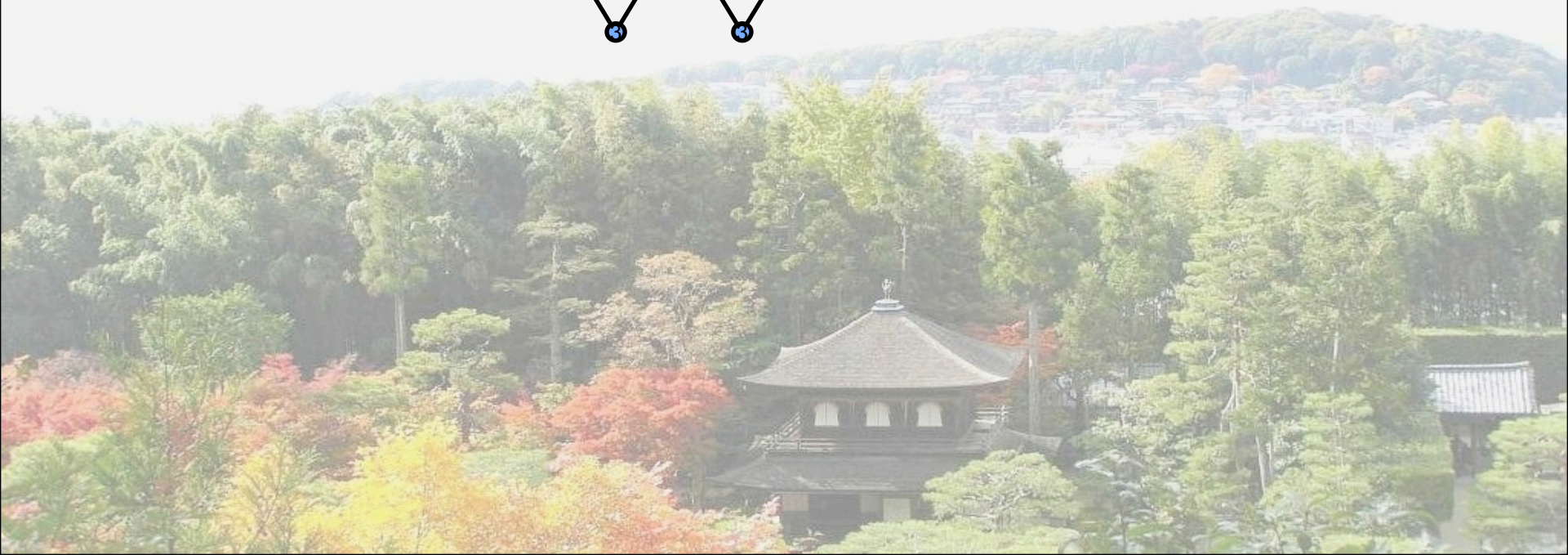
Kyoto
November 14, 2007

Magnetic Instability ?

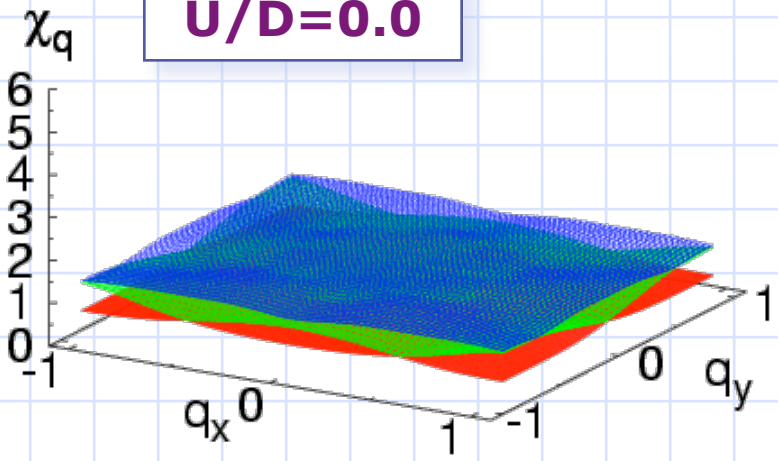




Magnetic susceptibility χ_q

T/D=1/30

U/D=0.0



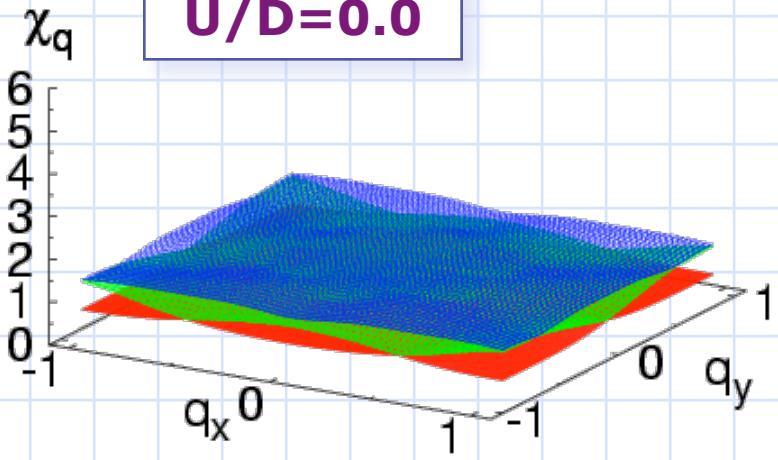
U/D=0.8

U/D=1.1

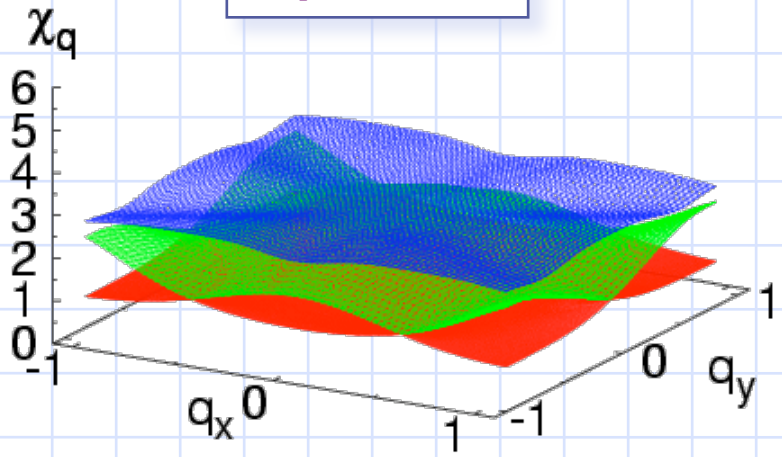
Magnetic susceptibility χ_q

T/D=1/30

U/D=0.0



U/D=0.8

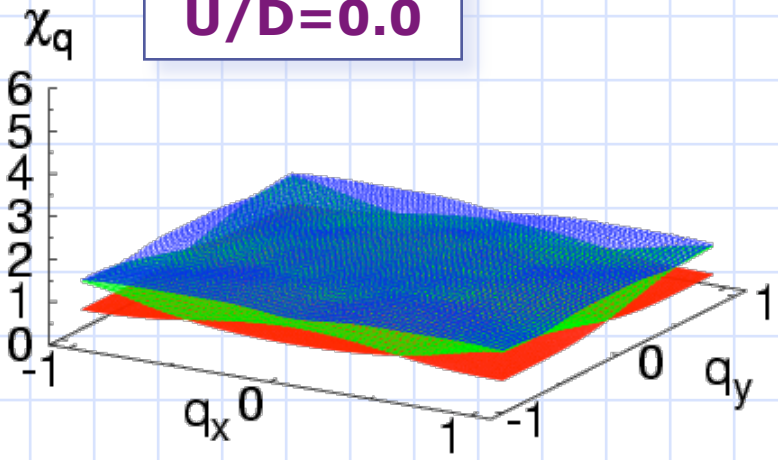


U/D=1.1

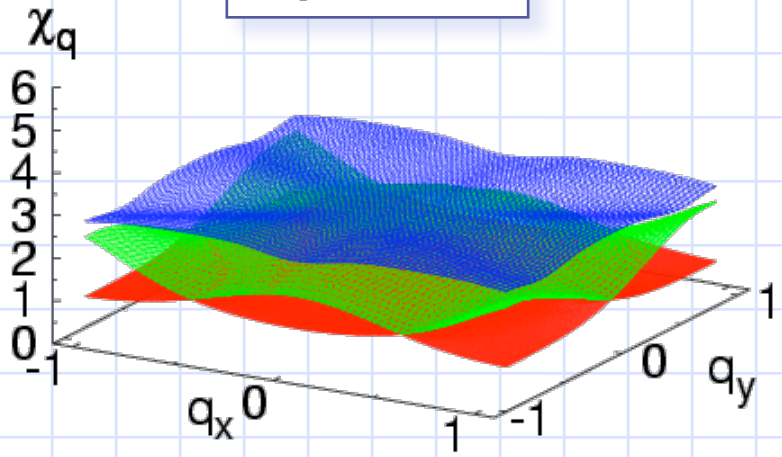
Magnetic susceptibility χ_q

T/D=1/30

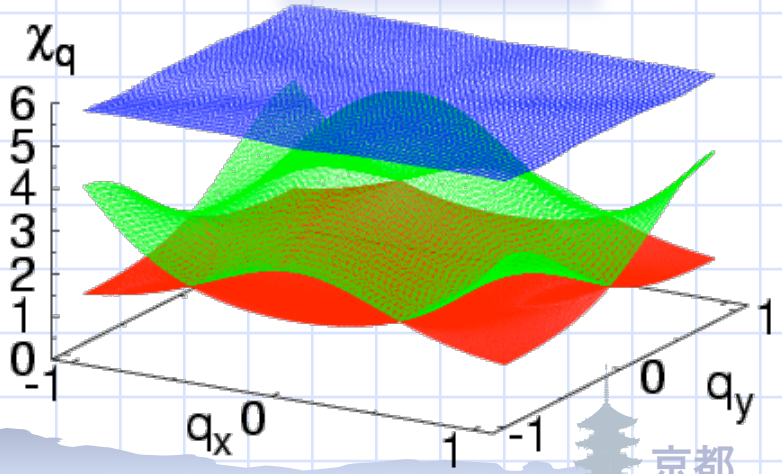
U/D=0.0



U/D=0.8



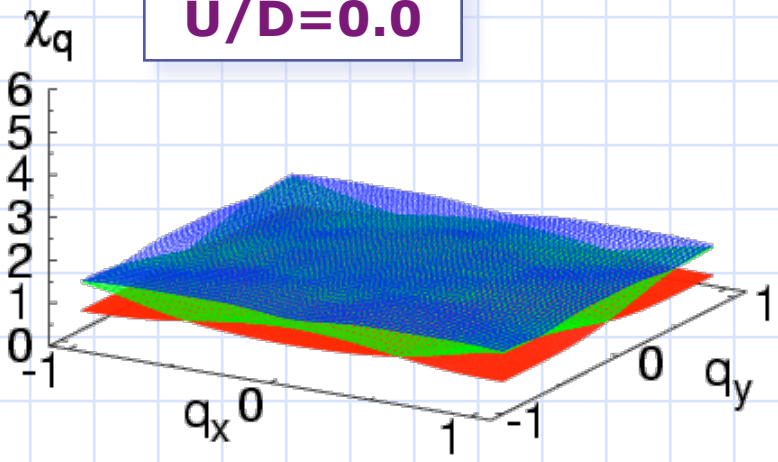
U/D=1.1



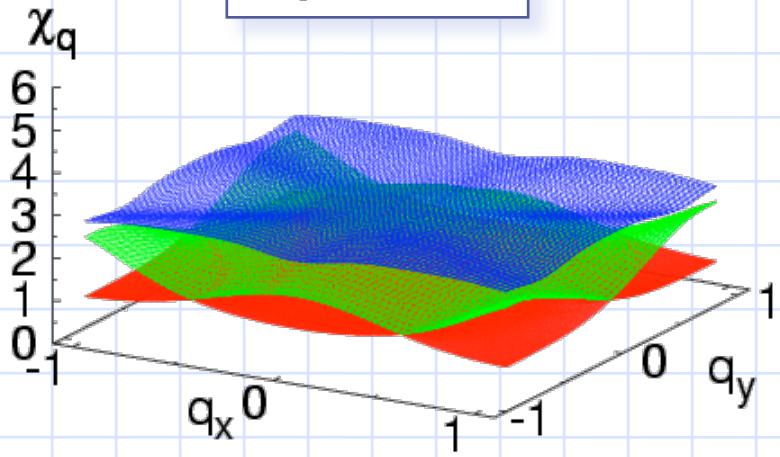
Magnetic susceptibility χ_q

T/D=1/30

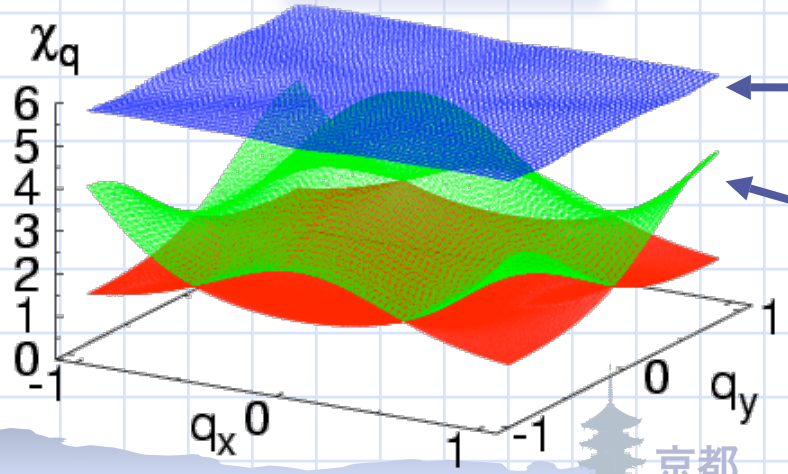
U/D=0.0



U/D=0.8



U/D=1.1



- **maximum**:
  q-dependence→ small
- **middle**:
  q=[0,0] → large

c.f. Imai et al, Bulut et al

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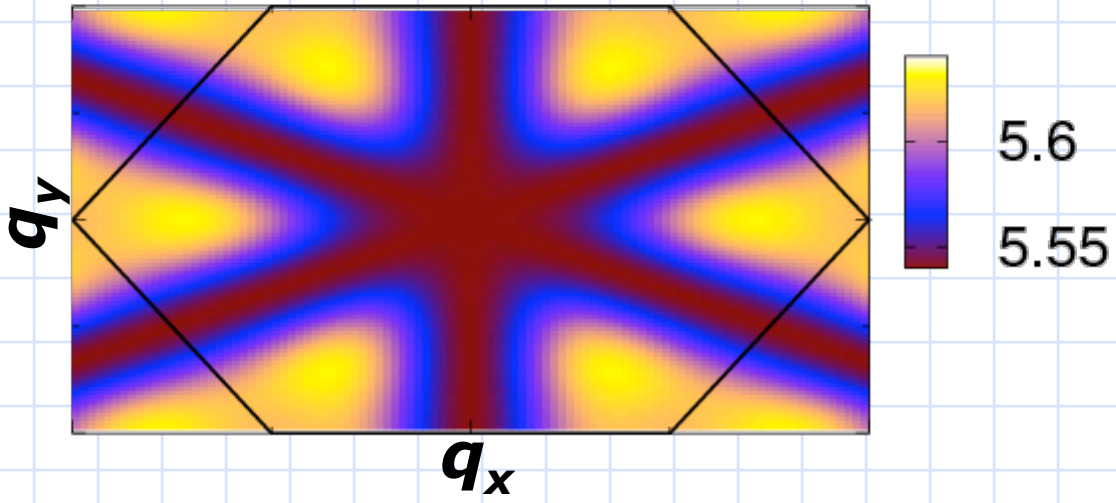
Maximum eigenvalues

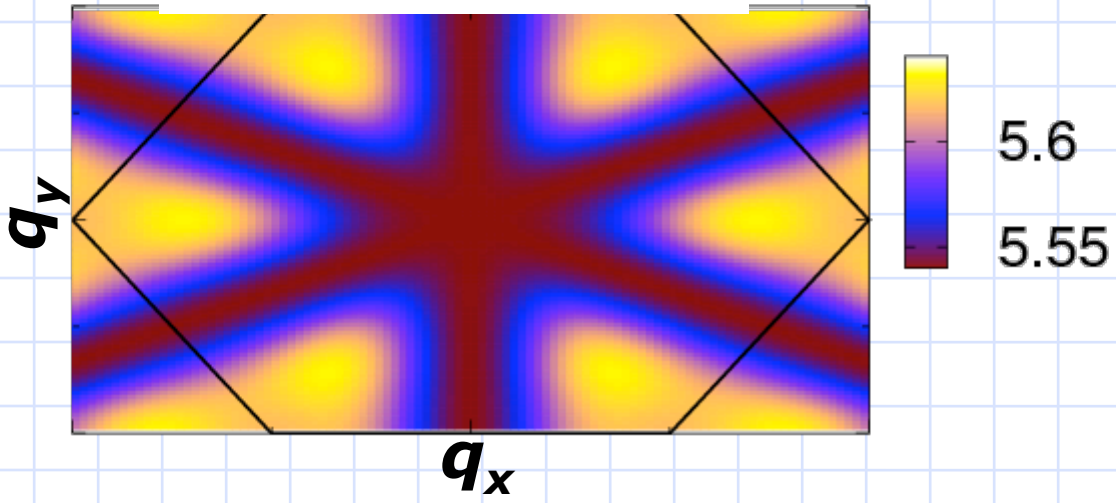
(temperature: T/W=1/30)



Maximum eigenvalues

(temperature: T/W=1/30)

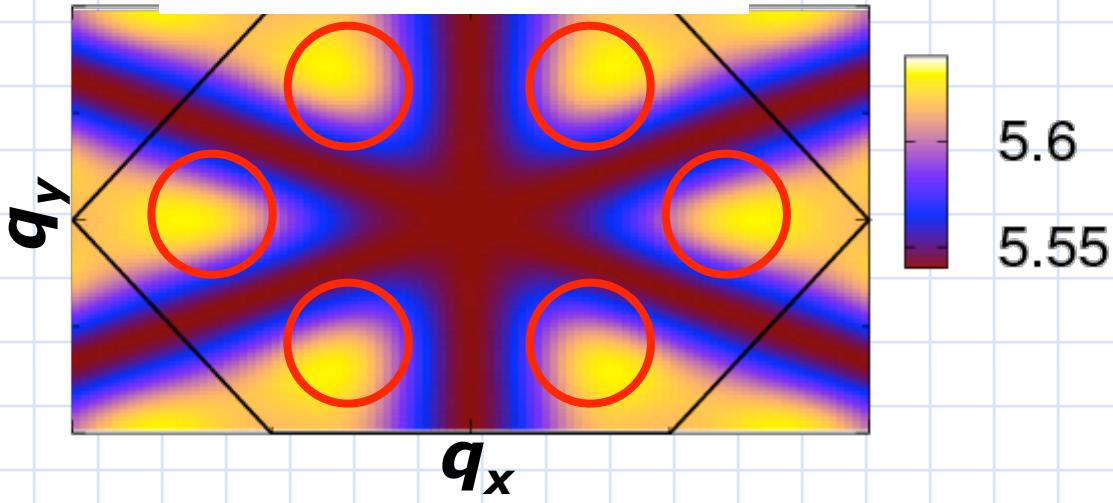
Metal: U/W=1.1



Maximum eigenvalues

(temperature: T/W=1/30)

Metal: U/W=1.1

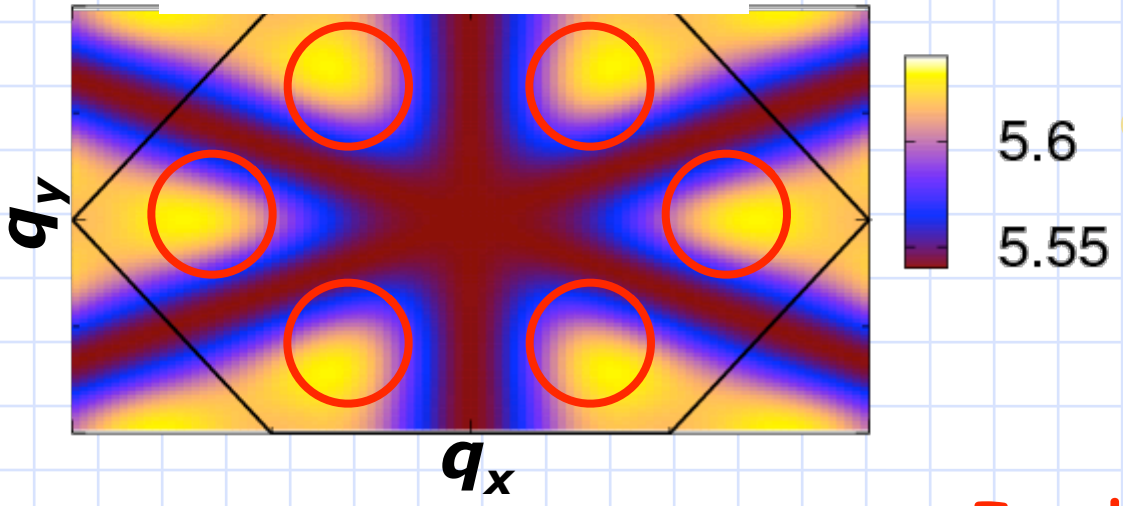


- Nesting of Fermi surface
- Maximum at six points

Maximum eigenvalues

(temperature: T/W=1/30)

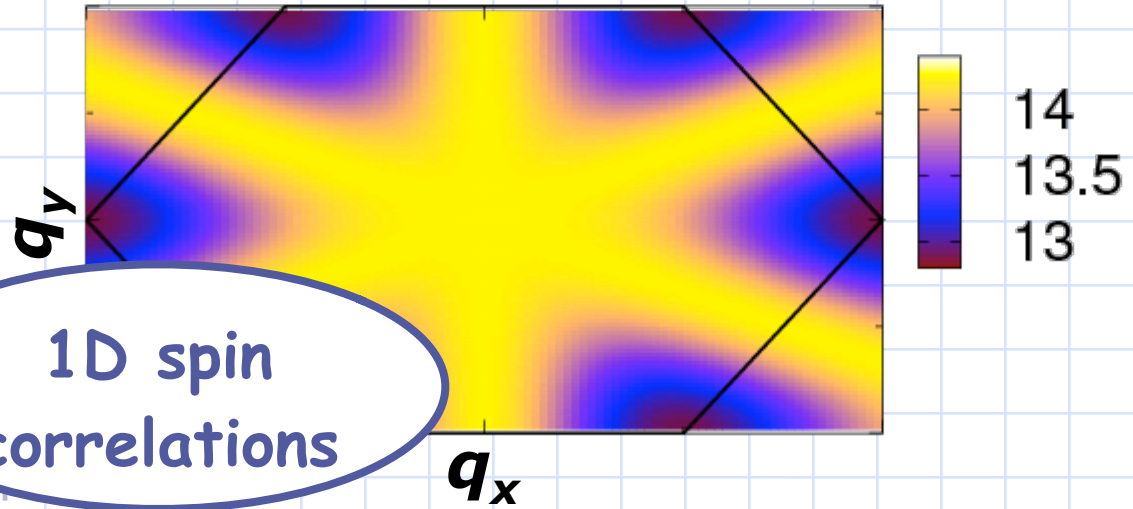
Metal: U/W=1.1



- Nesting of Fermi surface
- Maximum at six points

- n.n. spin correlation
- change in q-dependence !

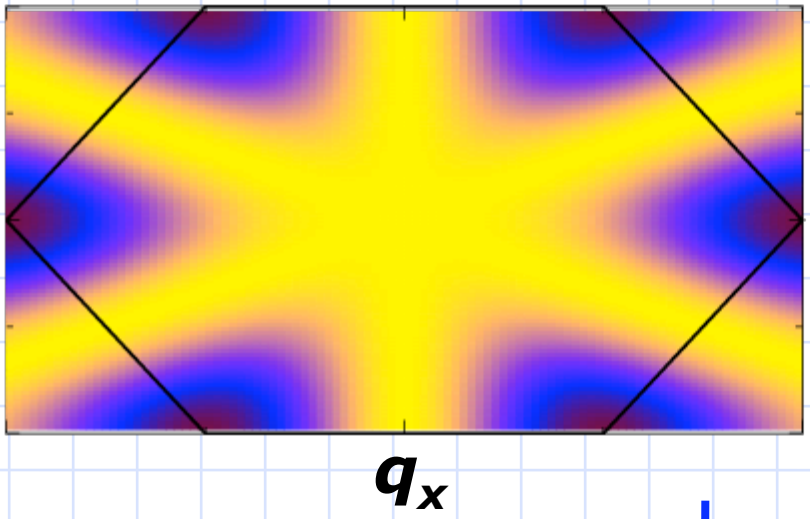
Insulating phase: U/W=1.4

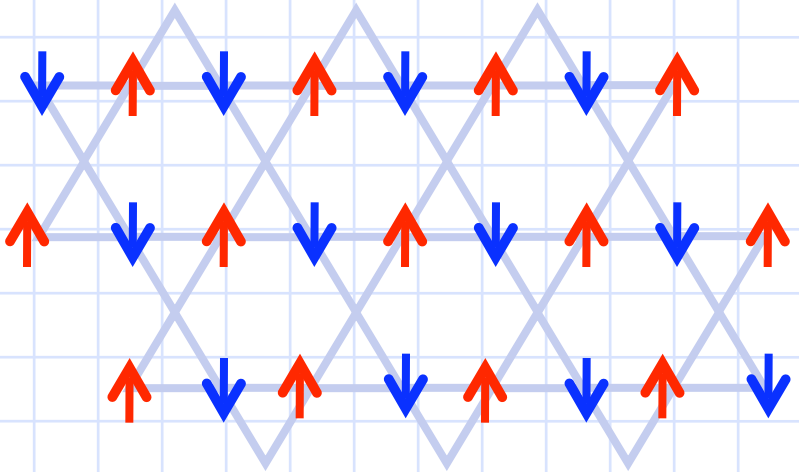


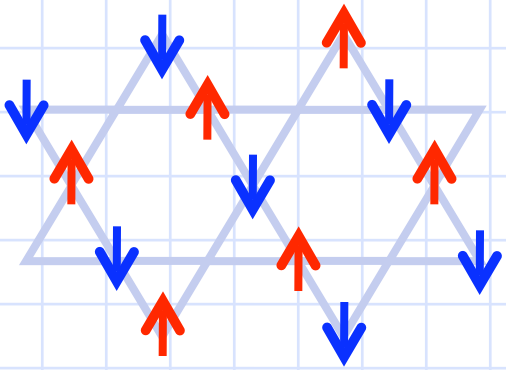
1D spin correlations

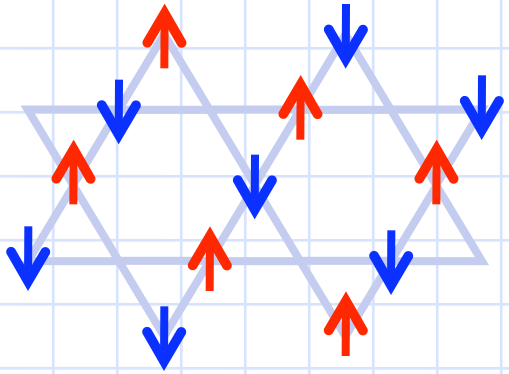
Dominant Spin Configurations

Mott phase



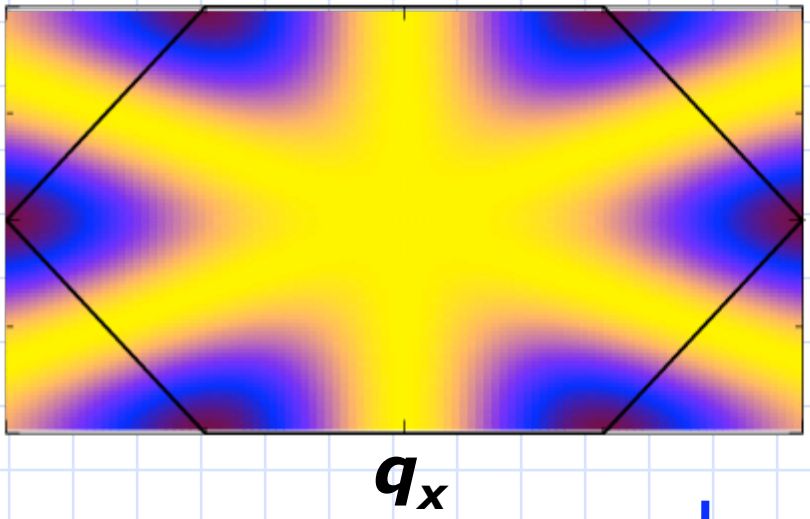


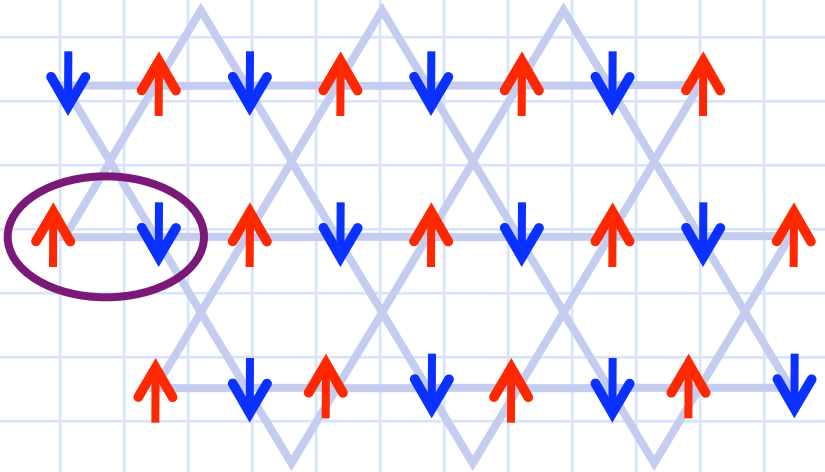


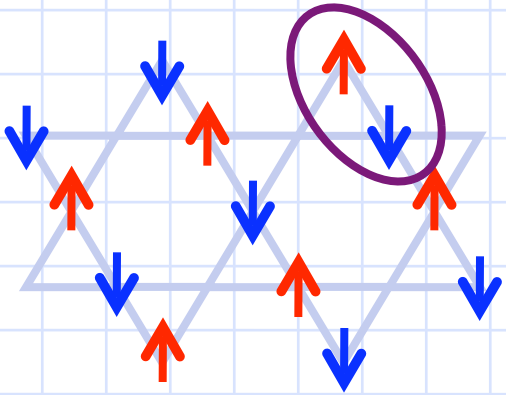


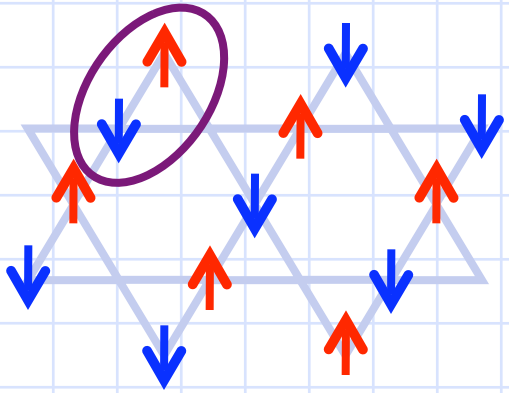
Dominant Spin Configurations

Mott phase





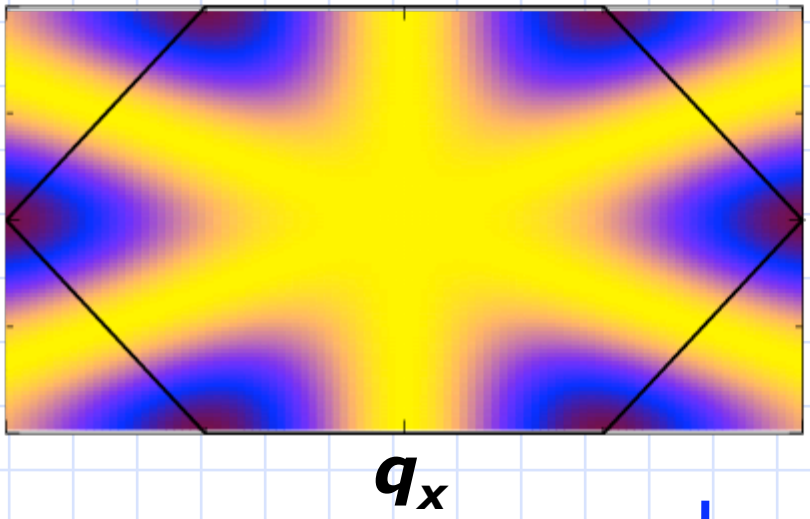


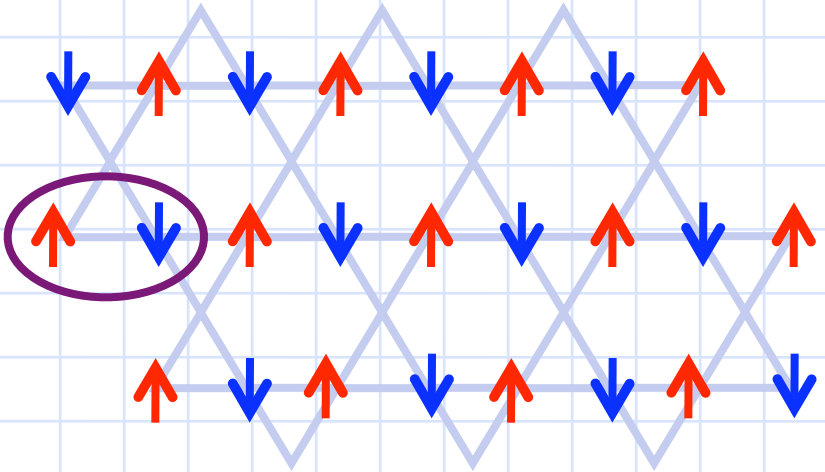


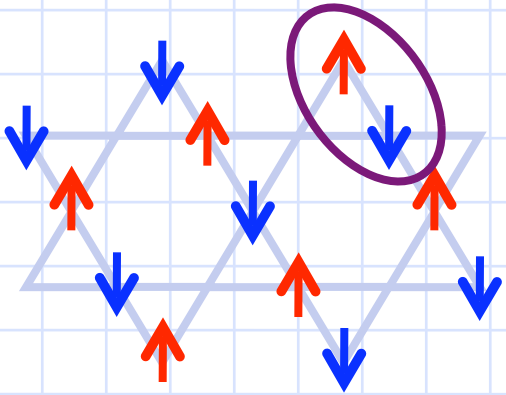
Short range
Pair correlations

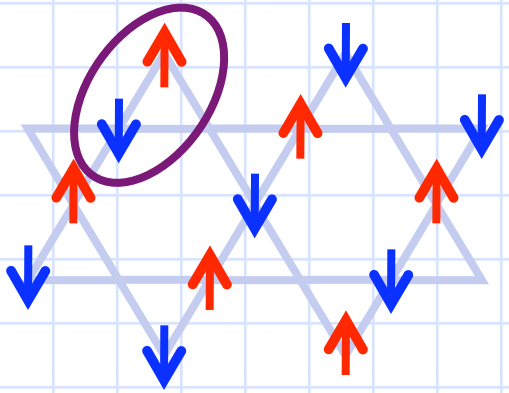
Dominant Spin Configurations

Mott phase







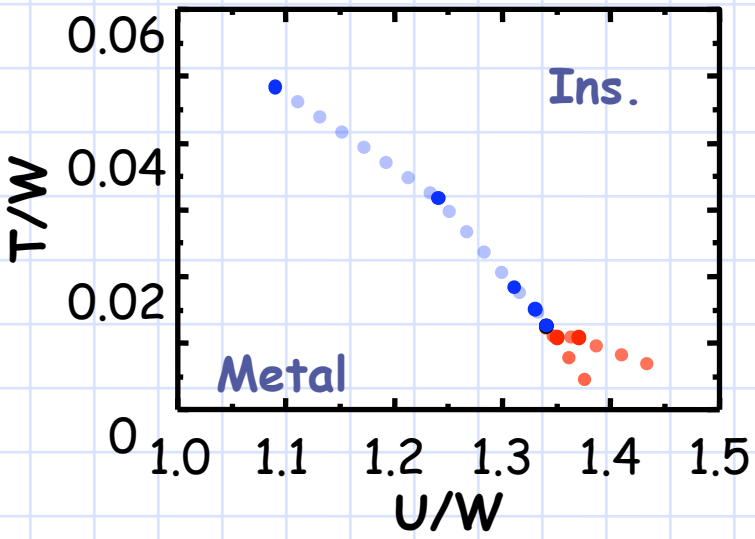


Short range
Pair correlations

Three AF-correlated 1D chains

Kagome lattice Hubbard model

- 1st order Mott transition
  - $U_c/W \sim 1.37$ (T/W=1/80)
- Metallic phase close to MIT

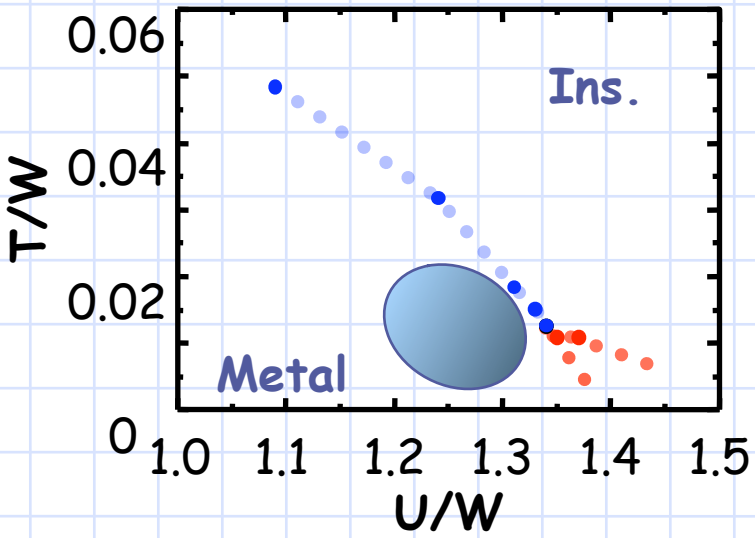


Kagome lattice Hubbard model

- 1st order Mott transition
  - $U_c/W \sim 1.37$ (T/W=1/80)
- Metallic phase close to MIT

frustration-induced heavy fermions

Enhanced spin correlations are masked by itineracy



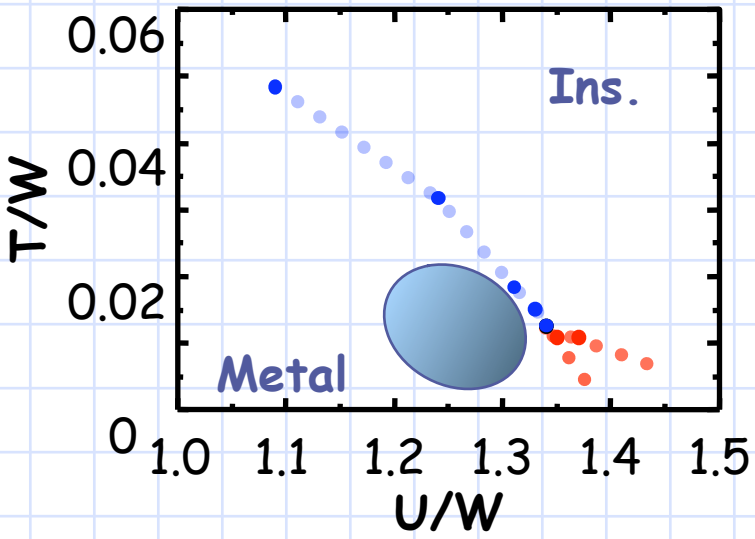
Kagome lattice Hubbard model

- 1st order Mott transition
  - $U_c/W \sim 1.37$ (T/W=1/80)
- Metallic phase close to MIT

frustration-induced heavy fermions

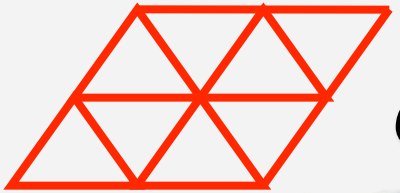
Enhanced spin correlations are masked by itineracy

Common to MT with frustration



Triangular Lattice

YKIS 07
Kyoto
November 14, 2007



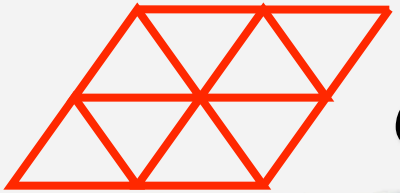
Organics

Ohashi et al. (2007)

YKIS 07
Kyoto
November 14, 2007

Triangular Lattice

Reentrant transition



Organics

Ohashi et al. (2007)

Organic conductors

◇ Correlated Electron Systems

◇ Simple electronic structure in k space

highly compressible

Pressure-induced !

Mott transitions
Superconductivity
Magnetism

Pressure-induced Mott transition

Band-width control

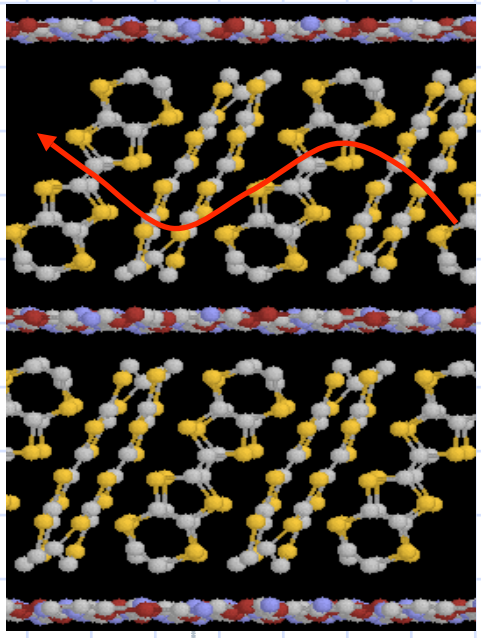
Kanoda group

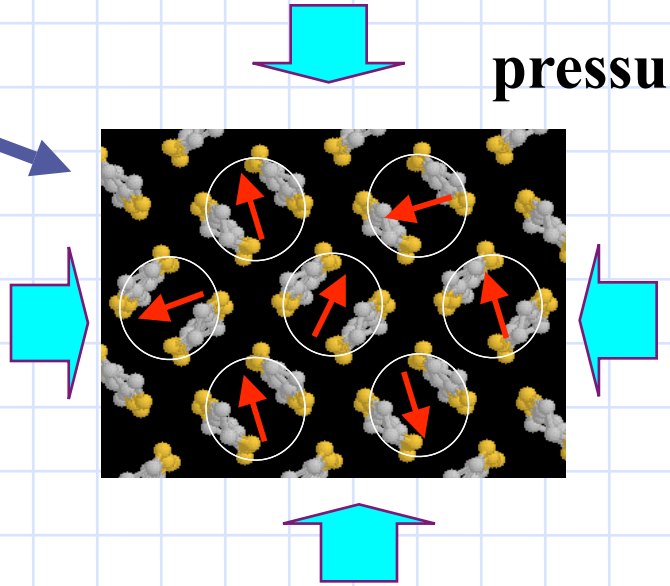
Quasi-2D organics κ-$(ET)_2Cu[N(CN)_2]Cl$

ET molecules

$Cu[N(CN)_2]Cl$

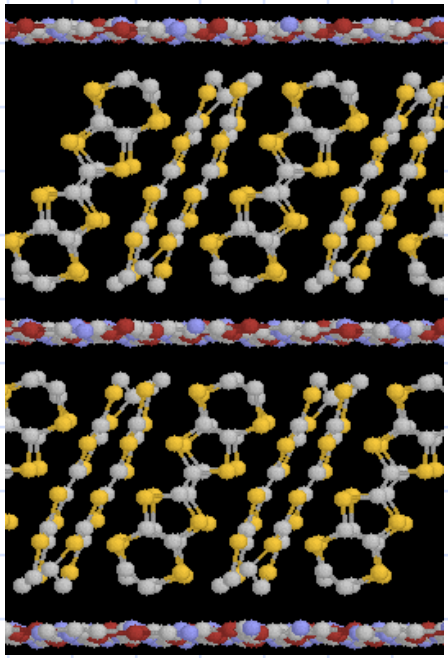
ET molecules

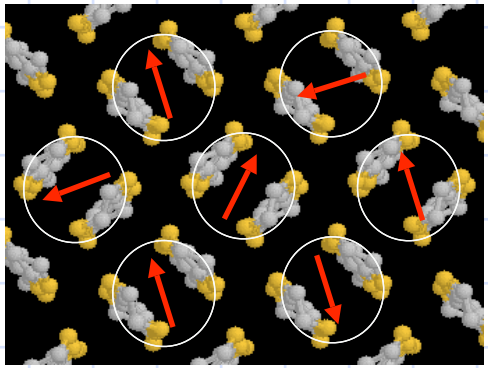




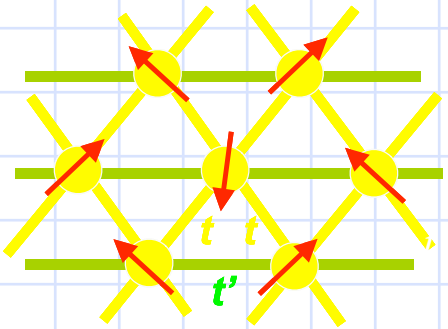
κ-$(ET)_2X$ organics Triangular lattice

Layer structure



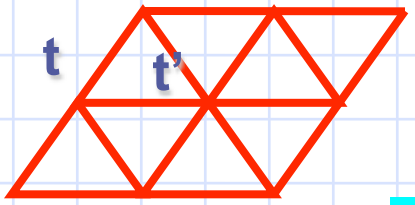


dimer model



Half-filling

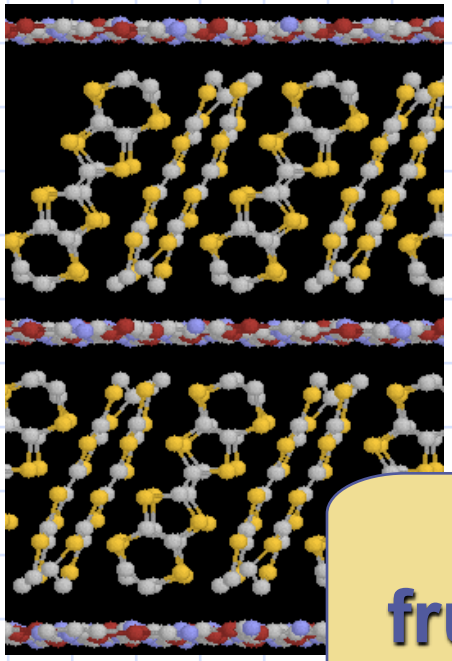
X	t'/t
$Cu_2(CN)_3$	1.06
$Cu[N(CN)_2]Cl$	0.75

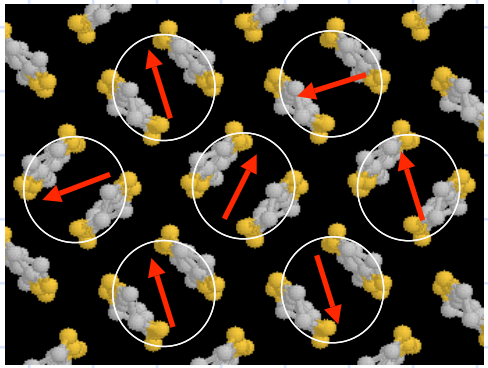


Anisotropic Triangular

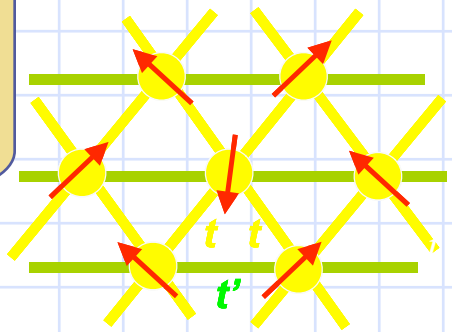
κ-$(ET)_2X$ organics Triangular lattice

Layer structure





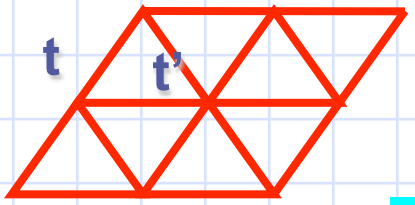
dimer model



Half-filling

Fully frustrated

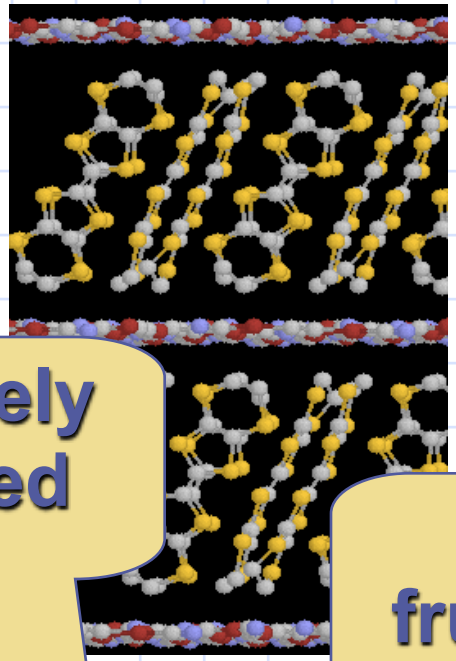
X	t'/t
$Cu_2(CN)_3$	1.06
$Cu[N(CN)_2]Cl$	0.75

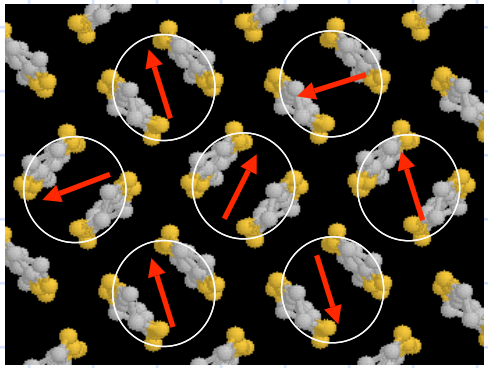


Anisotropic Triangular

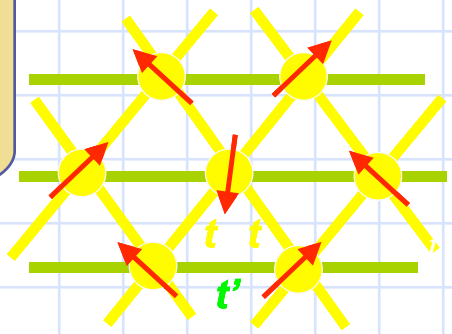
κ-$(ET)_2X$ organics Triangular lattice

Layer structure





dimer model



Half-filling

moderately frustrated

Fully frustrated

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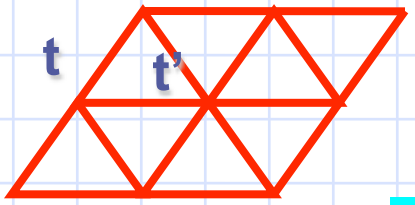


Anisotropic Triangular

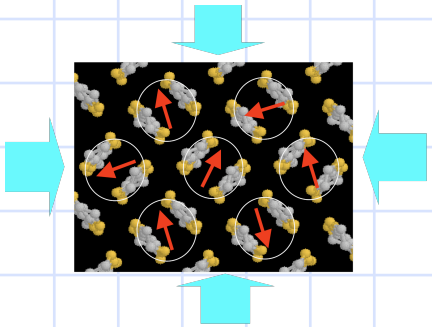
Mott transition by pressure

κ-$(ET)_2Cu[N(CN)_2]Cl$

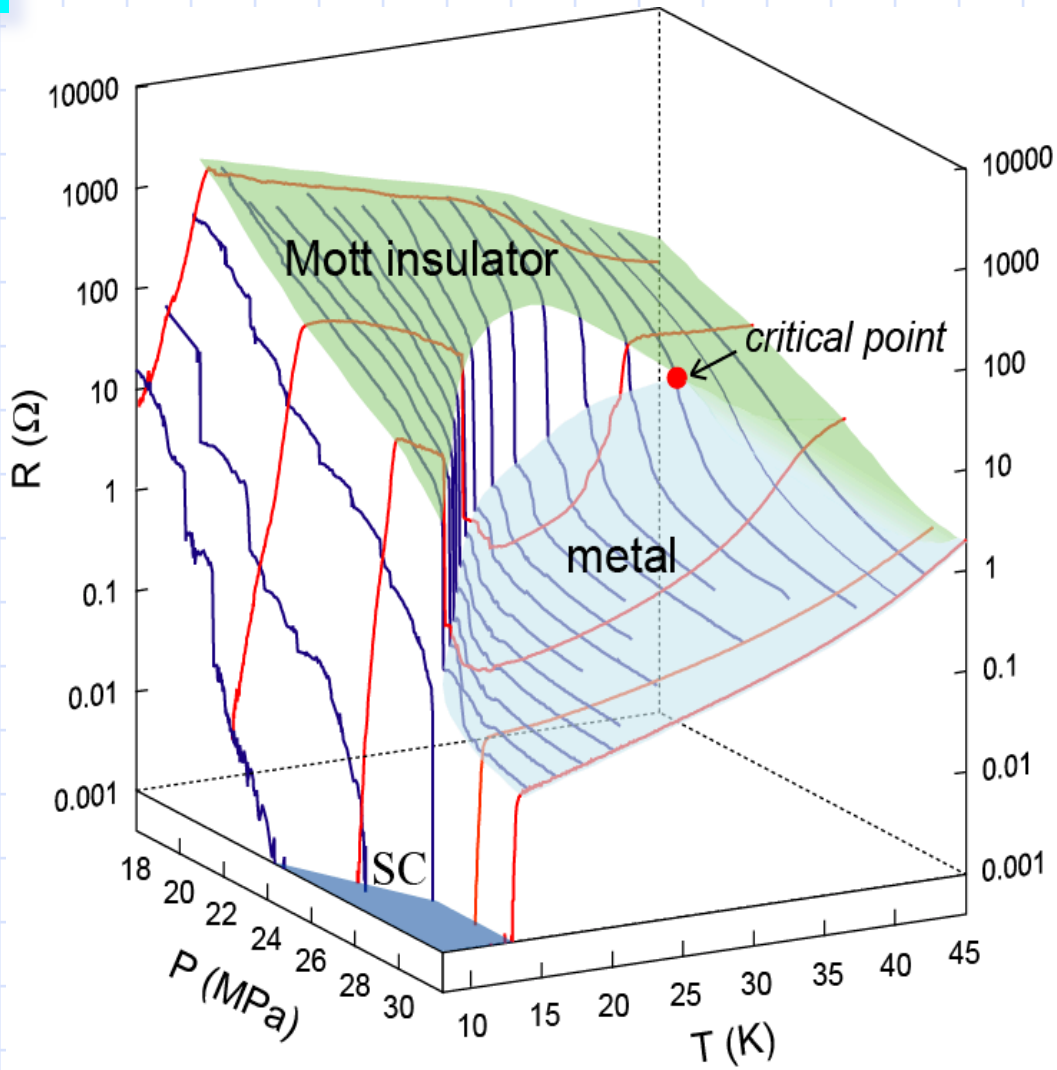
t'/t=0.75

Kanoda group

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

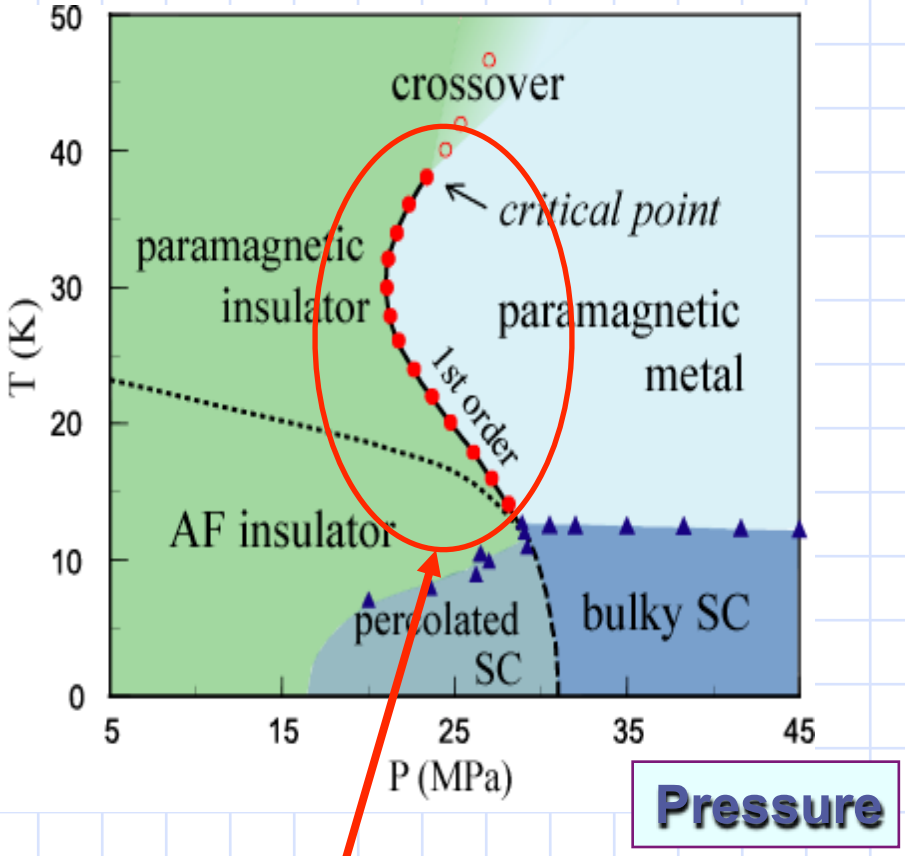


Resistance

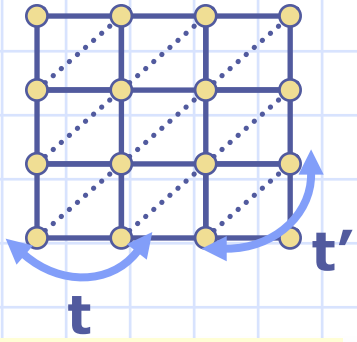


κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

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



Pressure



t'/t =0.8

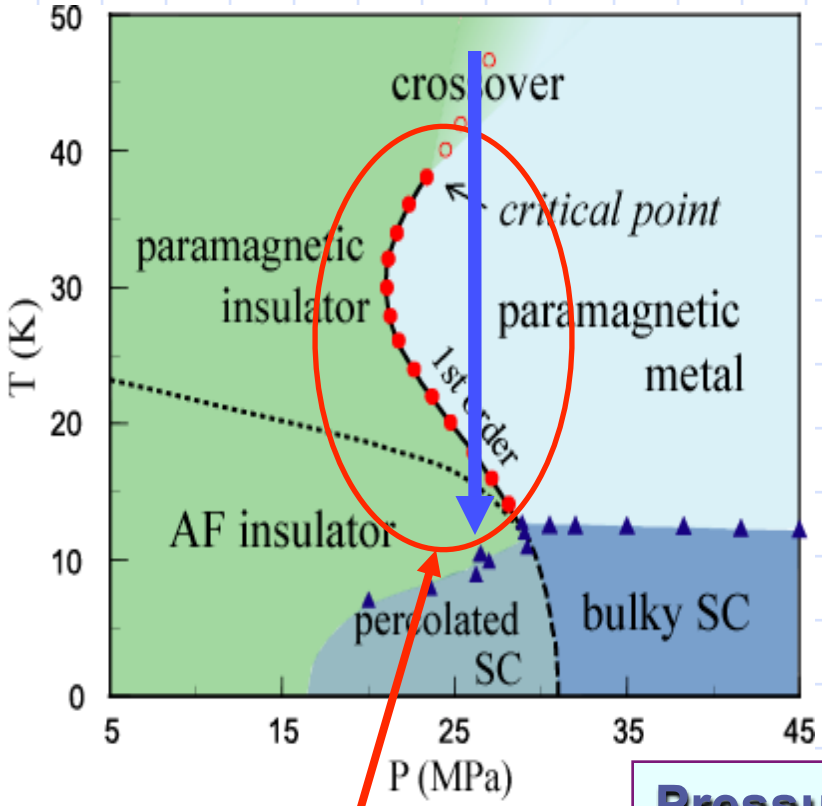
moderately frustrated

Finite-T Mott transition

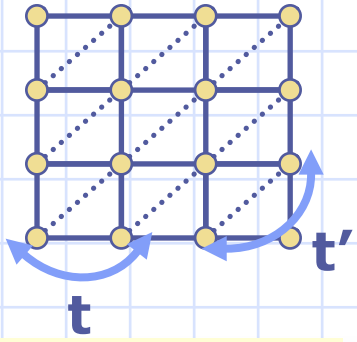
Reentrant behavior

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

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



Pressure



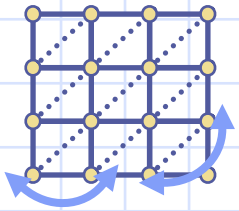
t'/t =0.8

moderately frustrated

Finite-T Mott transition

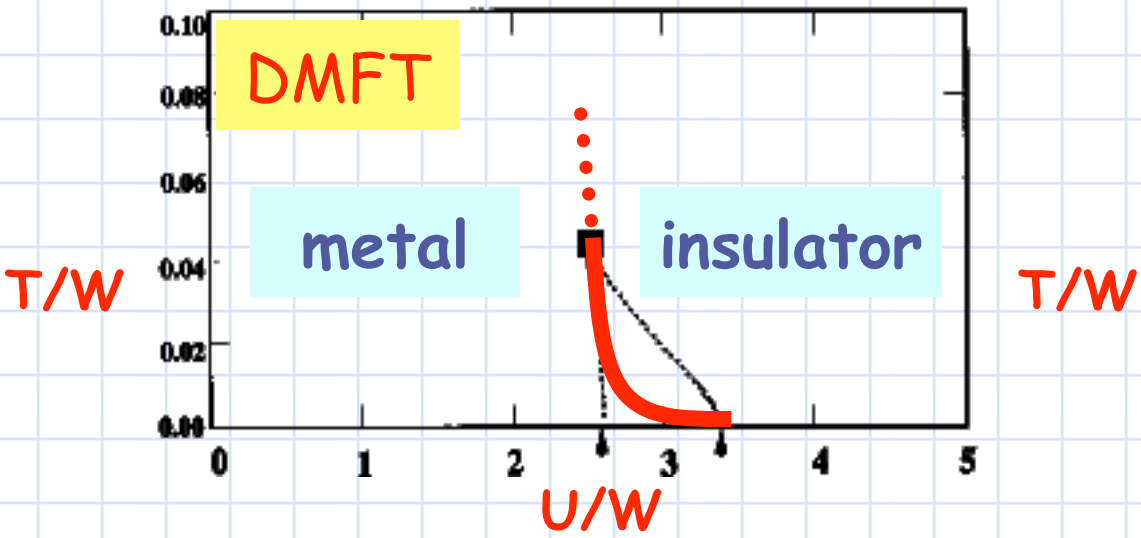
Reentrant behavior

Itineracy vs Frustration



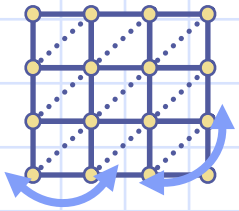
Basic & Naive question

D=∞ Hubbard model

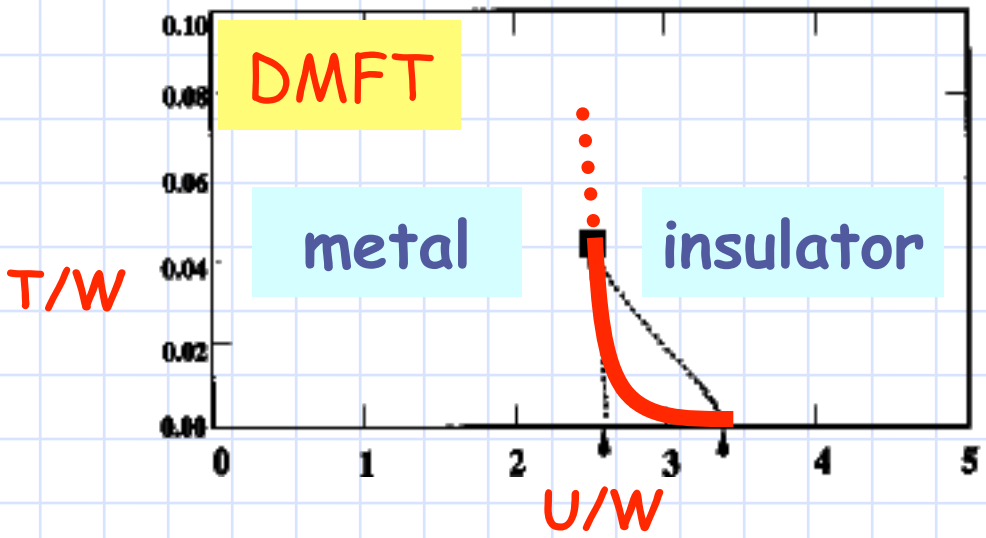


Georges et al., RMP, 68, 13 (1996)

Basic & Naive question



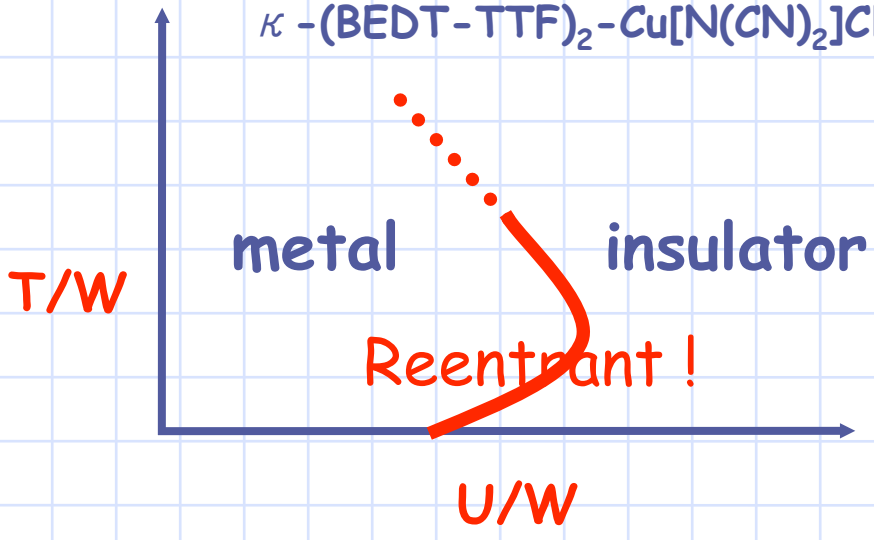
D=∞ Hubbard model



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

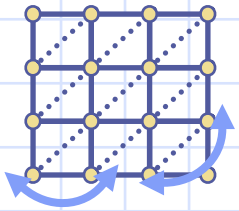
organics

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

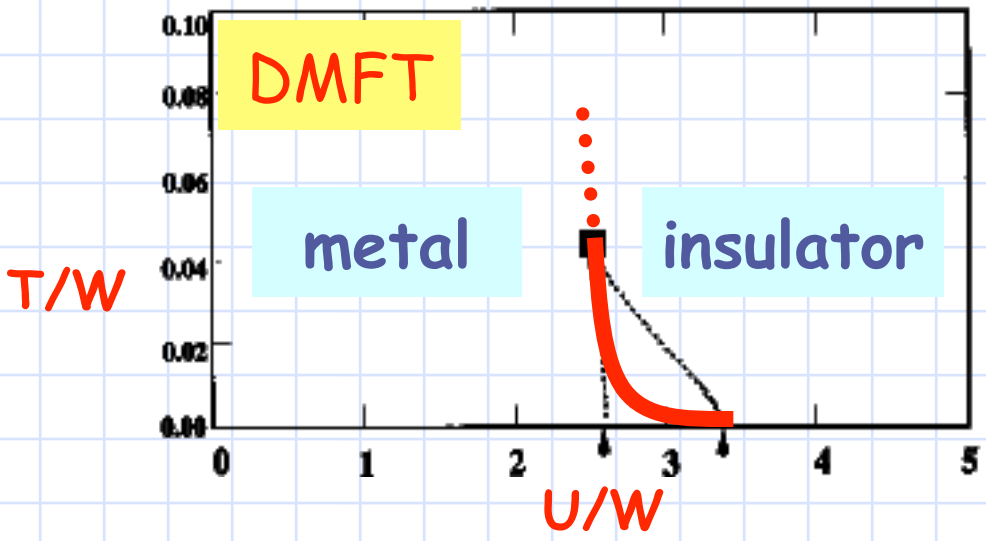


$\propto$ (pressure)$^{-1}$

Basic & Naive question



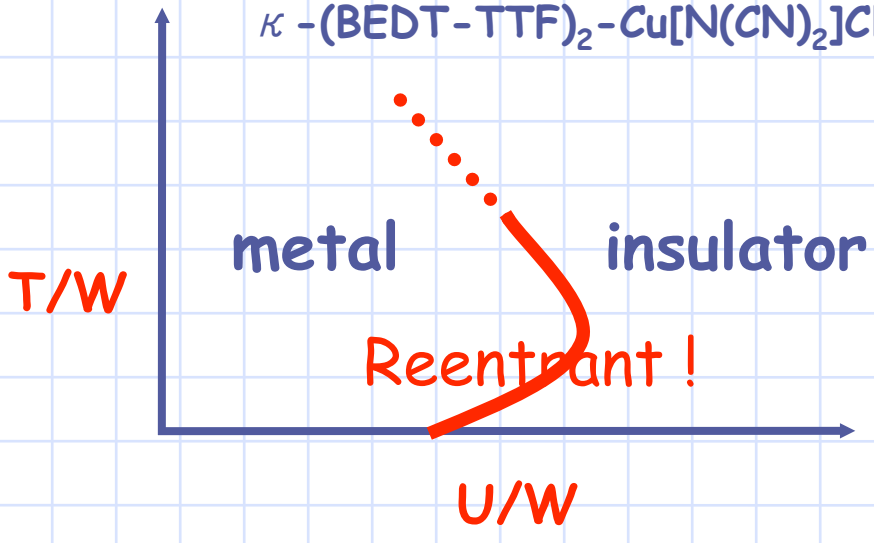
D=∞ Hubbard model



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

organics

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



Effects of frustration

→ Cluster (Cellular-DMFT)

YKIS 07
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November 14, 2007

Cellular DMFT treatment

YKIS 07
Kyoto
November 14, 2007

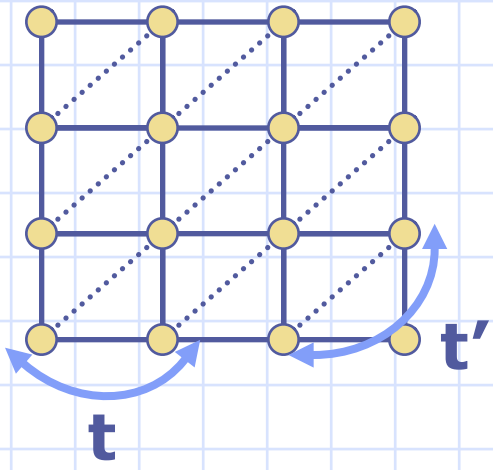
Cellular DMFT treatment

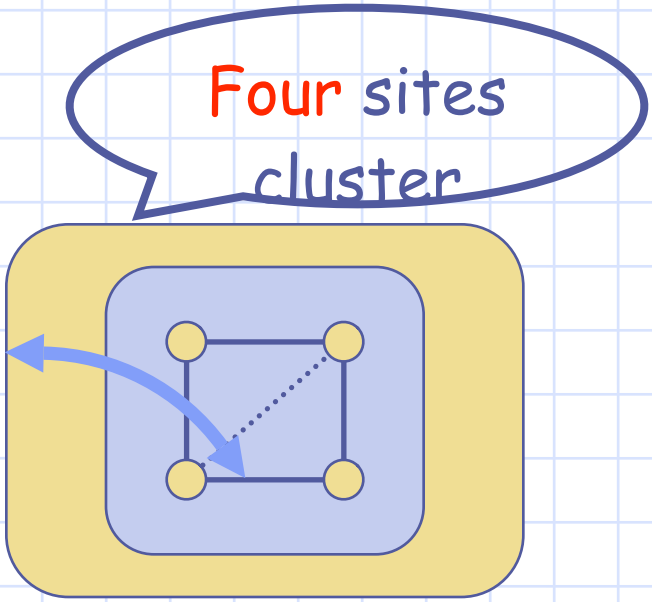
Reentrant Mott transition

Magnetic transition

Cellular-DMFT

Original Hubbard model





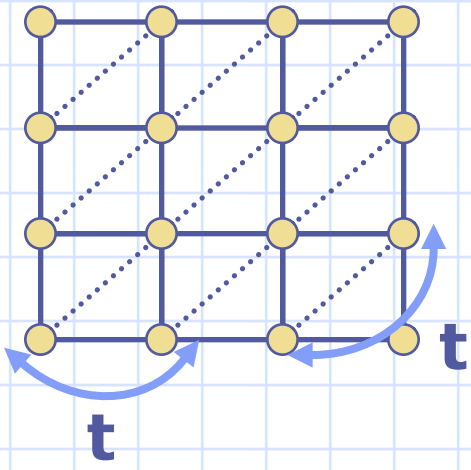
Effective cluster model

QMC method

(Hirsh-Fye algorism)

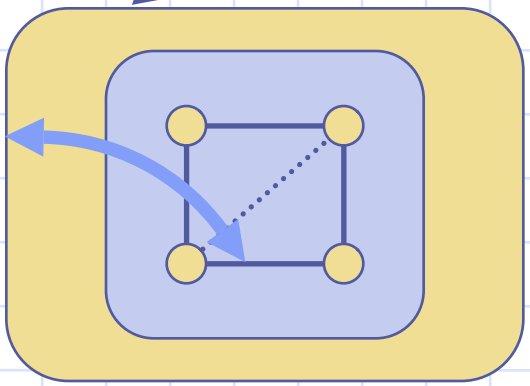
Cellular-DMFT

Original Hubbard model



Self-
consisten
t

Four sites
cluster



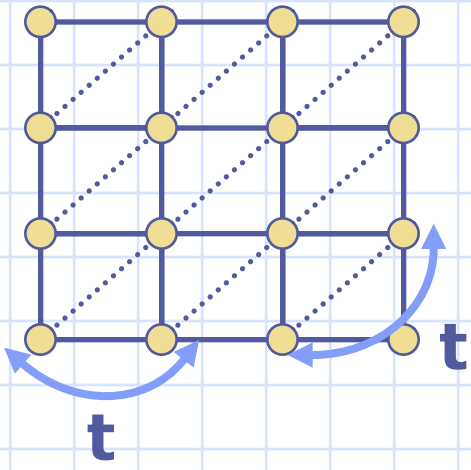
Effective cluster model

QMC method

(Hirsh-Fye algorism)

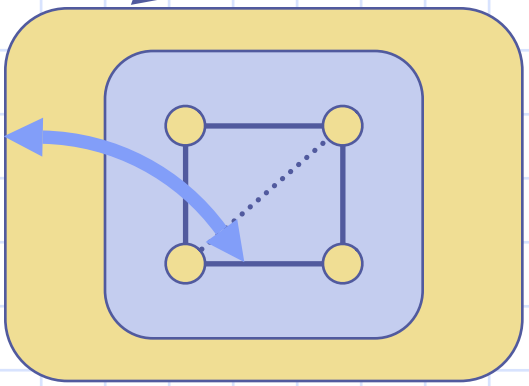
Cellular-DMFT

Original Hubbard model



Self-consisten t

Four sites cluster



Effective cluster model

t'/t=0: square lattice

t'/t=1: triangular lattice

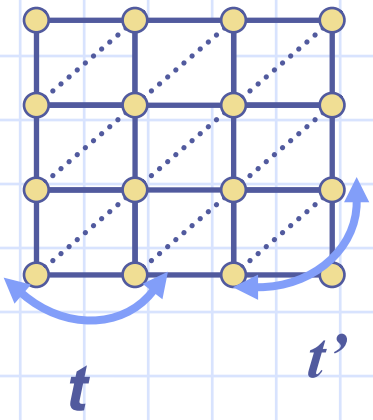
QMC method

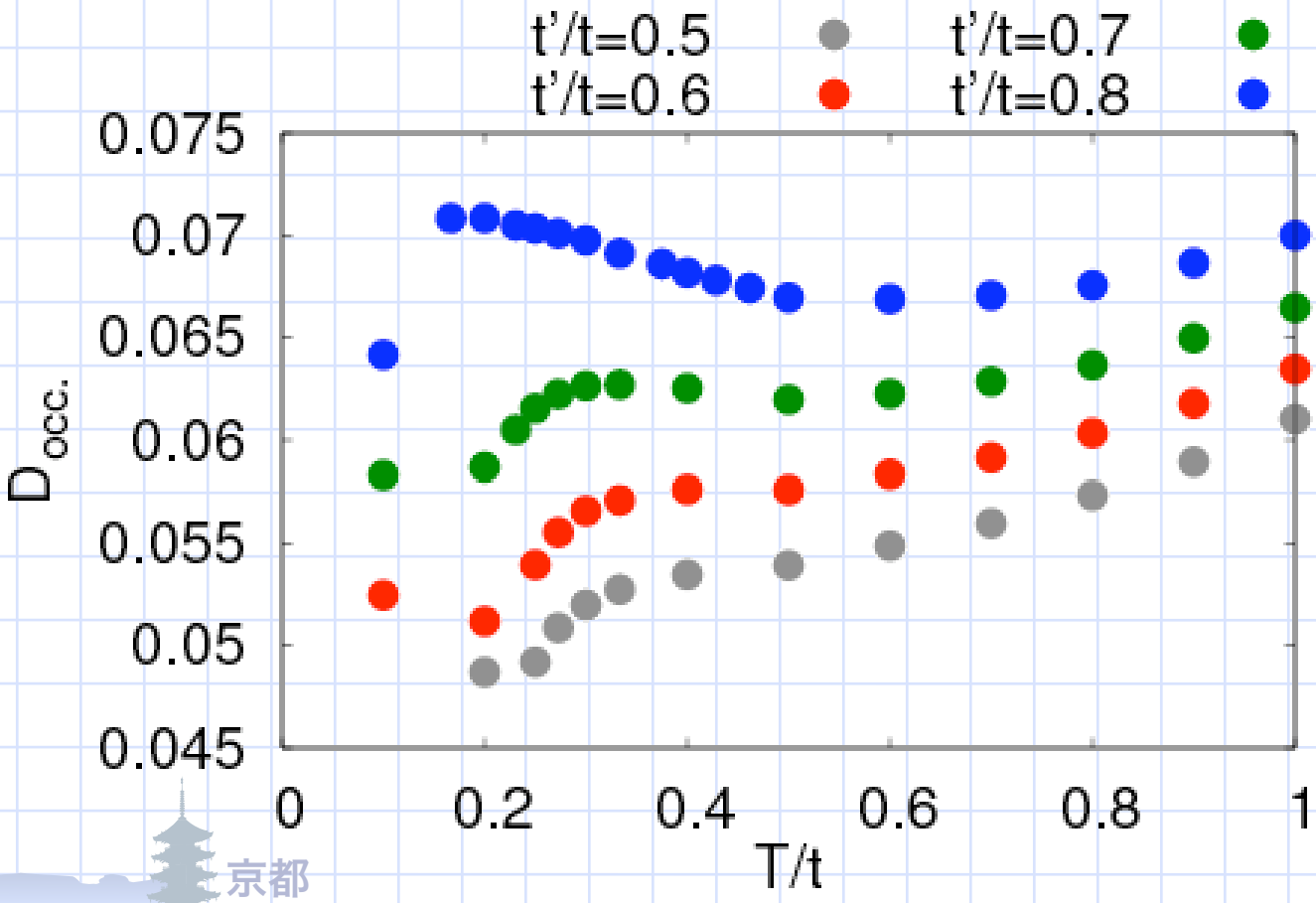
(Hirsh-Fye algorism)

Nonmonotonic T-dependence

Celluler DMFT

U/t = 8



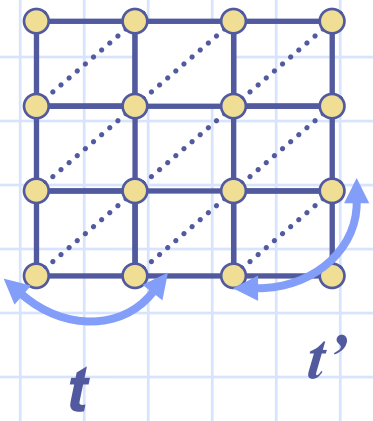


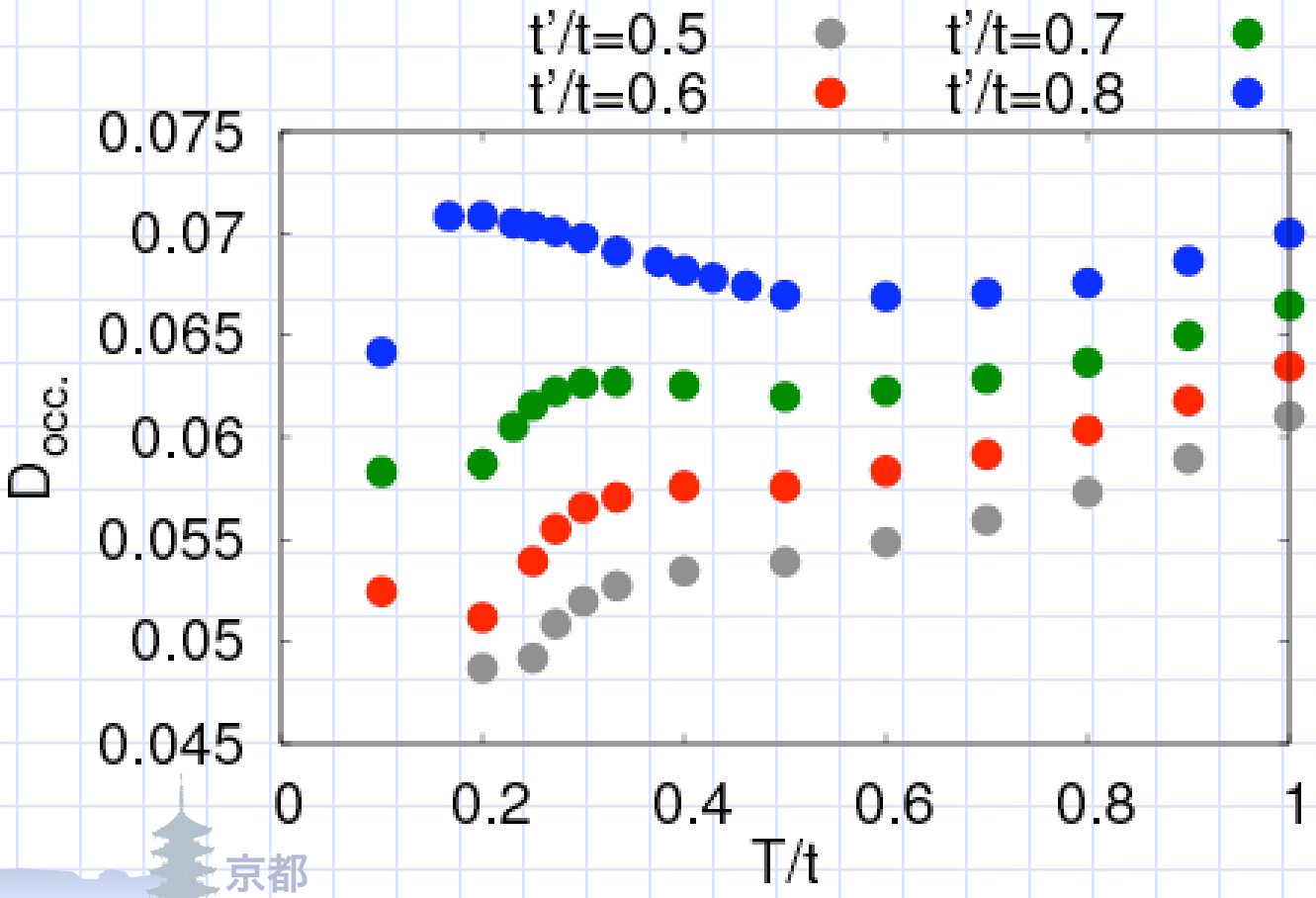
Nonmonotonic T-dependence

Celluler DMFT

Double occupancy

U/t = 8



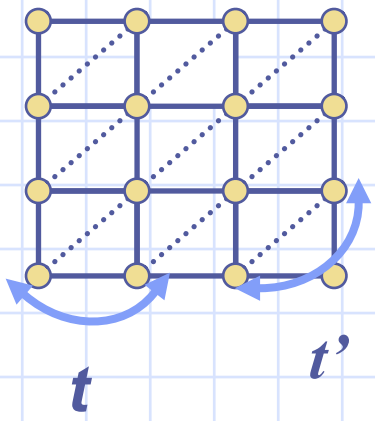


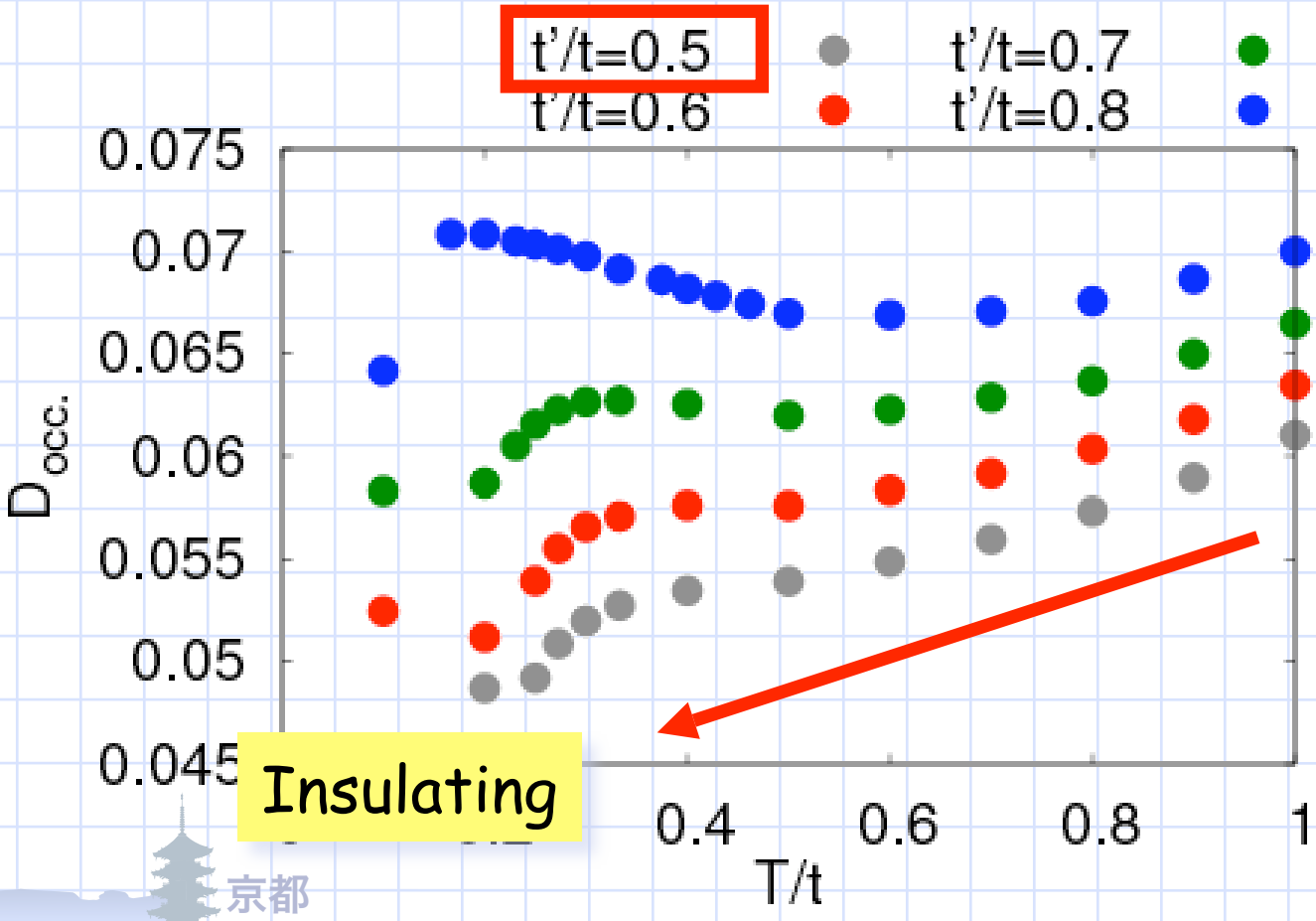
Nonmonotonic T-dependence

Celluler DMFT

Double occupancy

U/t = 8



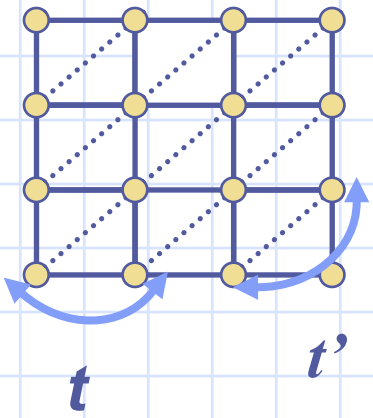


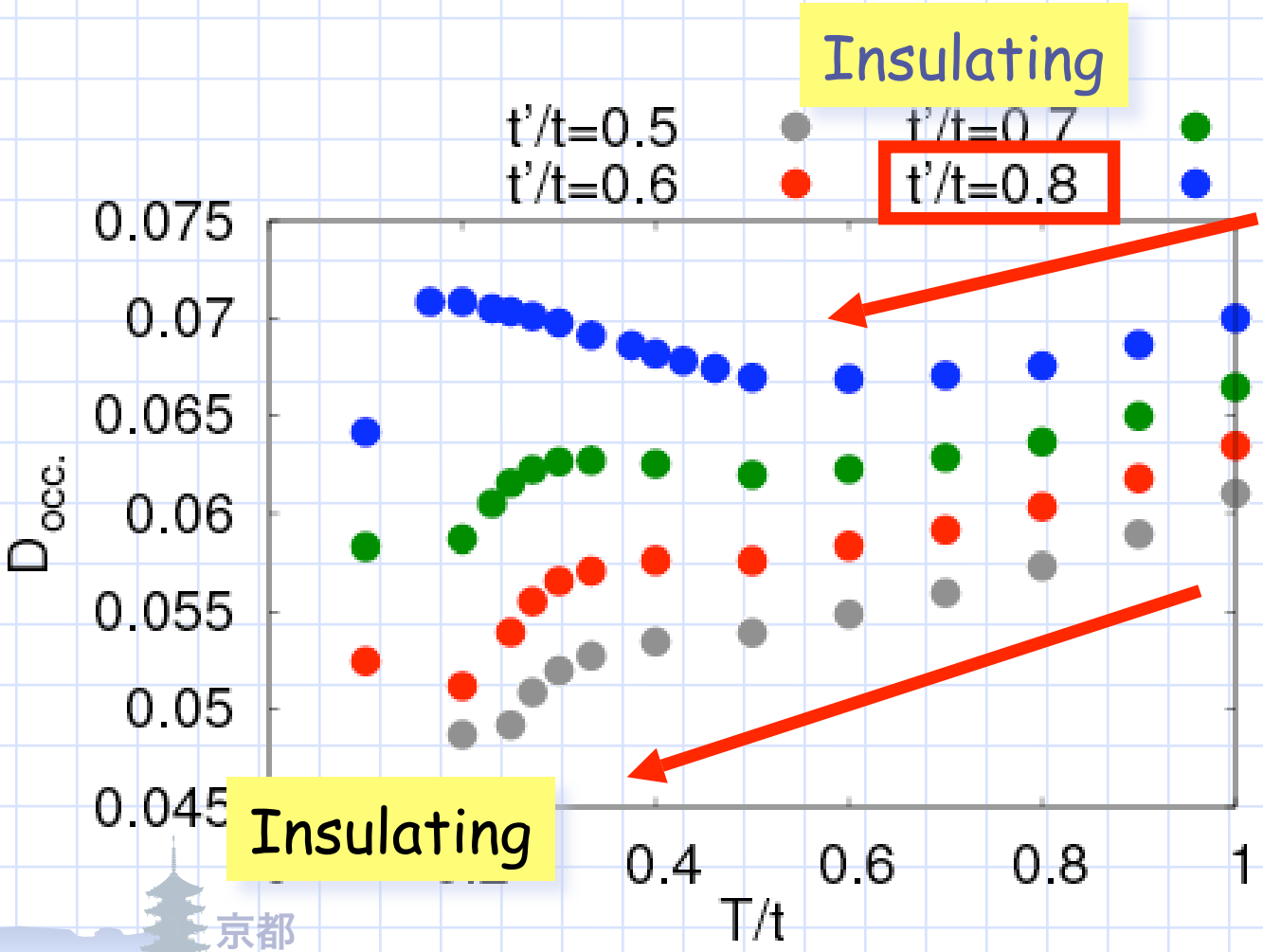
Nonmonotonic T-dependence

Celluler DMFT

Double occupancy

U/t = 8



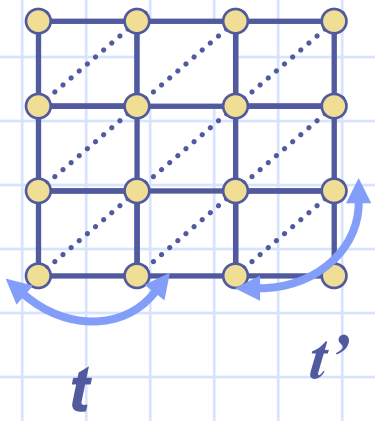


Nonmonotonic T-dependence

Celluler DMFT

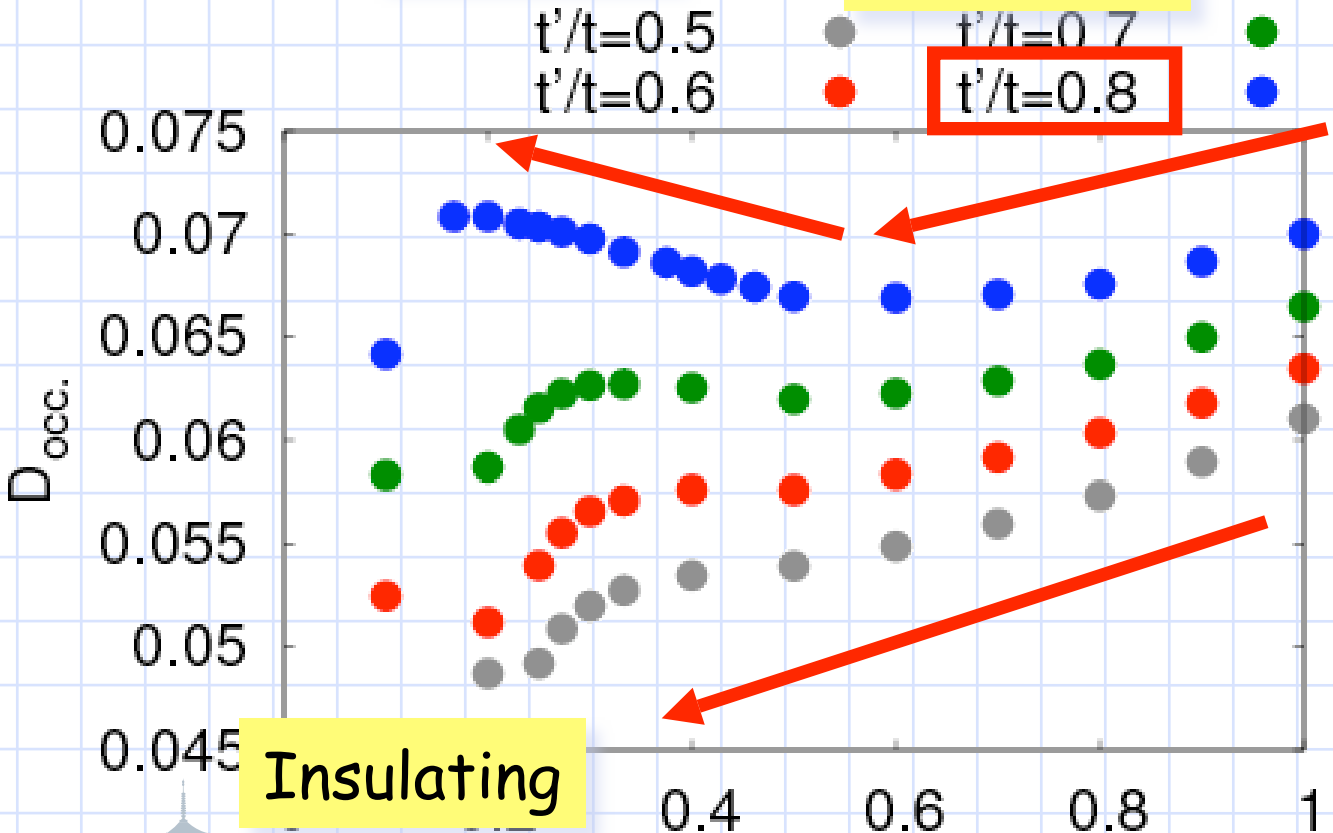
Double occupancy

U/t = 8



Metallic

Insulating



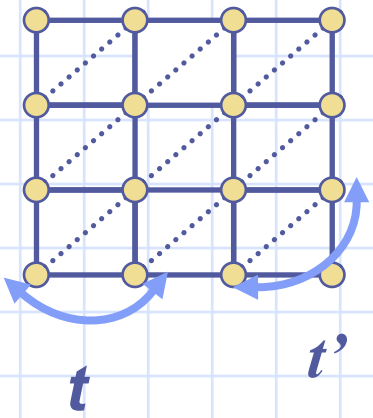
Insulating

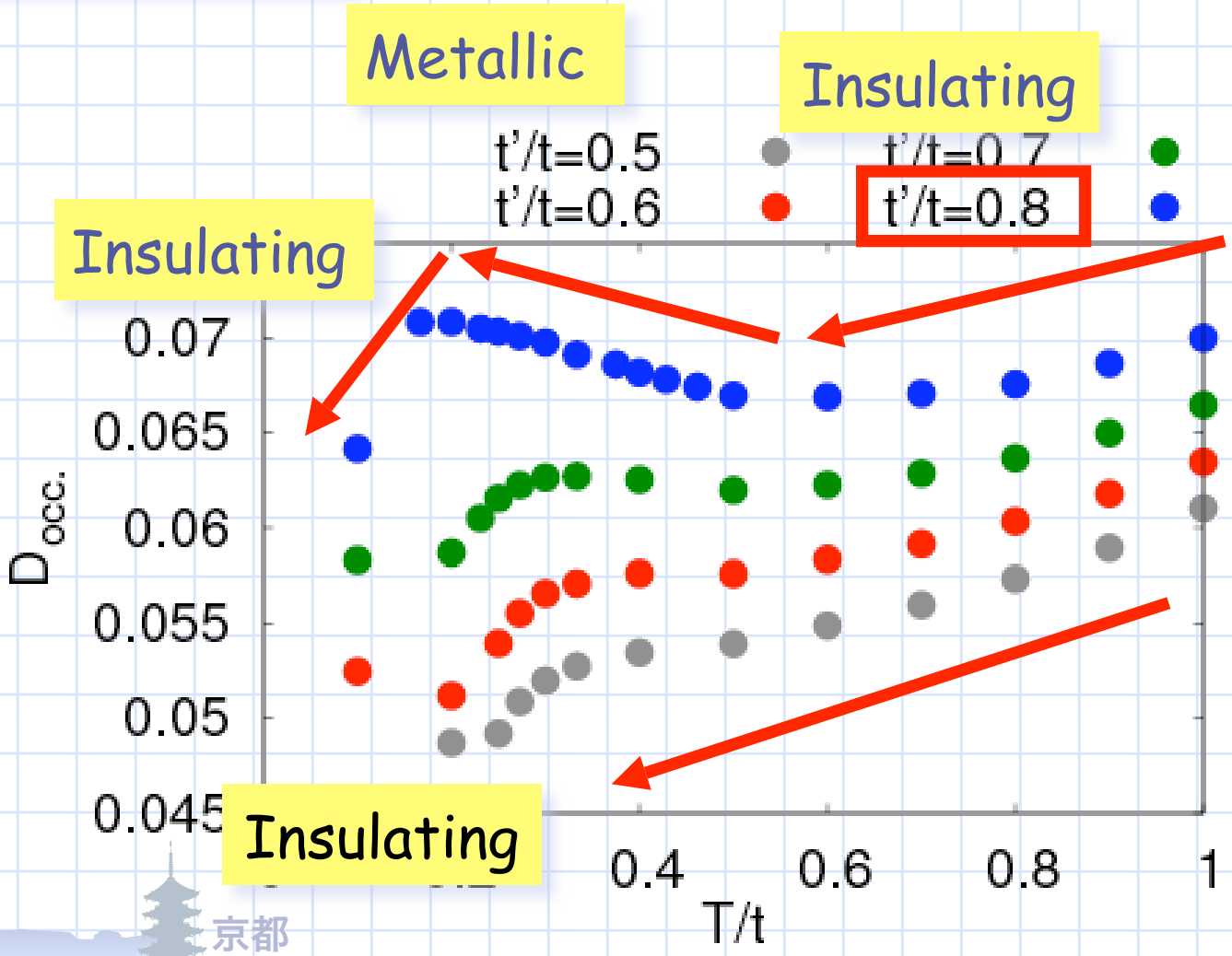
Nonmonotonic T-dependence

Celluler DMFT

Double occupancy

U/t = 8



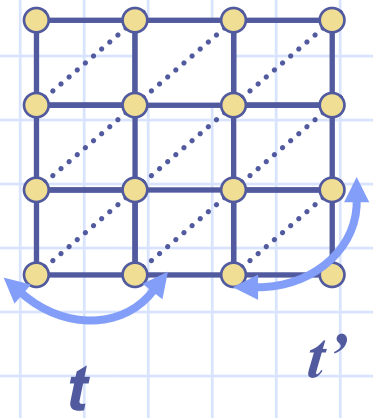


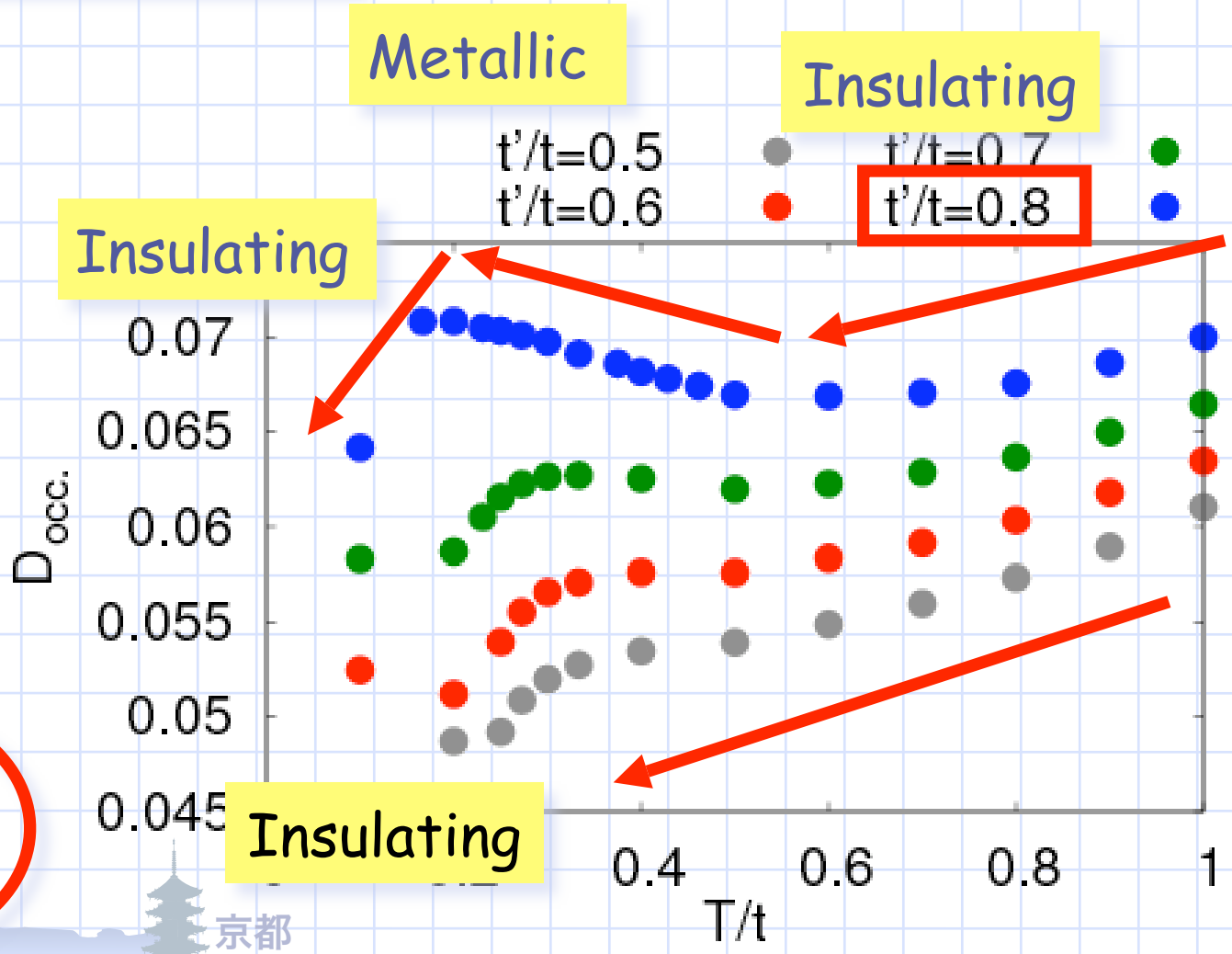
Nonmonotonic T-dependence

Celluler DMFT

Double occupancy

U/t = 8

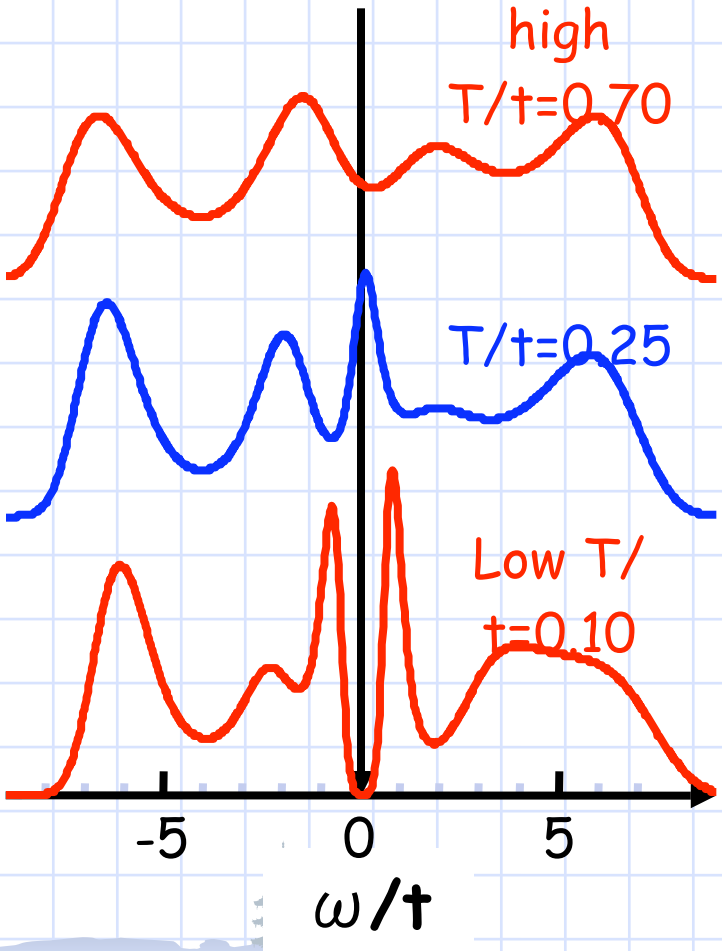




focus
t'/t=0.8

Density of states

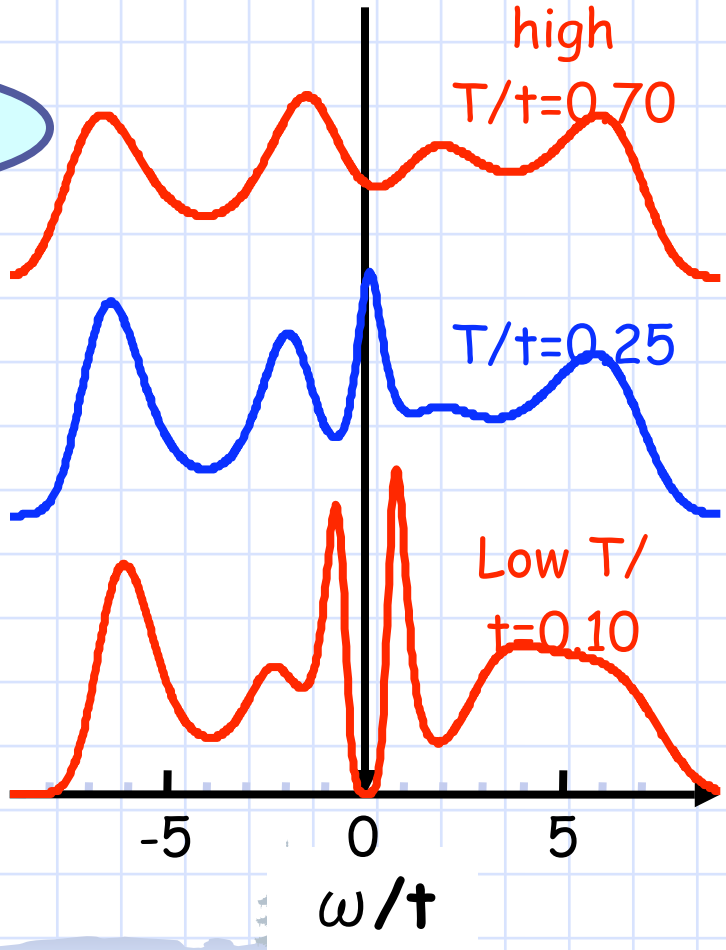
U/t = 8 t'/t=0.8



Density of states

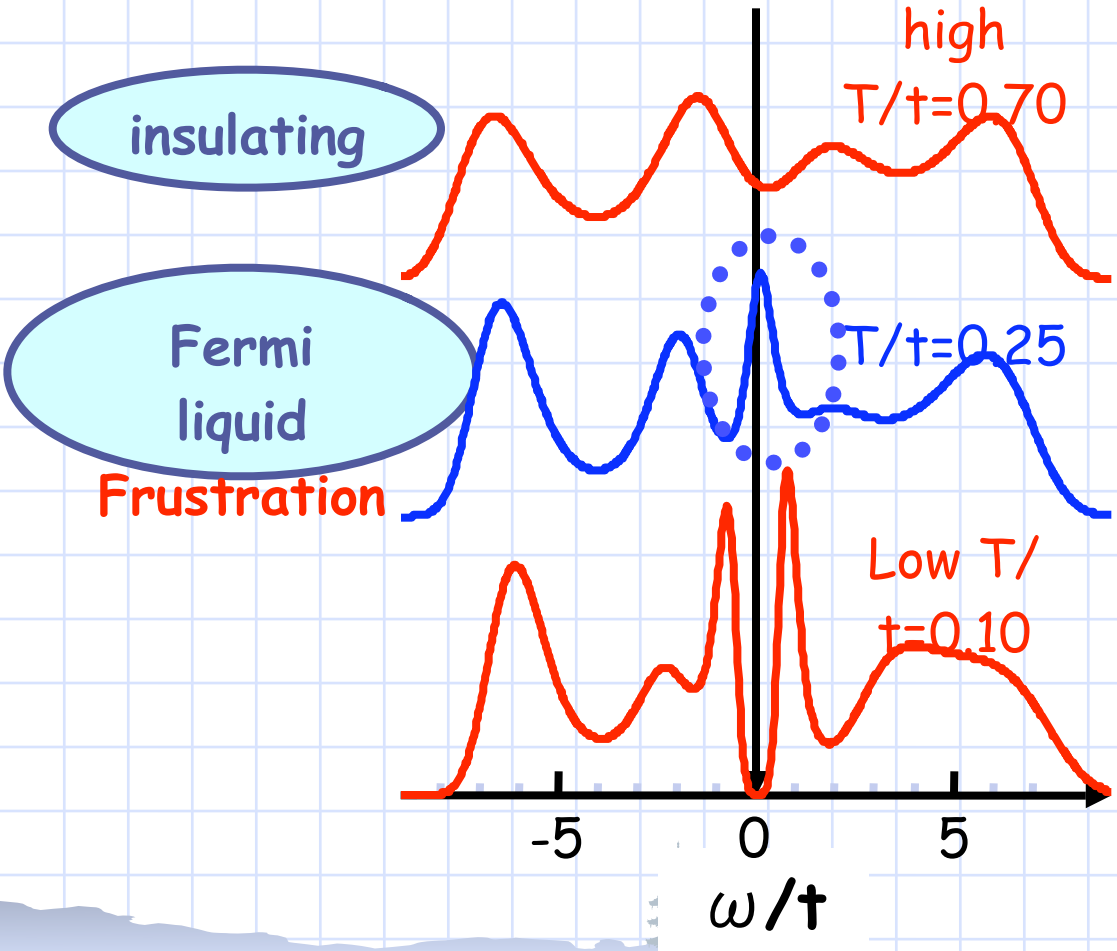
U/t = 8 t'/t=0.8

insulating



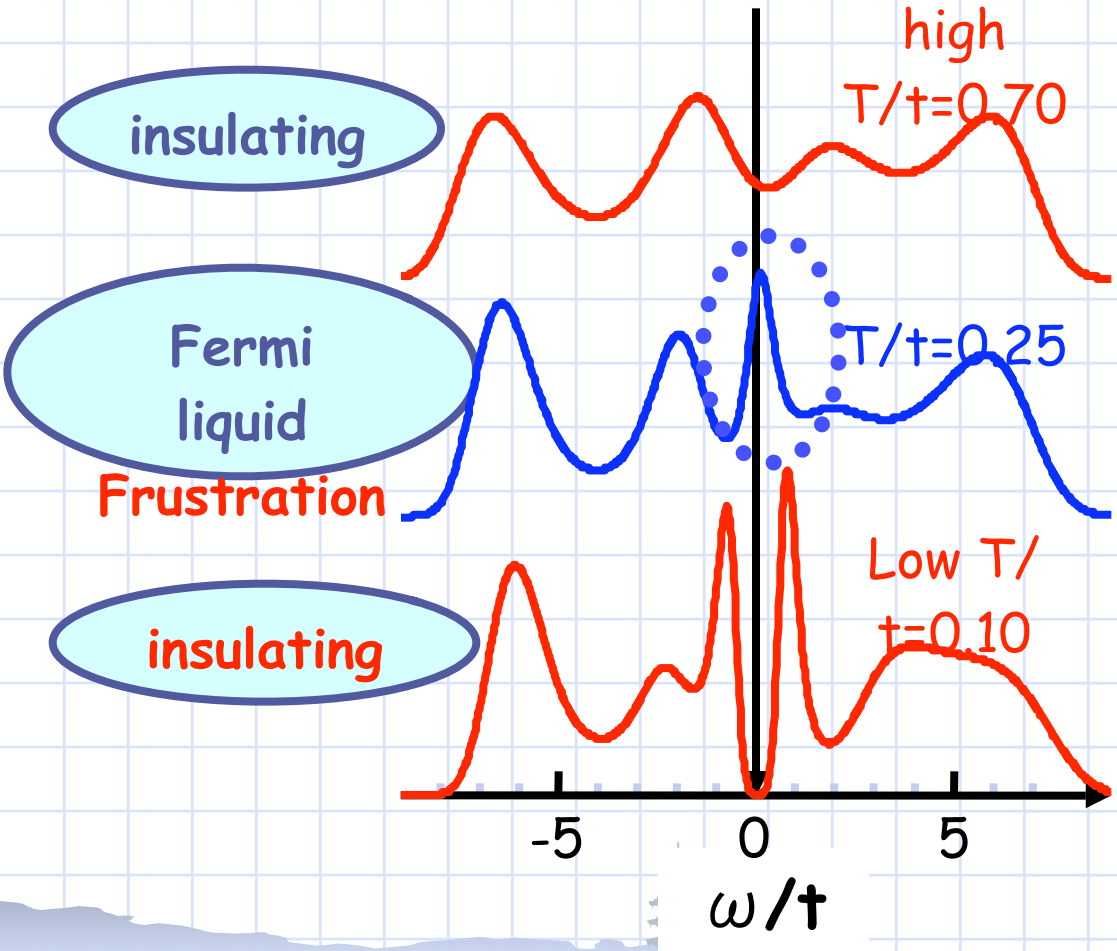
Density of states

U/t = 8 t'/t=0.8



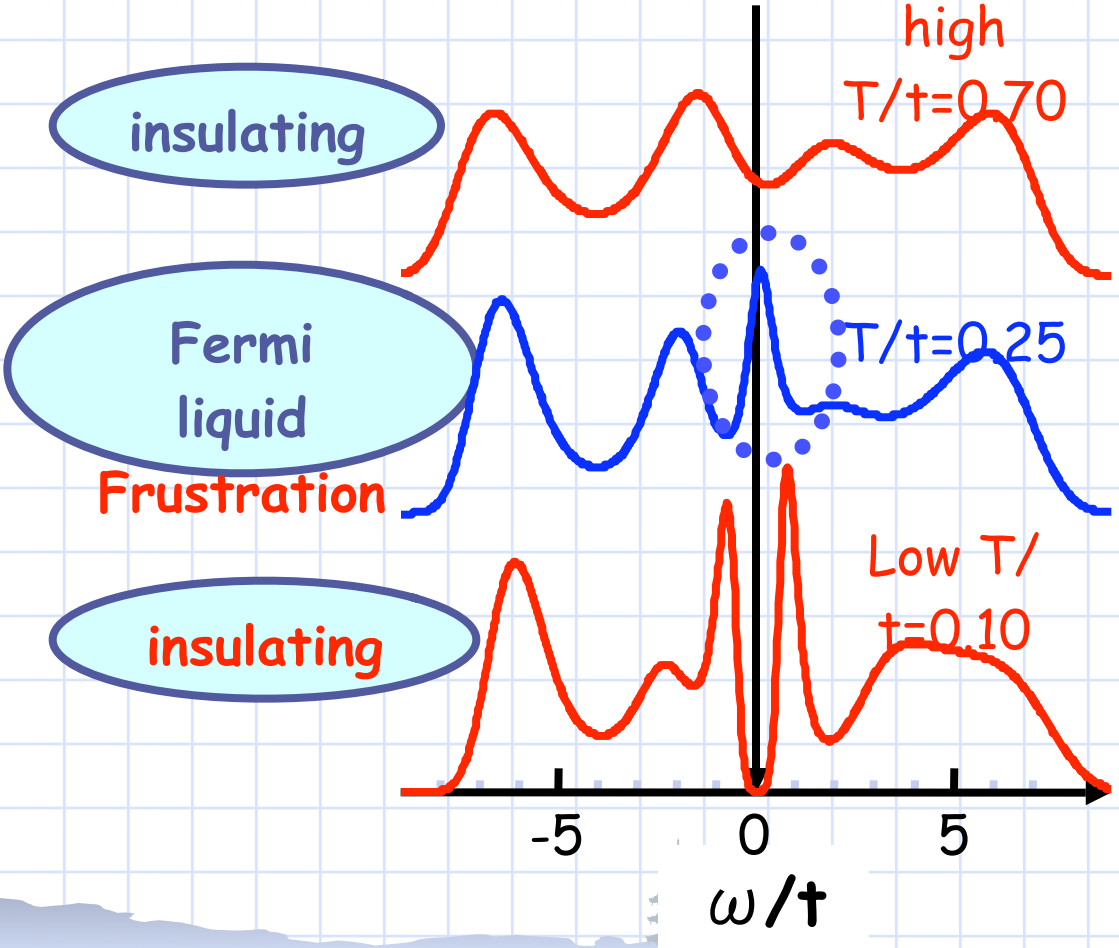
Density of states

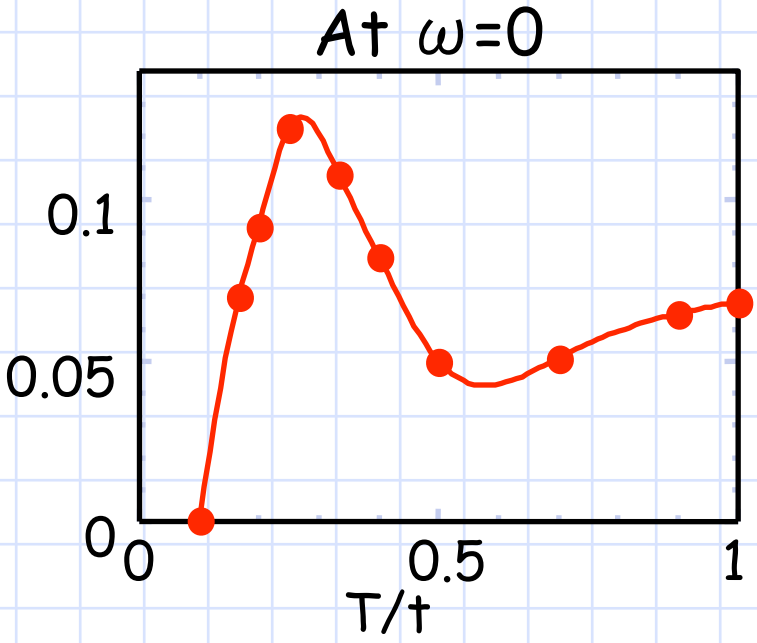
U/t = 8 t'/t=0.8



Density of states

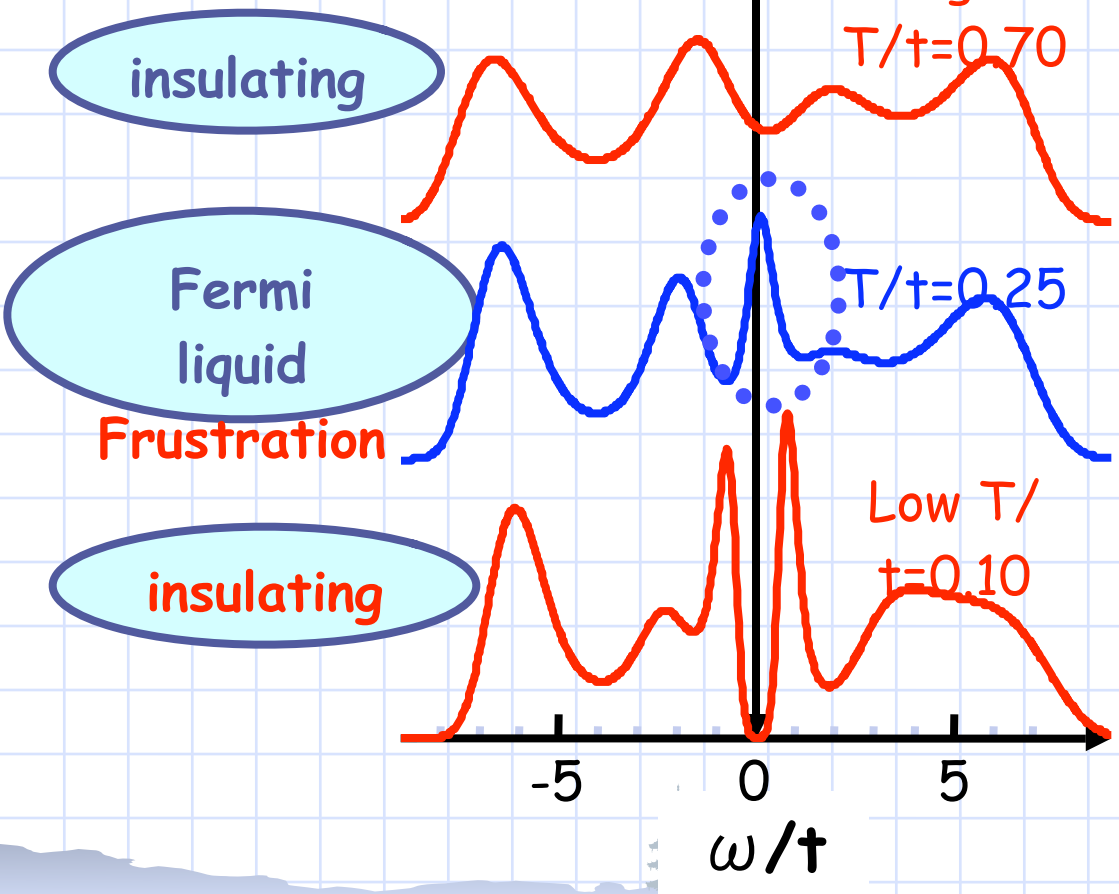
U/t = 8 t'/t=0.8

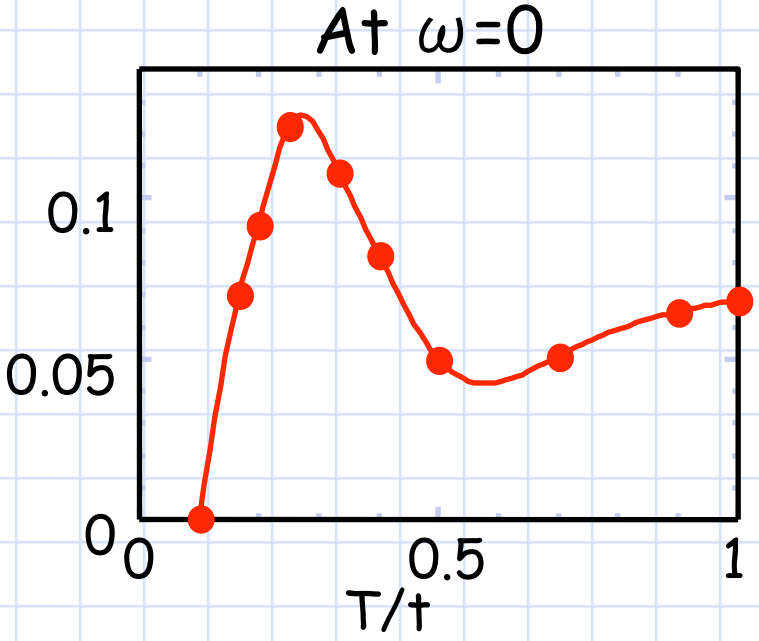


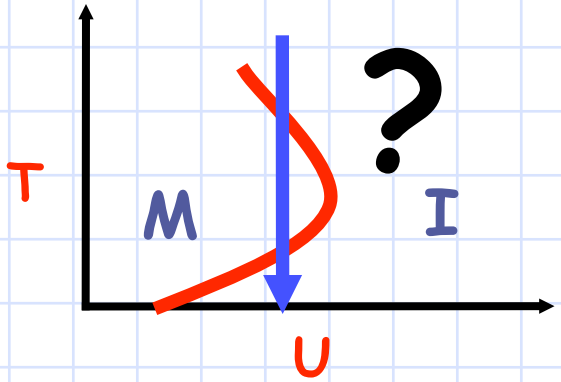


Density of states

U/t = 8 t'/t=0.8

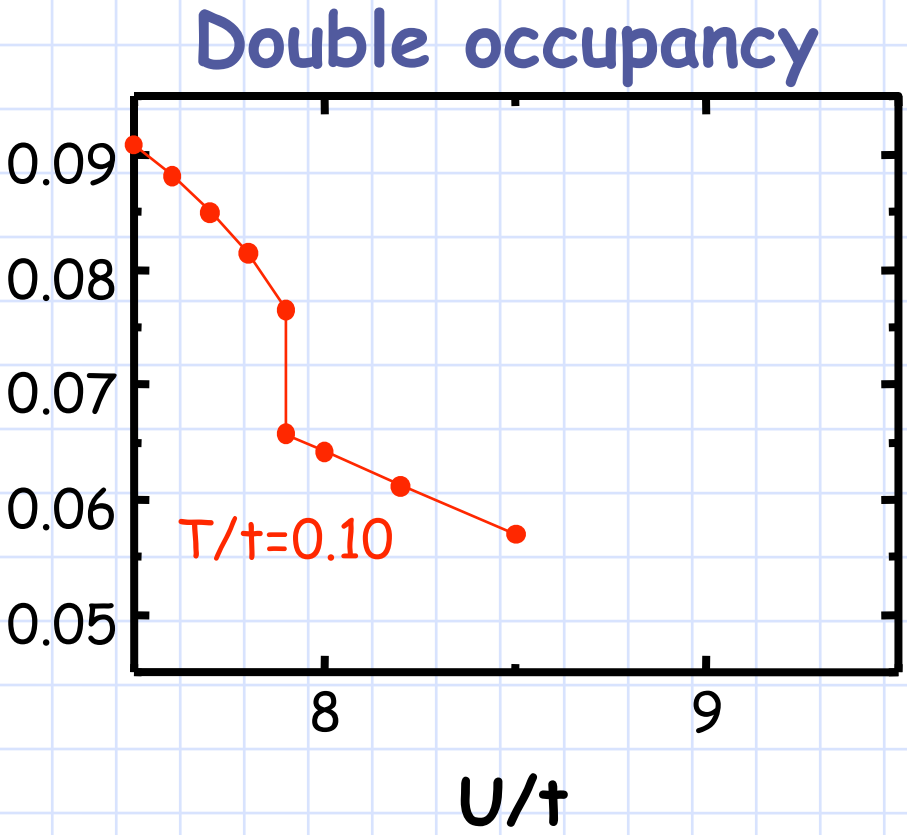






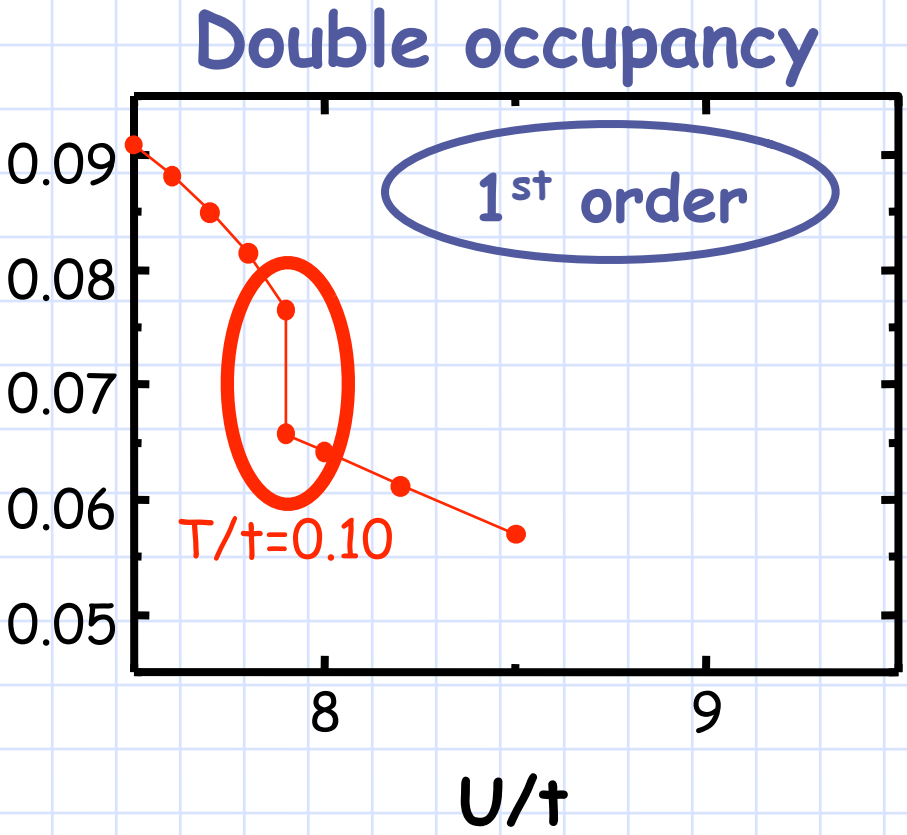
Mott transition

t'/t=0.8



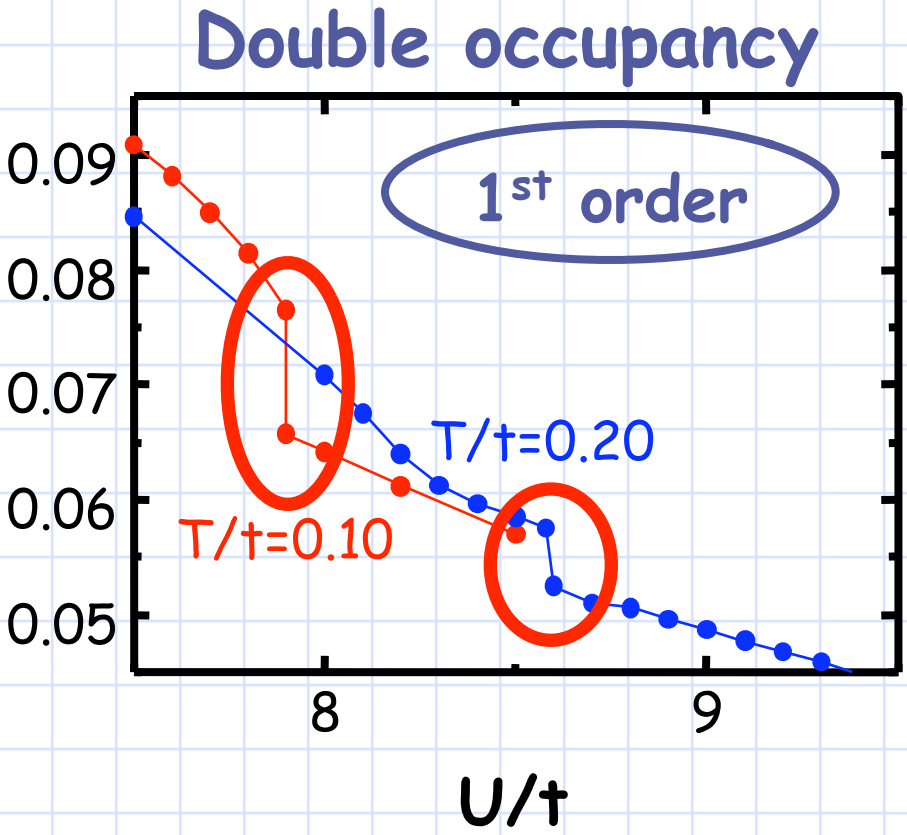
Mott transition

t'/t=0.8



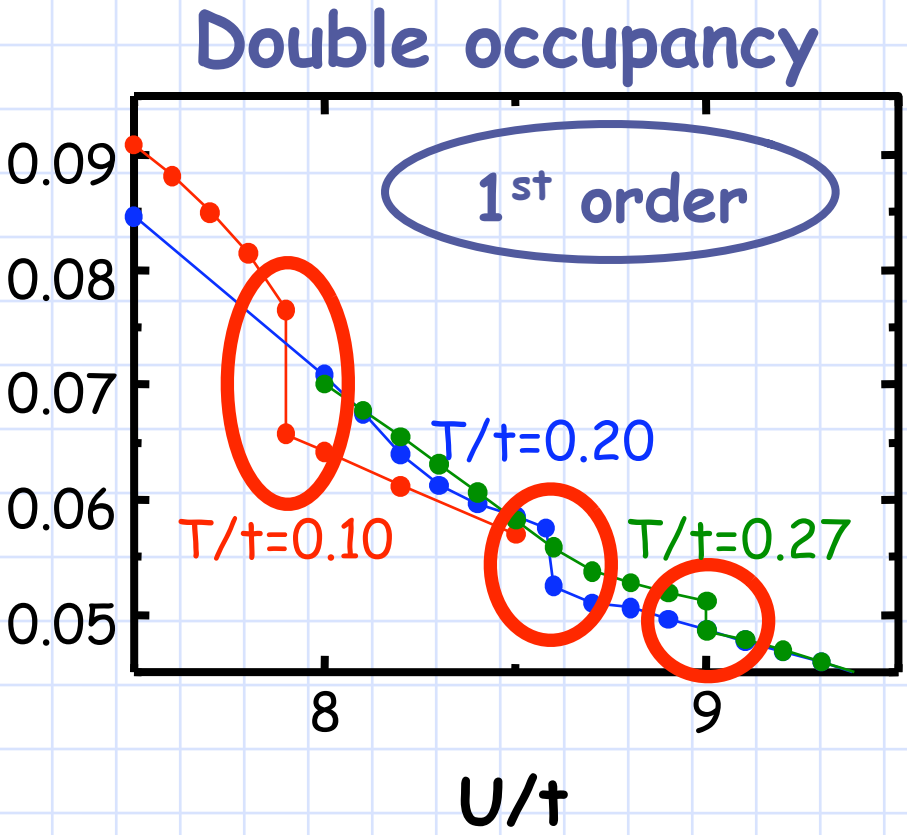
Mott transition

t'/t=0.8



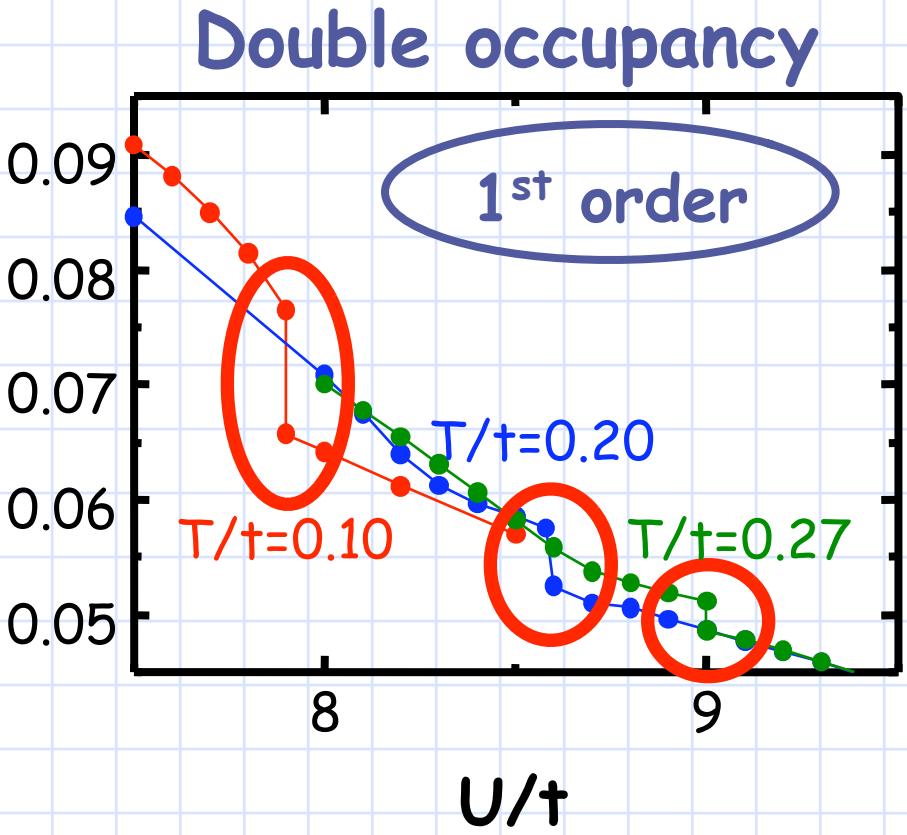
Mott transition

t'/t=0.8



Mott transition

t'/t=0.8

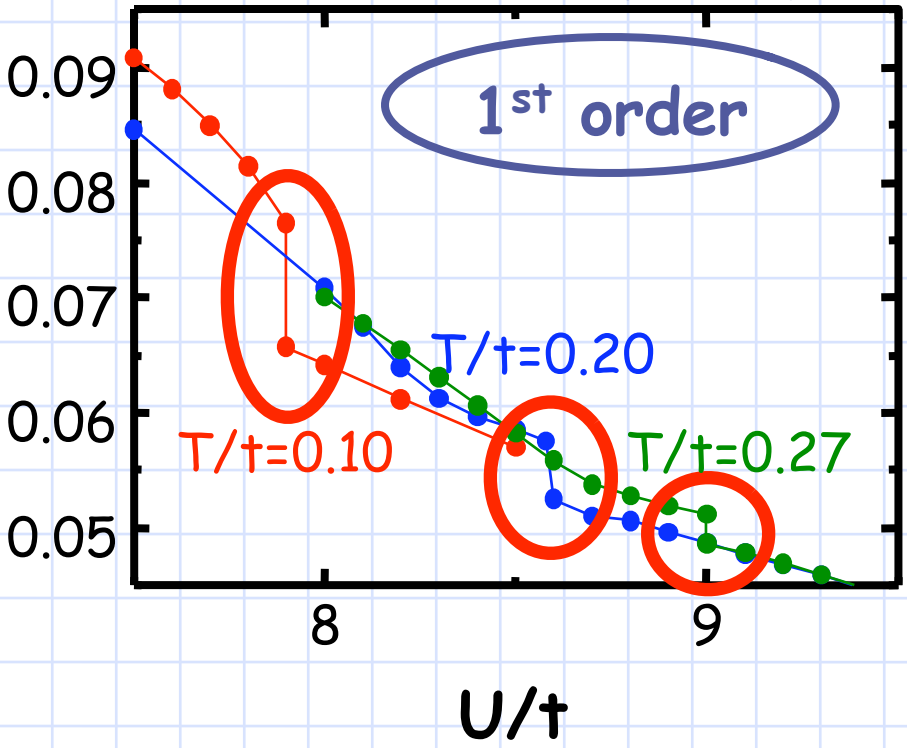


U_c increases with T

Mott transition

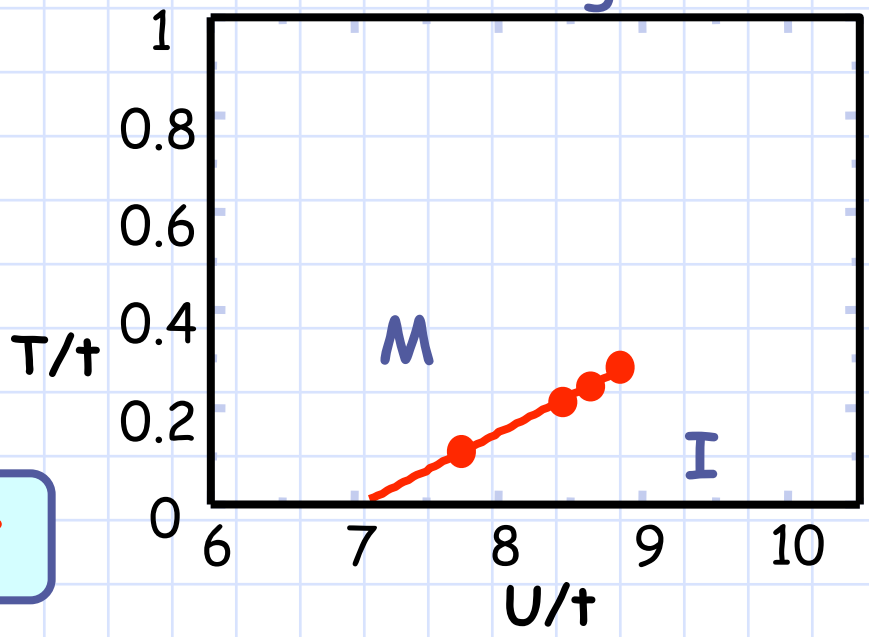
t'/t=0.8

Double occupancy



Contrasted to DMFT

Phase diagram

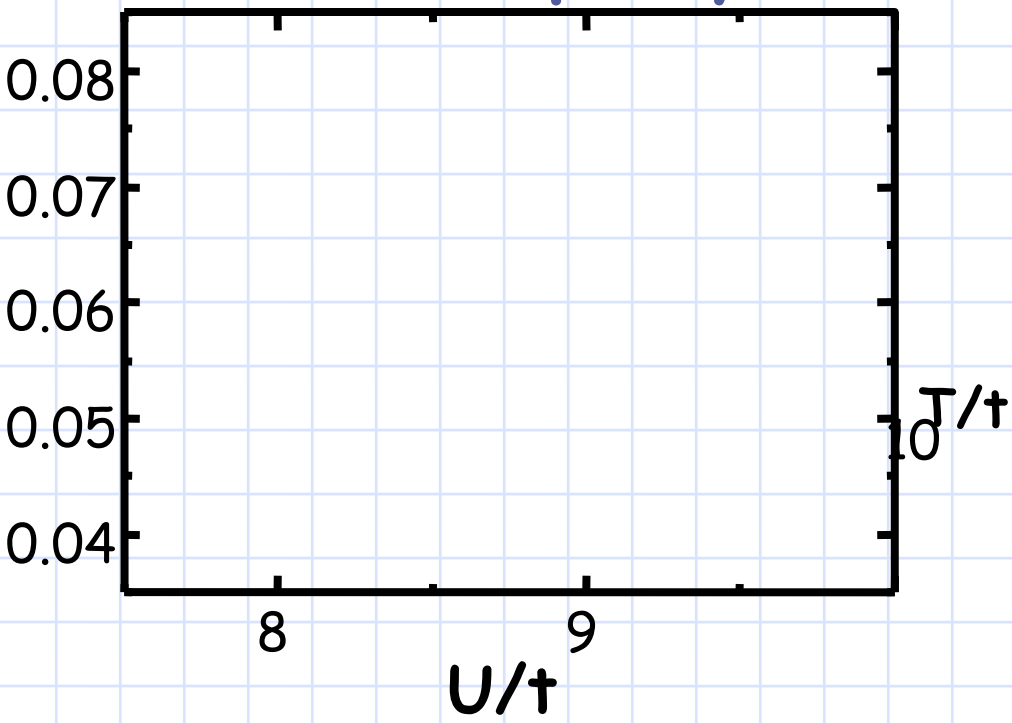


U_c increases with T

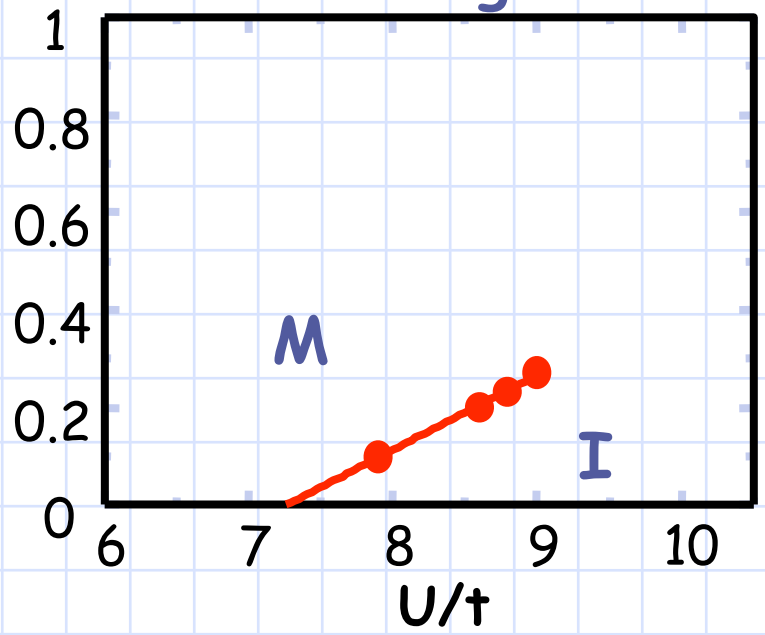
High-temperature behavior

t'/t=0.8

Double occupancy



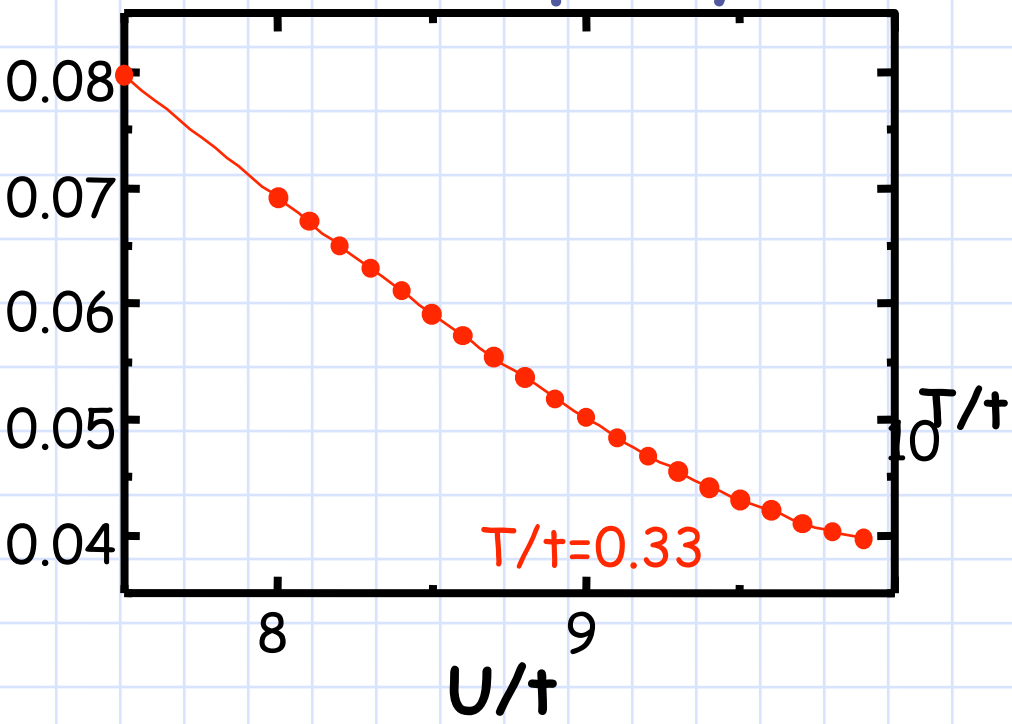
Phase diagram



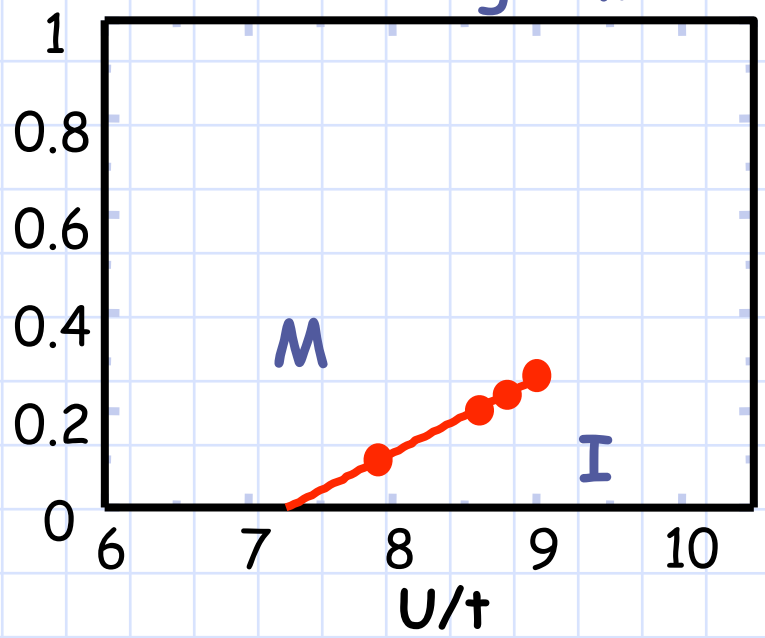
High-temperature behavior

t'/t=0.8

Double occupancy



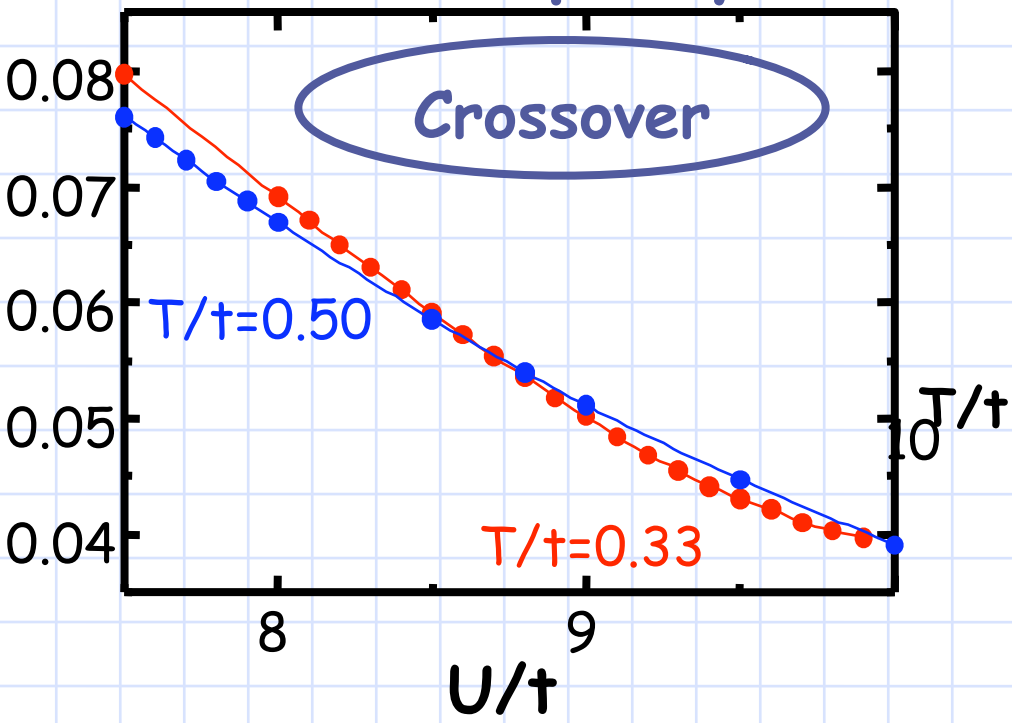
Phase diagram



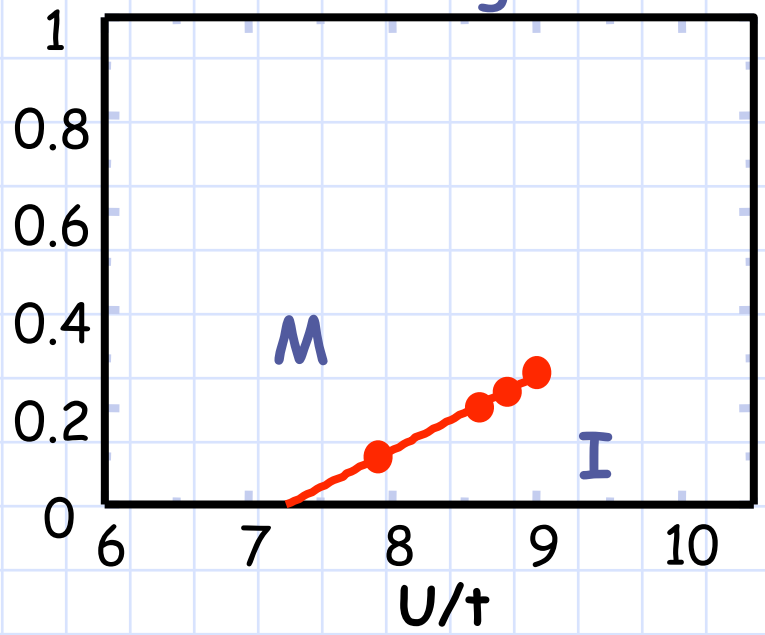
High-temperature behavior

t'/t=0.8

Double occupancy

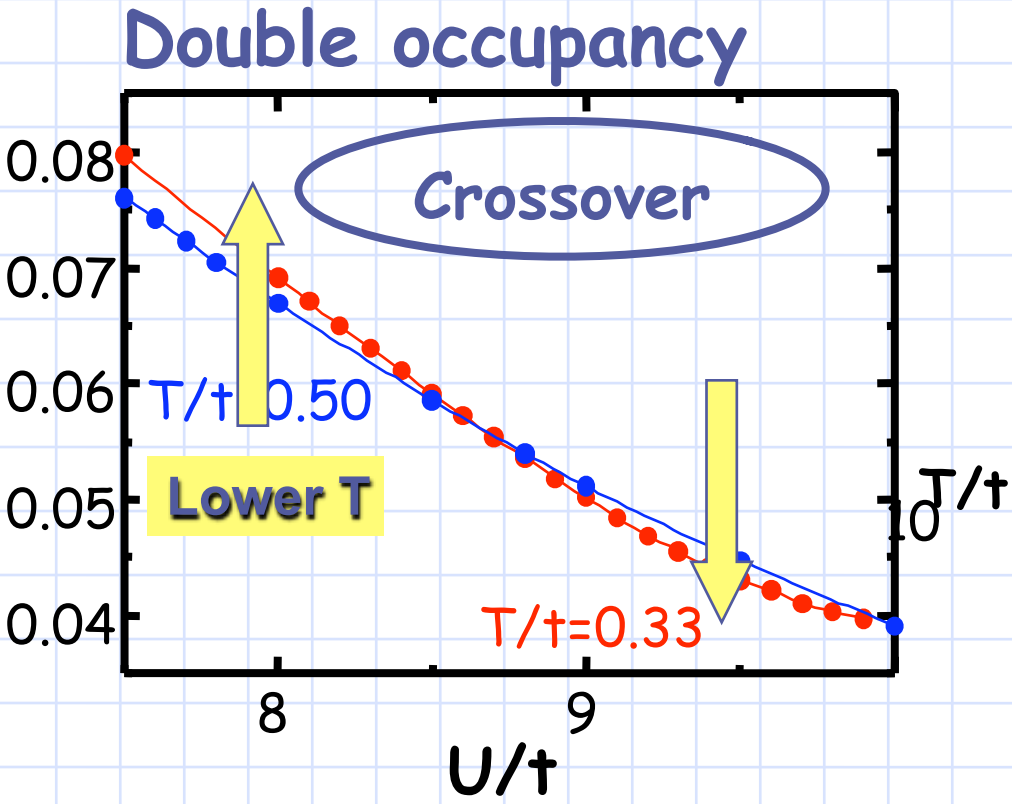


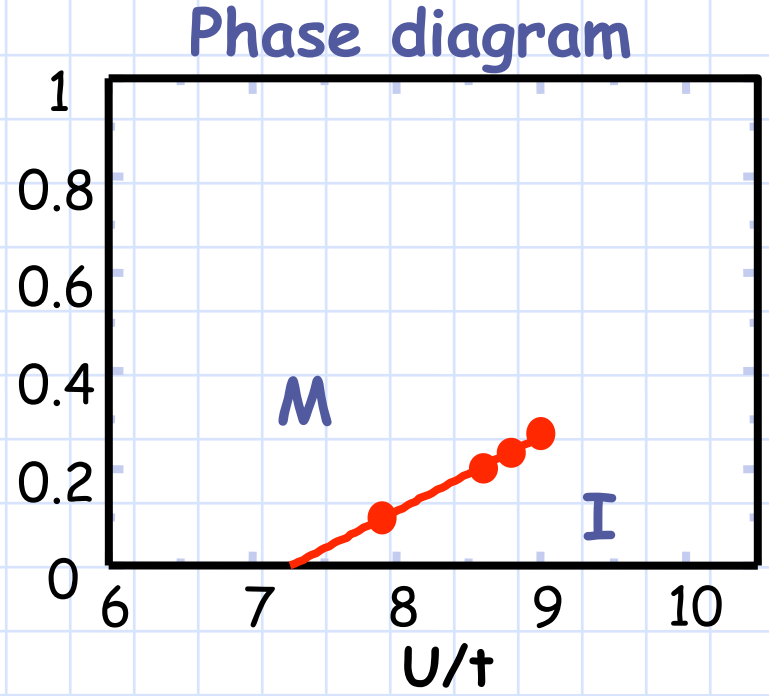
Phase diagram



High-temperature behavior

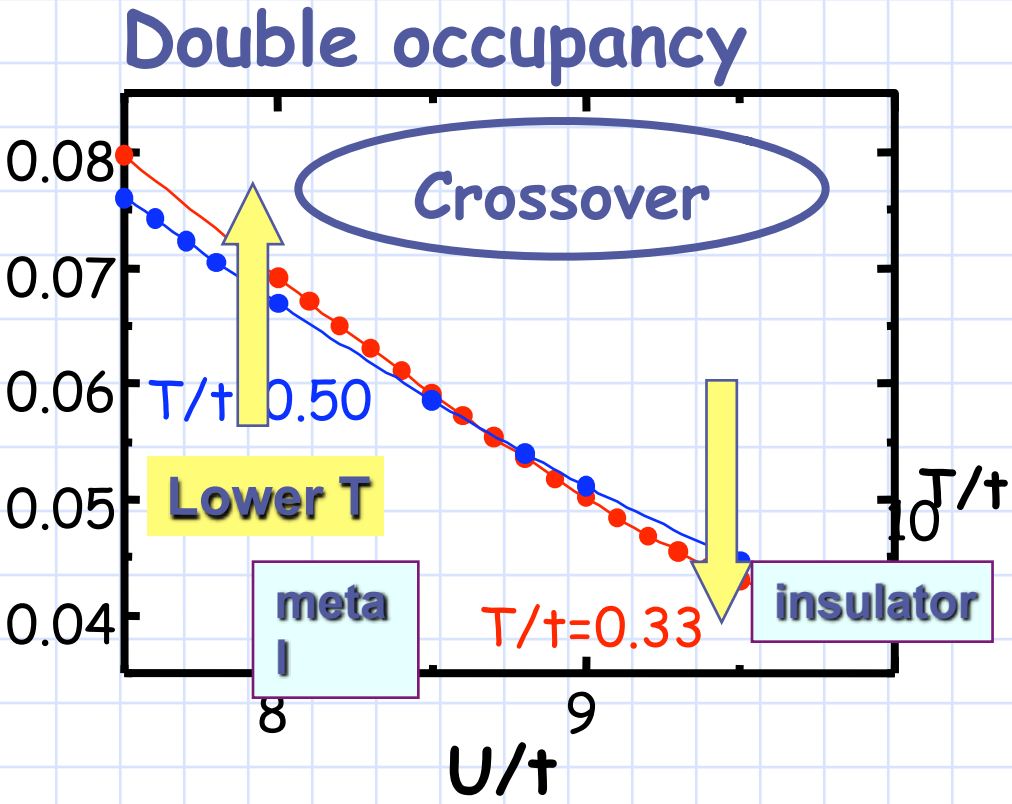
t'/t=0.8

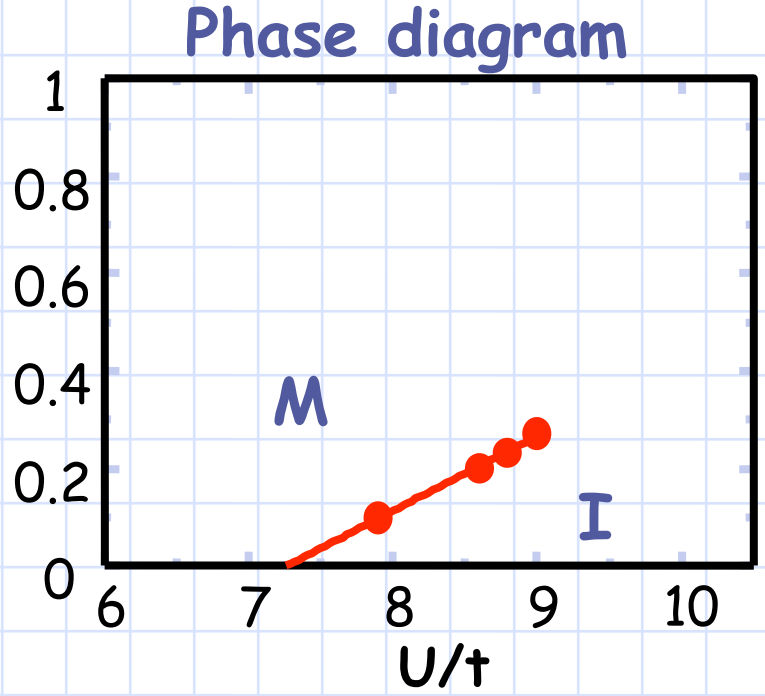




High-temperature behavior

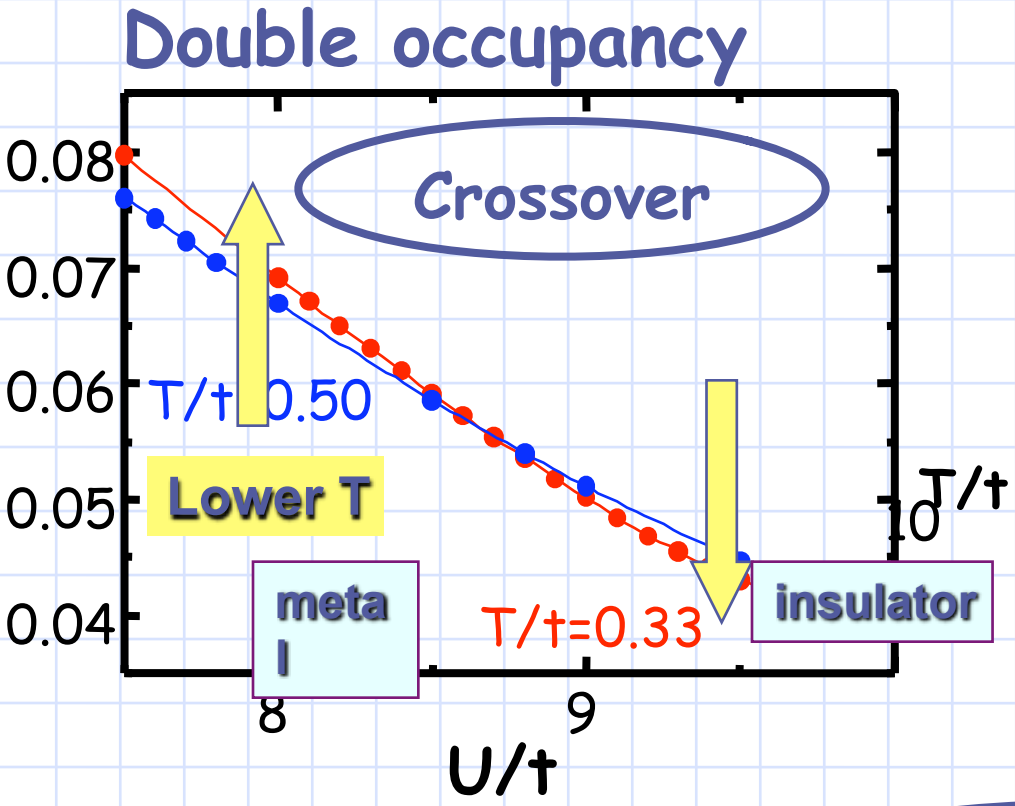
t'/t=0.8

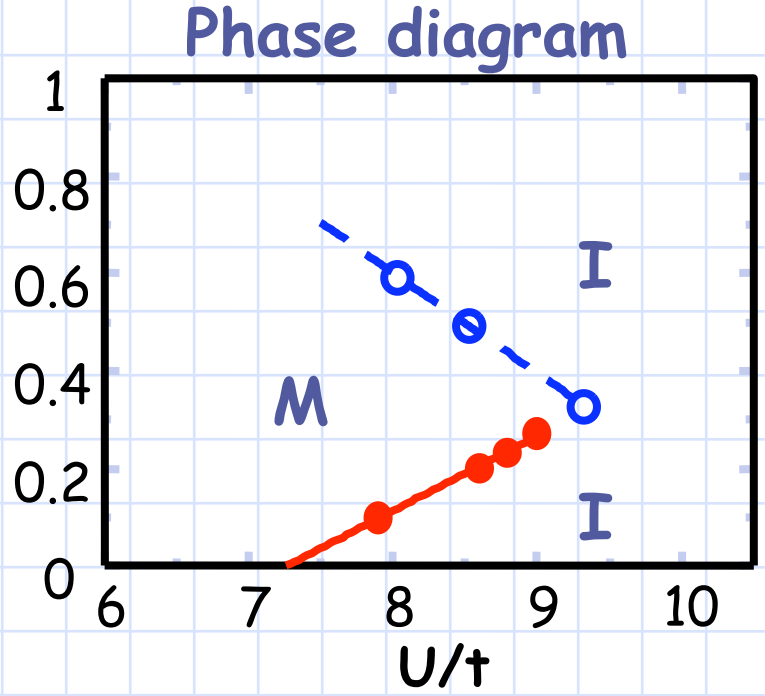




High-temperature behavior

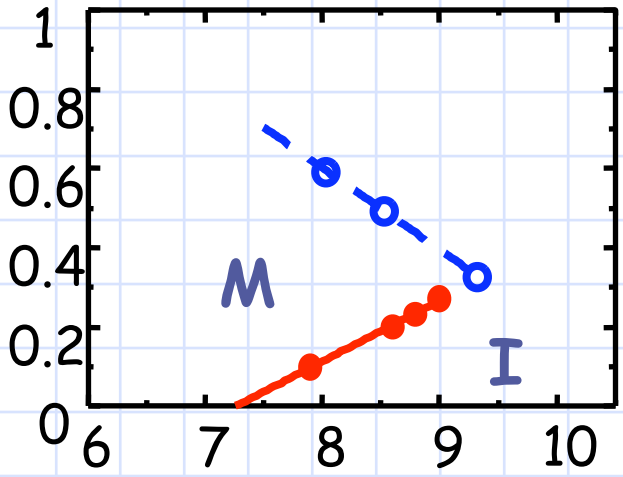
t'/t=0.8

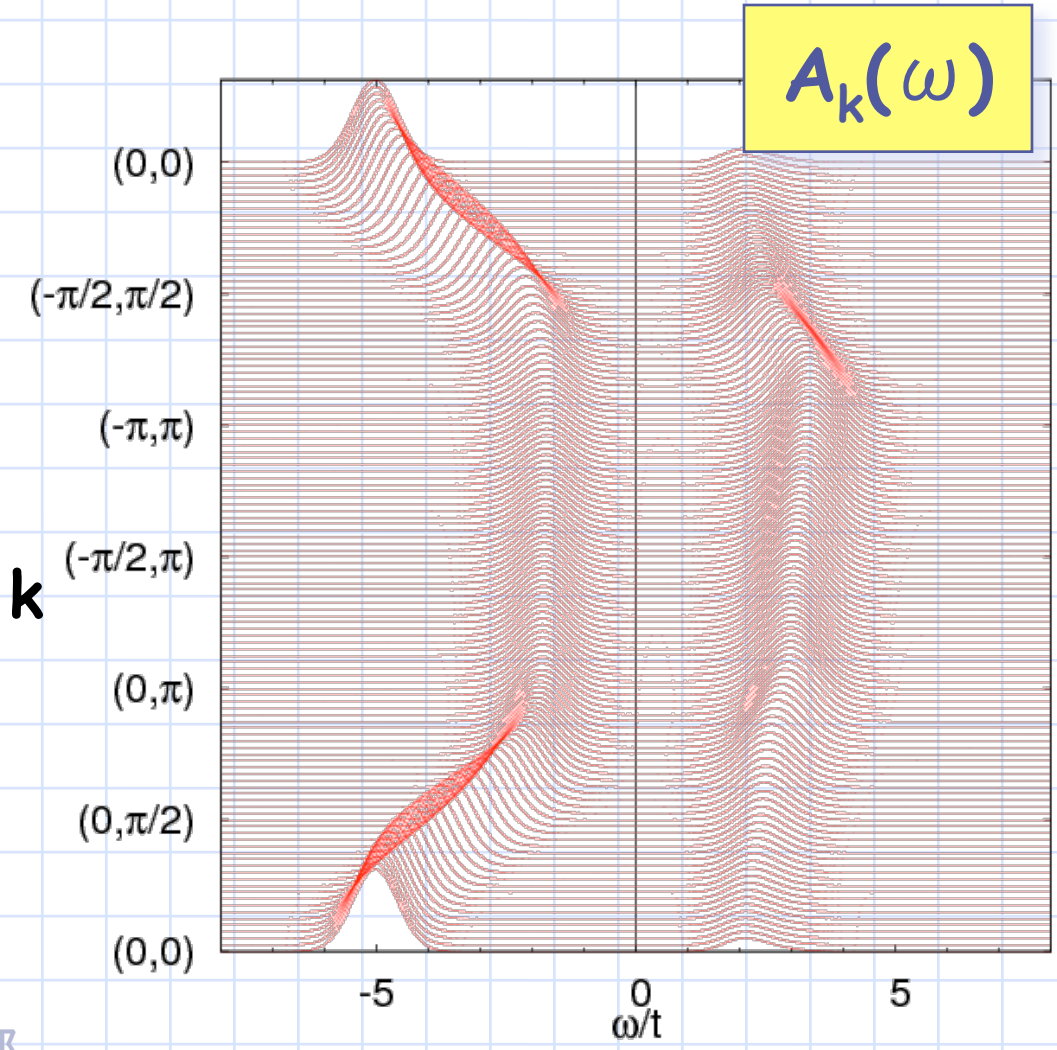




Reentrant !

k-dependent spectral function



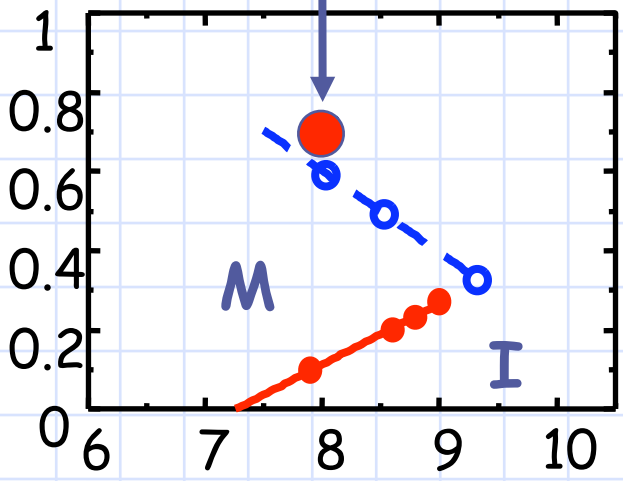


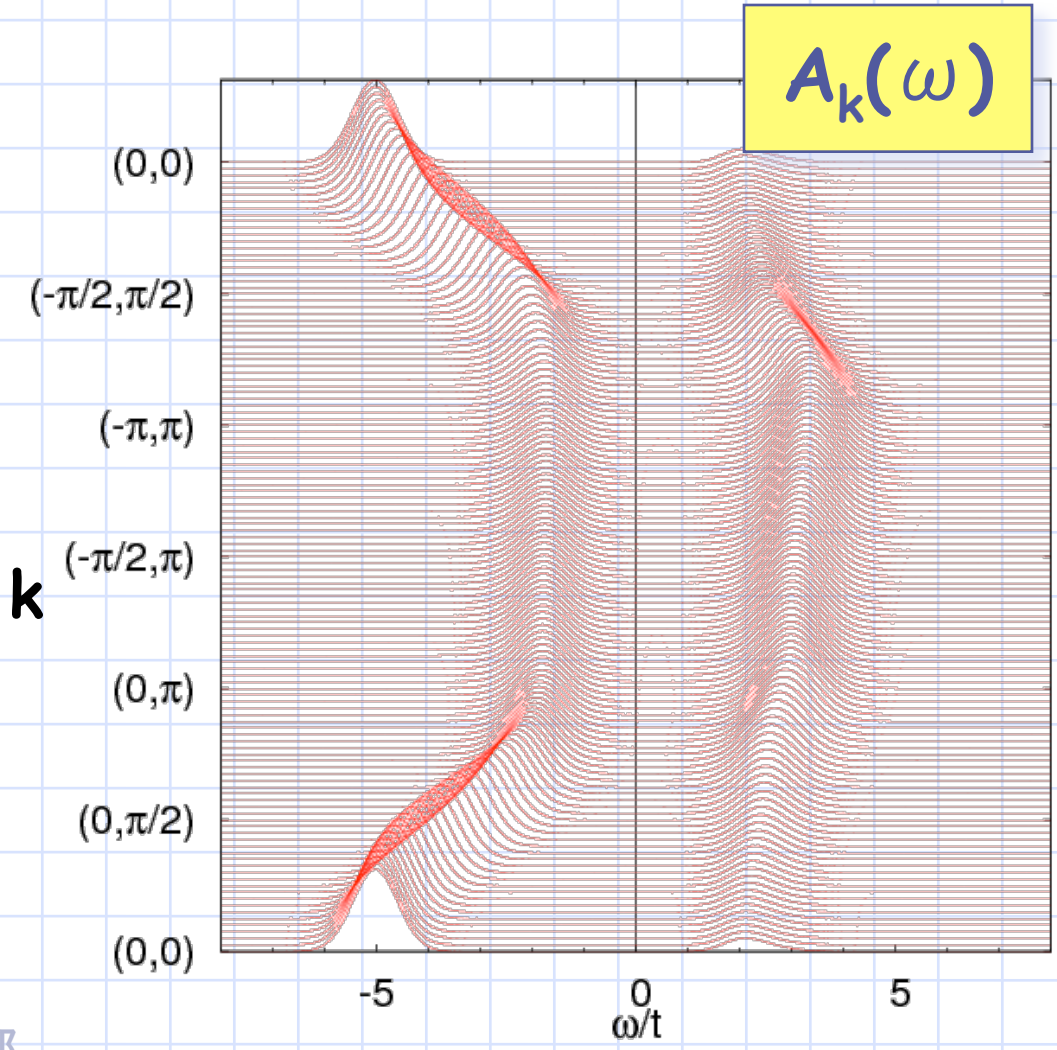
k-dependent spectral function

High T

U/t=0.8, t'/t=0.8,

T/t=0.7



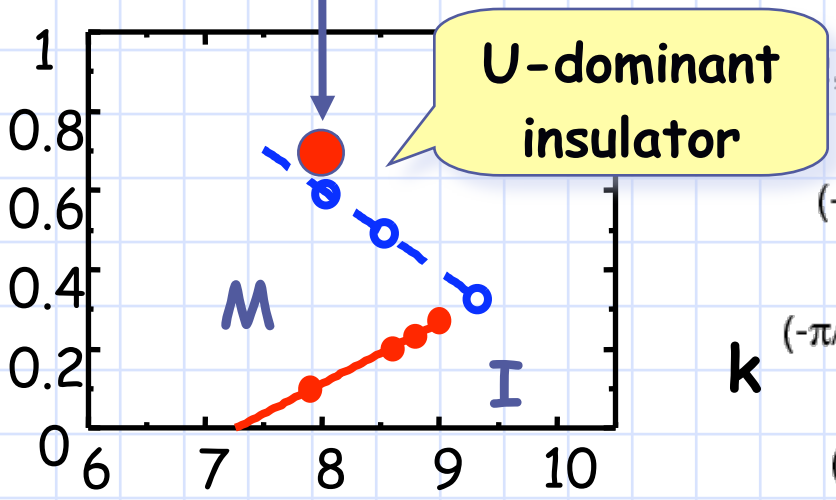


k-dependent spectral function

High T

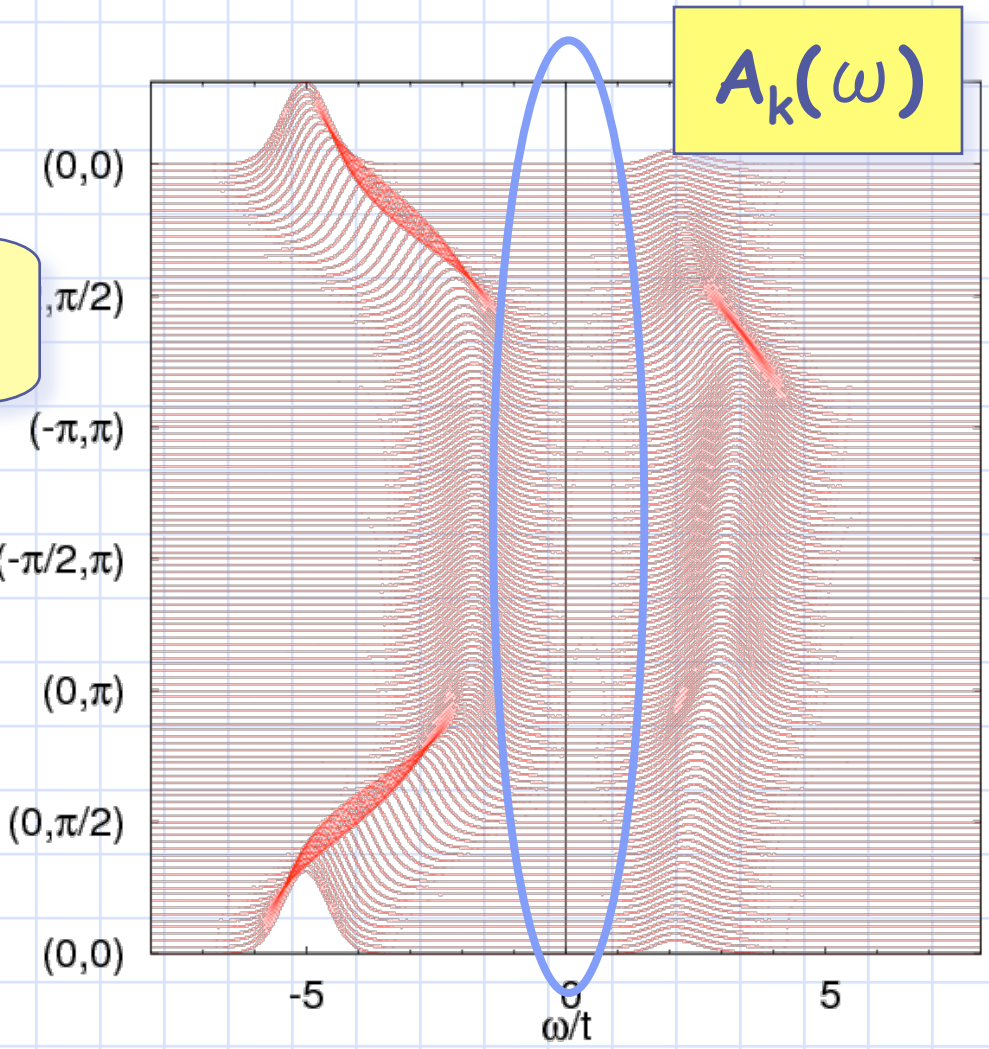
U/t=0.8, t'/t=0.8,

T/t=0.7

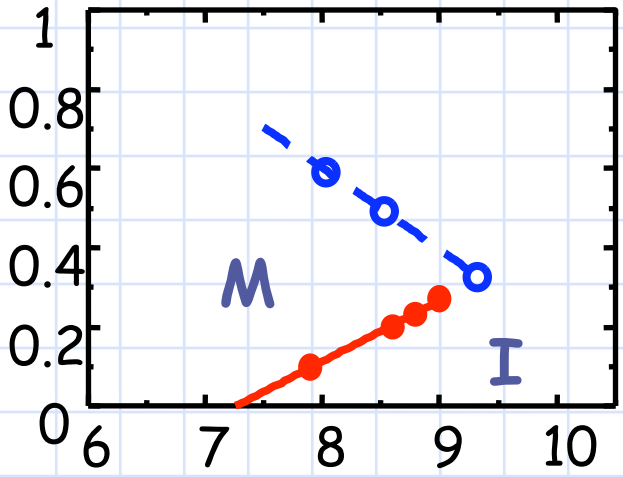


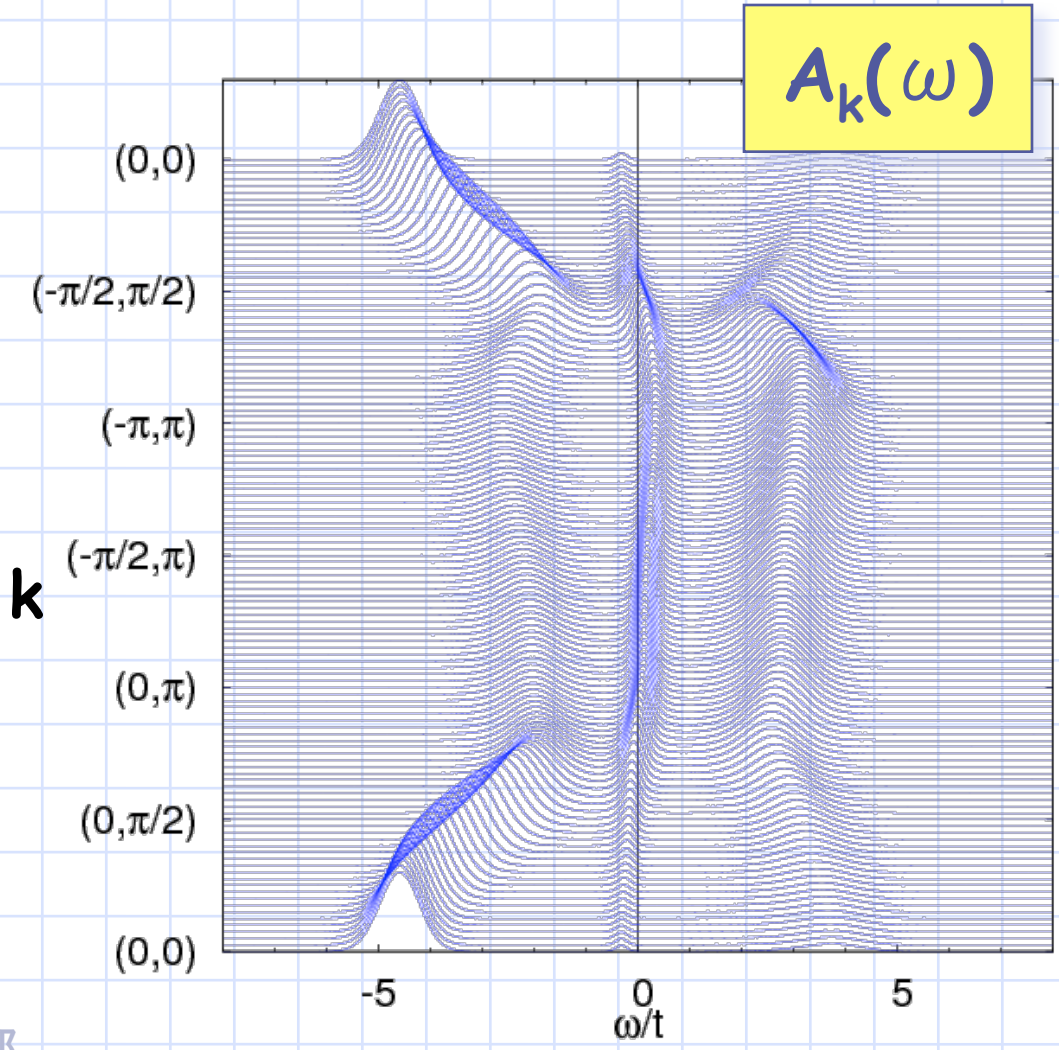
U-dominant insulator

No quasi-particles



k-dependent spectral function



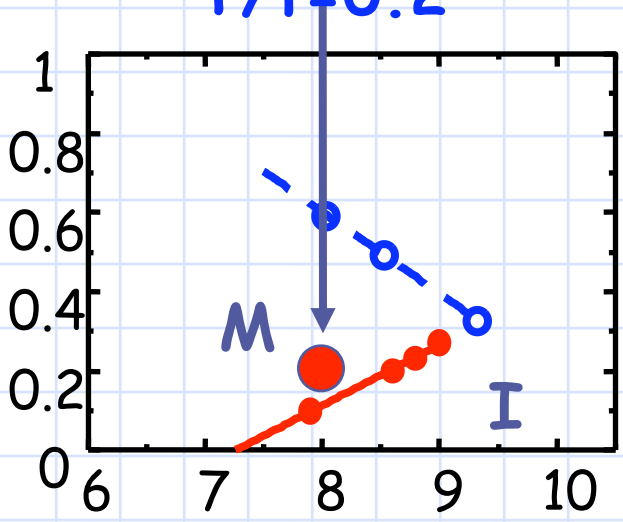


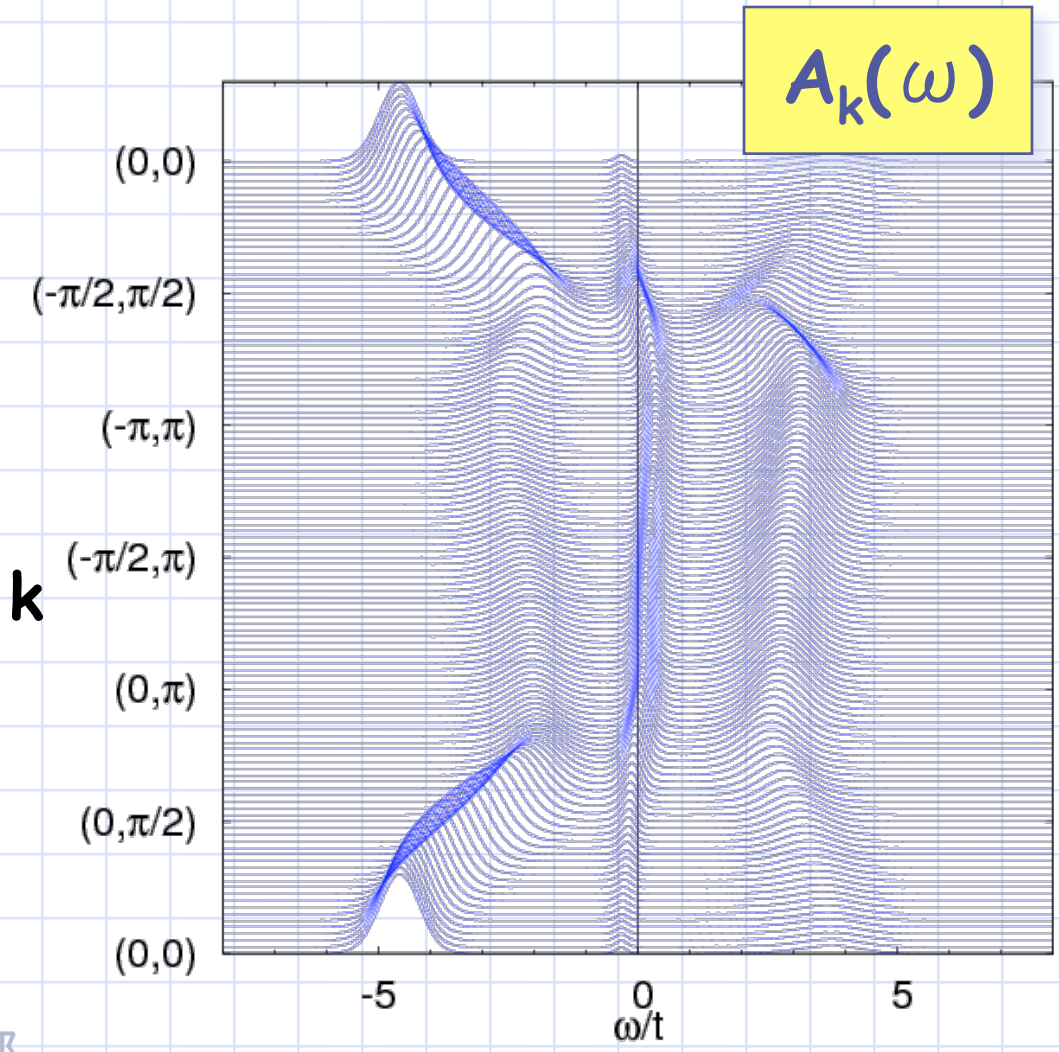
k-dependent spectral function

Intermediate T

U/t=0.8, t'/t=0.8,

T/t=0.2



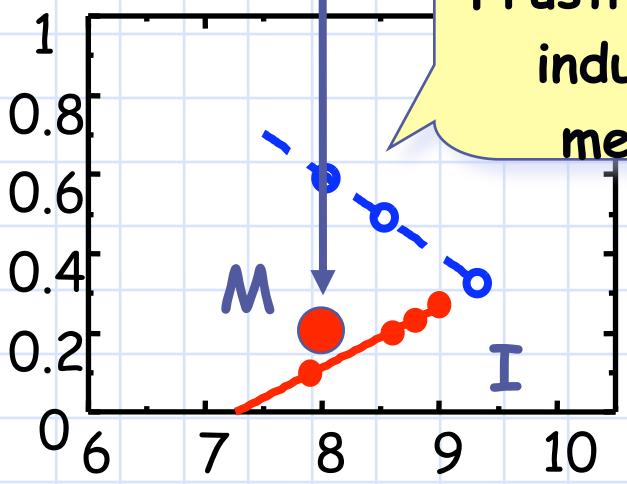


k-dependent spectral function

Intermediate T

U/t=0.8, t'/t=0.8,

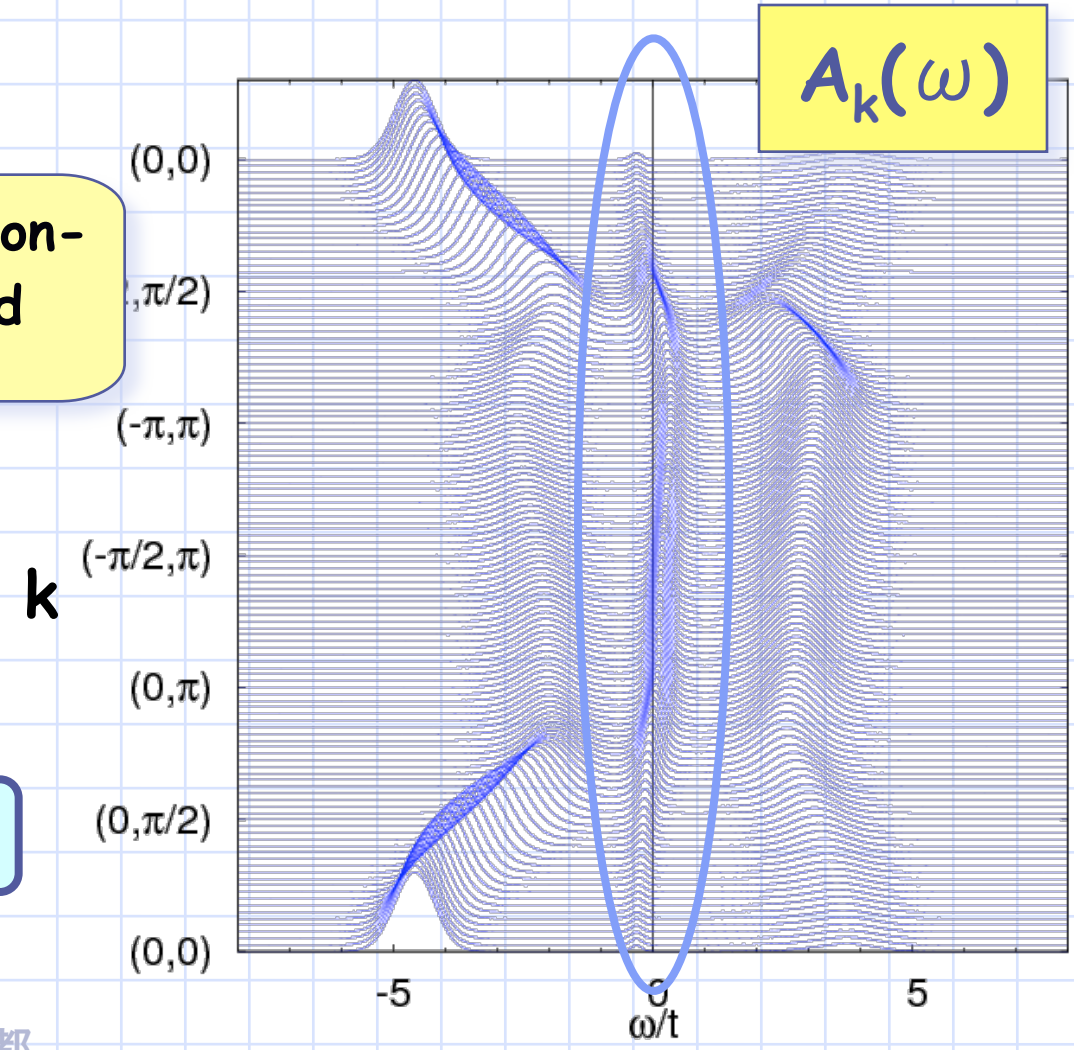
T/t=0.2



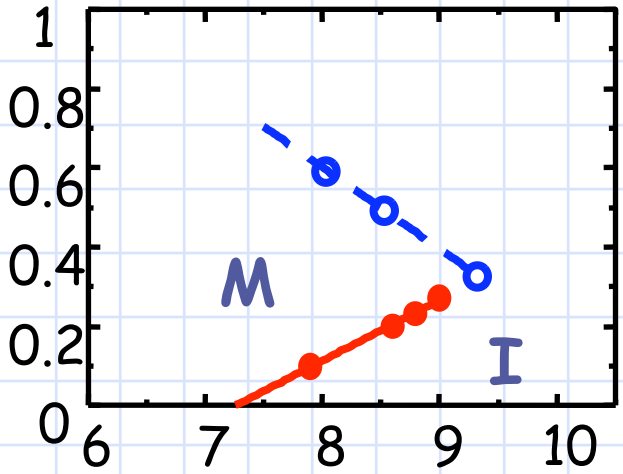
Frustration-induced metal

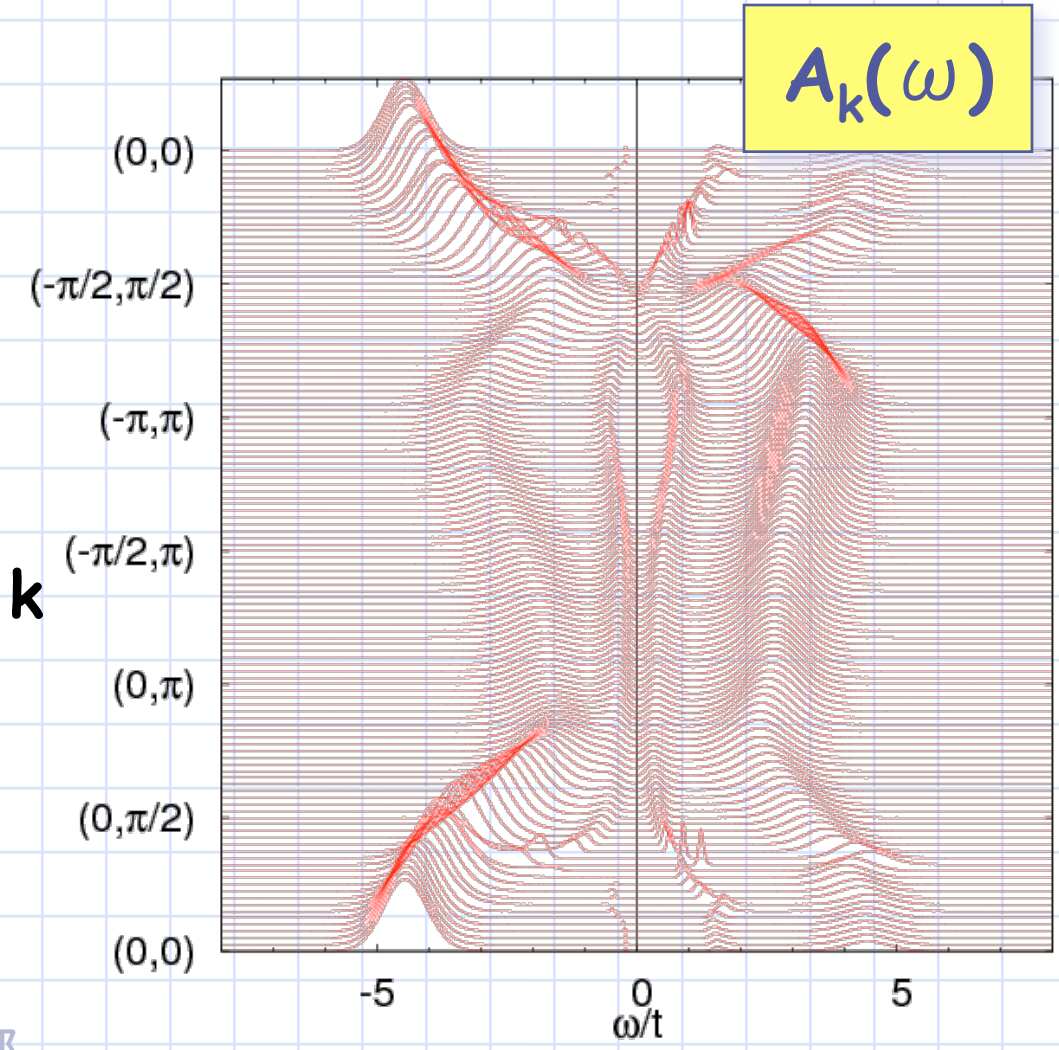
Quasi-particles

frustration



k-dependent spectral function



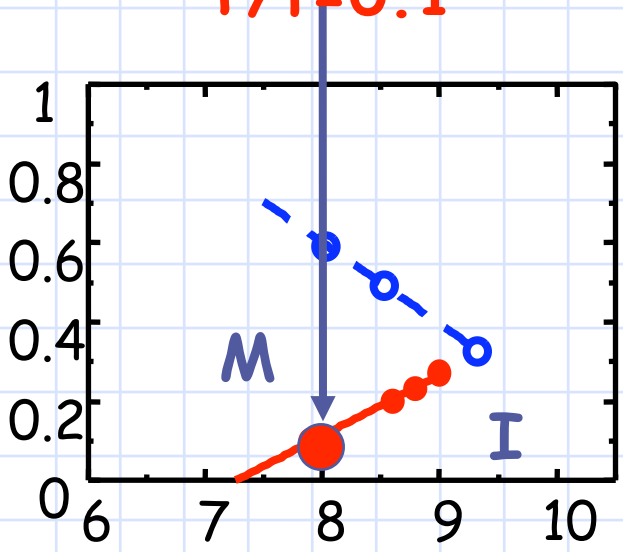


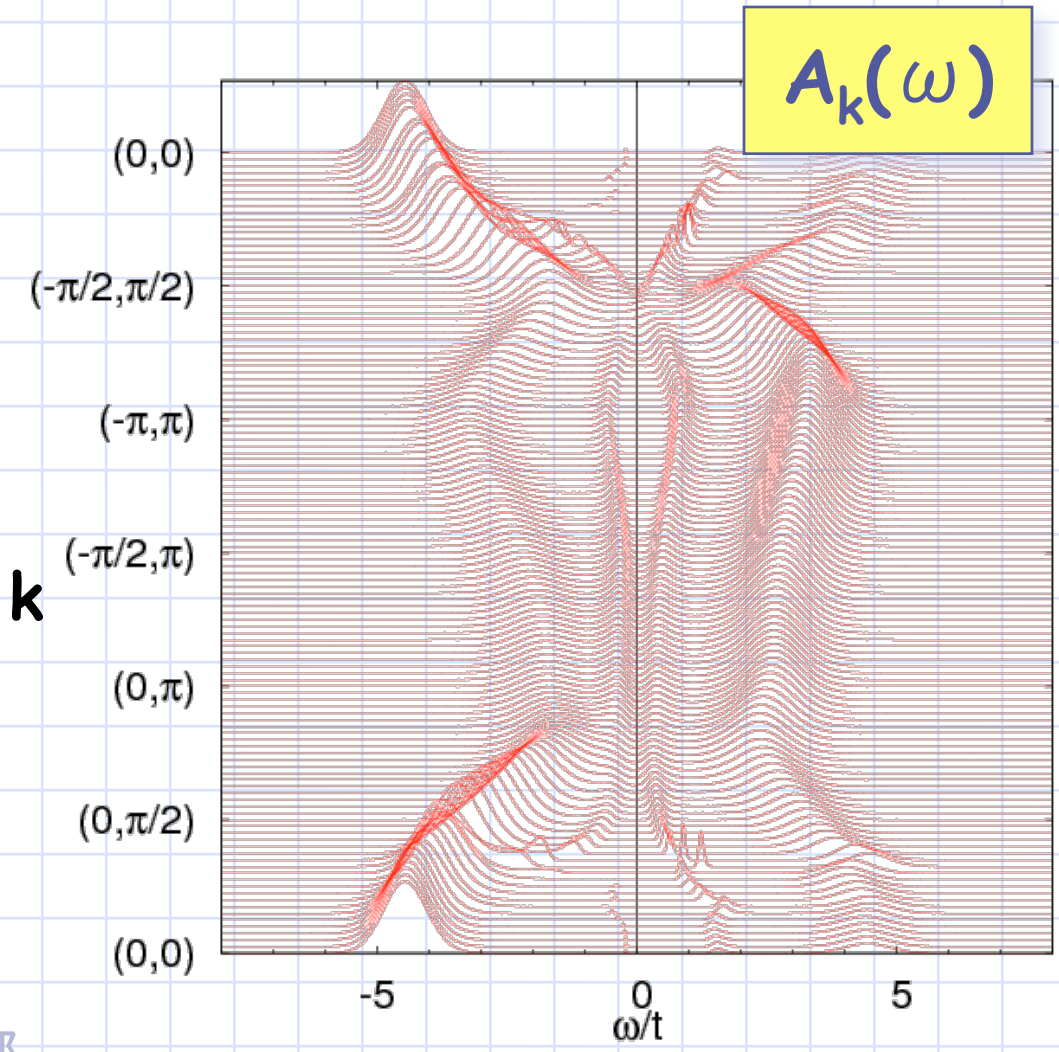
k-dependent spectral function

Low T

U/t=0.8, t'/t=0.8,

T/t=0.1



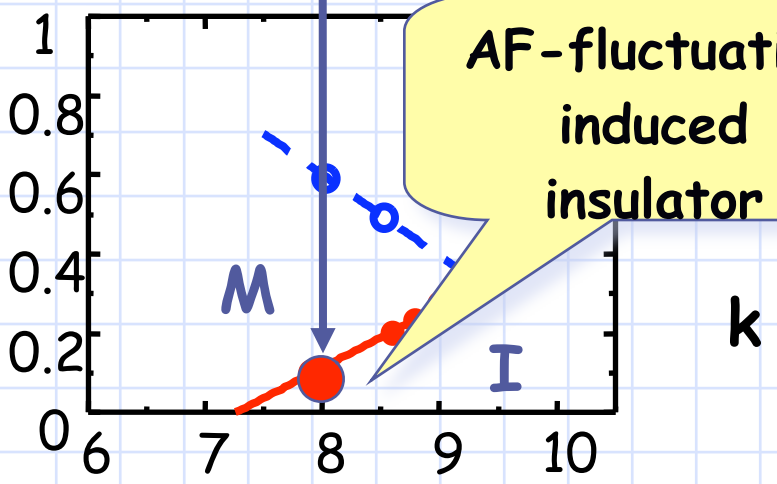


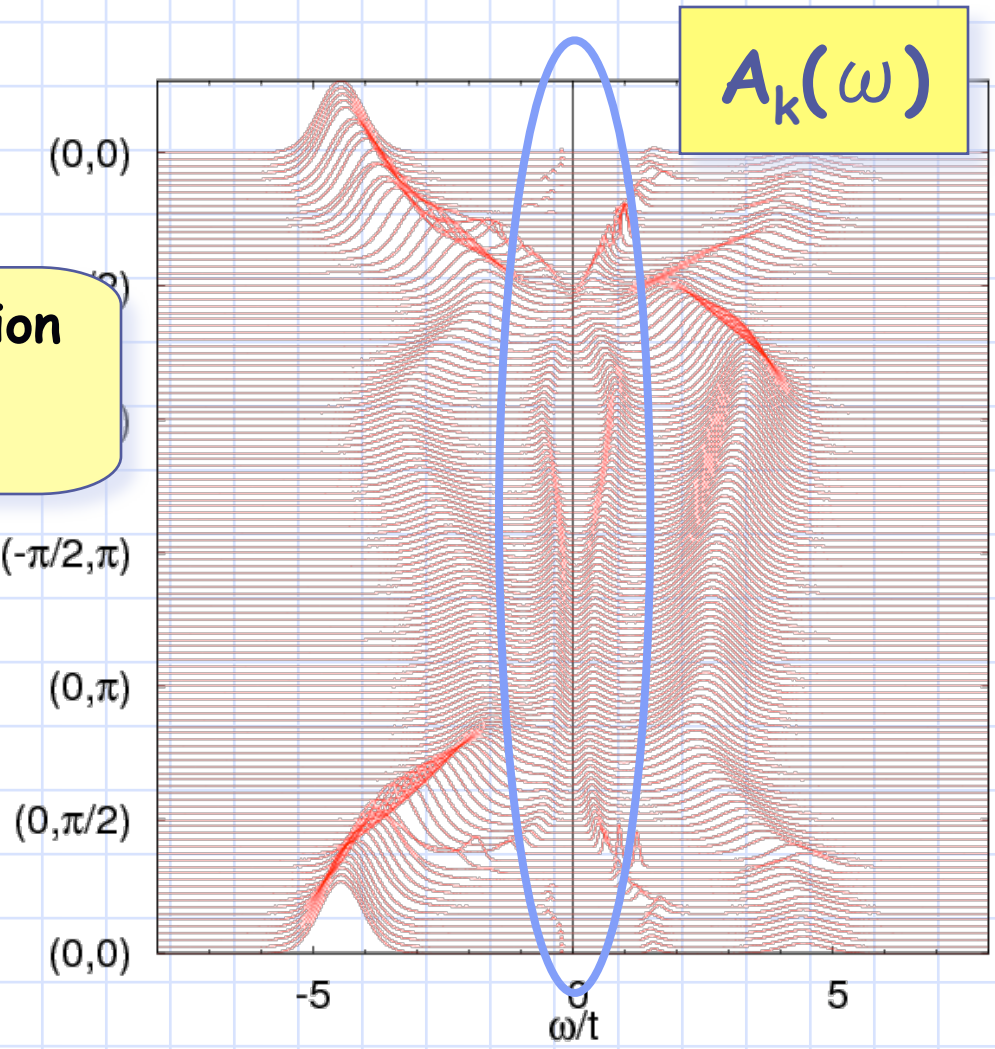
k-dependent spectral function

Low T

U/t=0.8, t'/t=0.8,

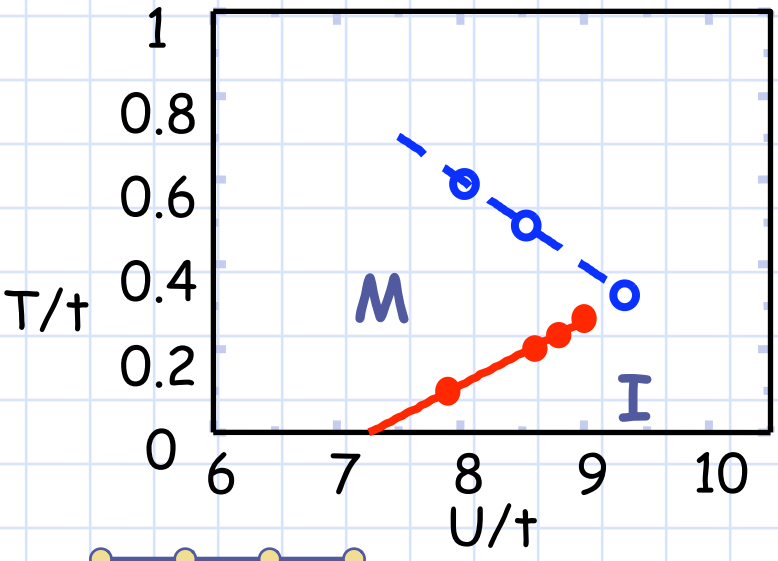
T/t=0.1

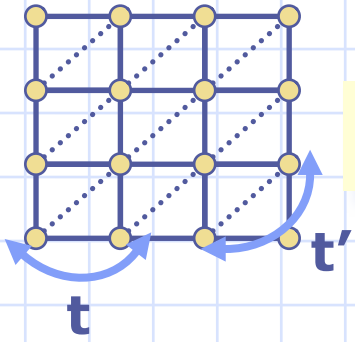




- splitting of QP peak
- different from high T

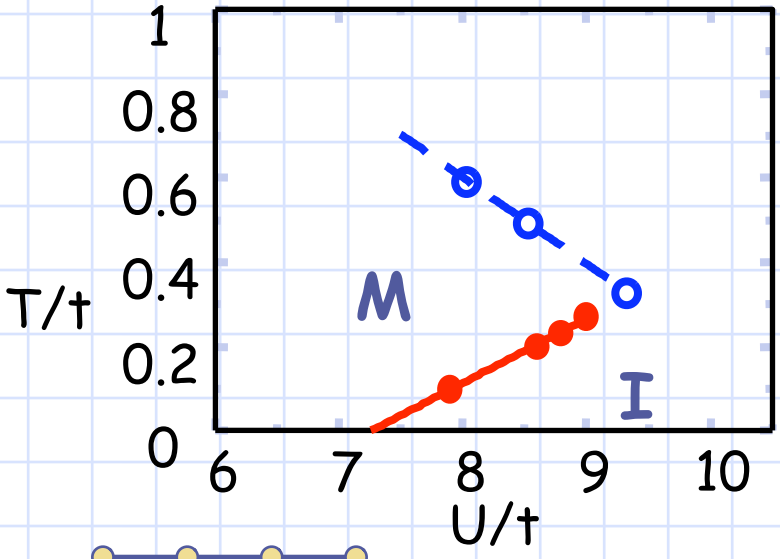
Phase diagram

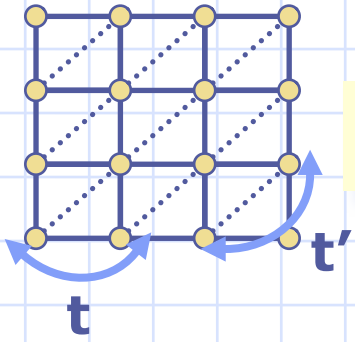




t'/t =0.8

Phase diagram

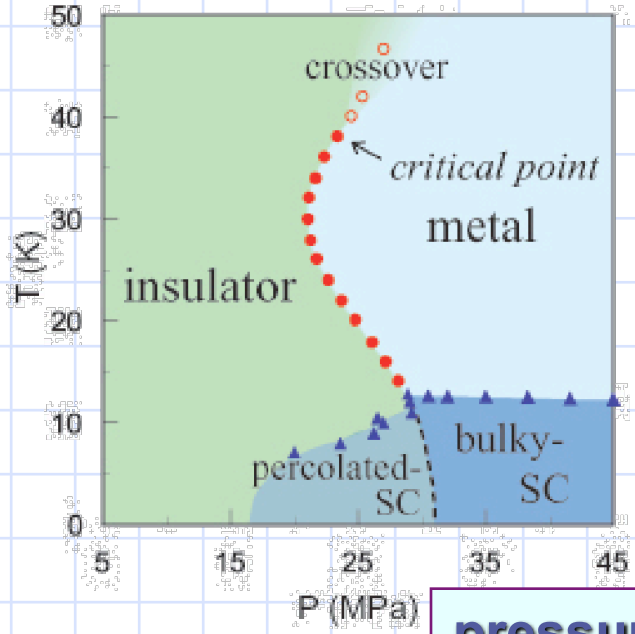




t'/t =0.8

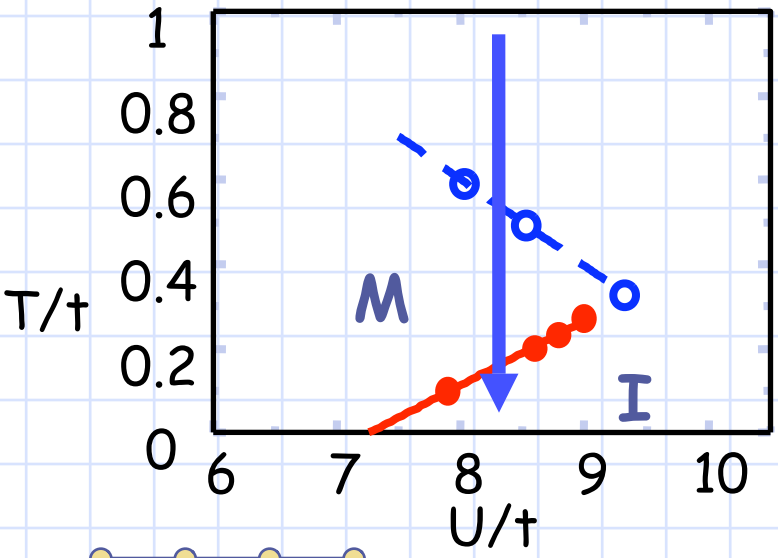
Kanoda group

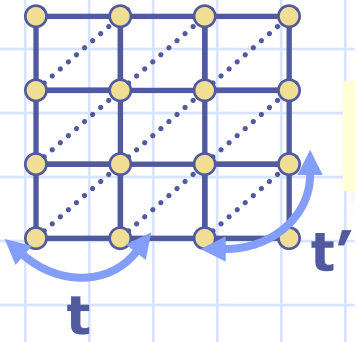
κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



pressure

Phase diagram

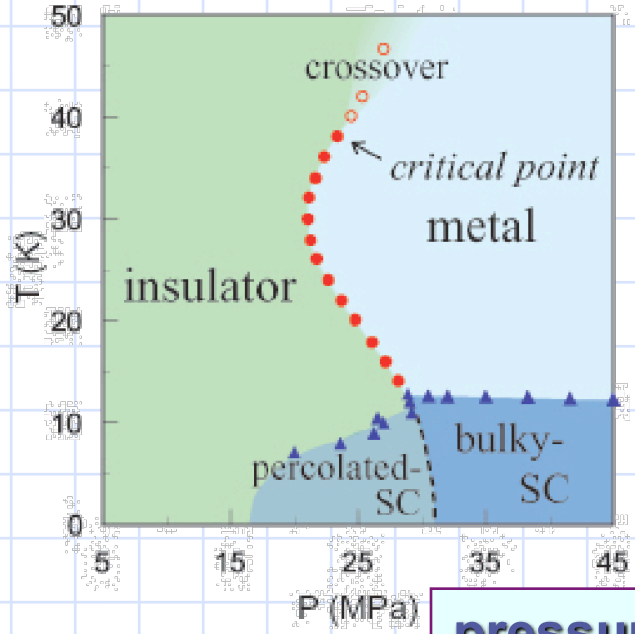




t'/t =0.8

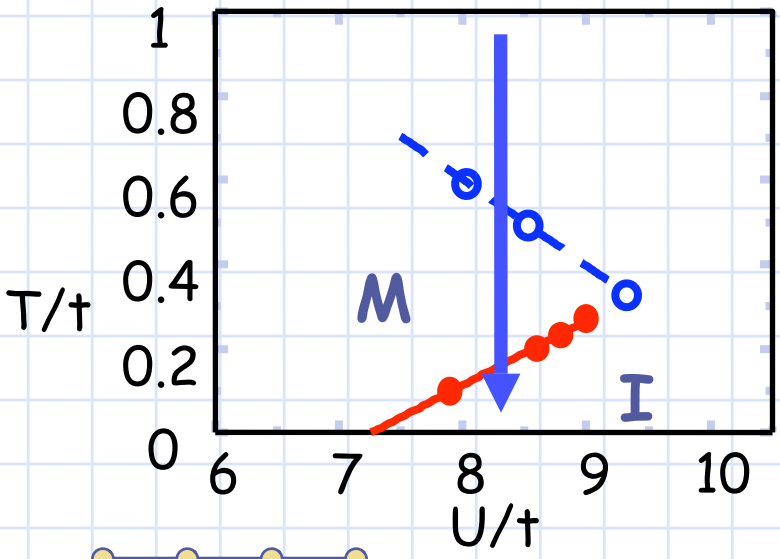
Kanoda group

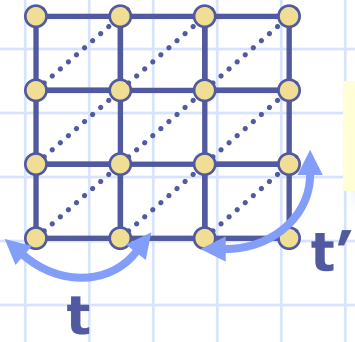
κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



pressure

Phase diagram

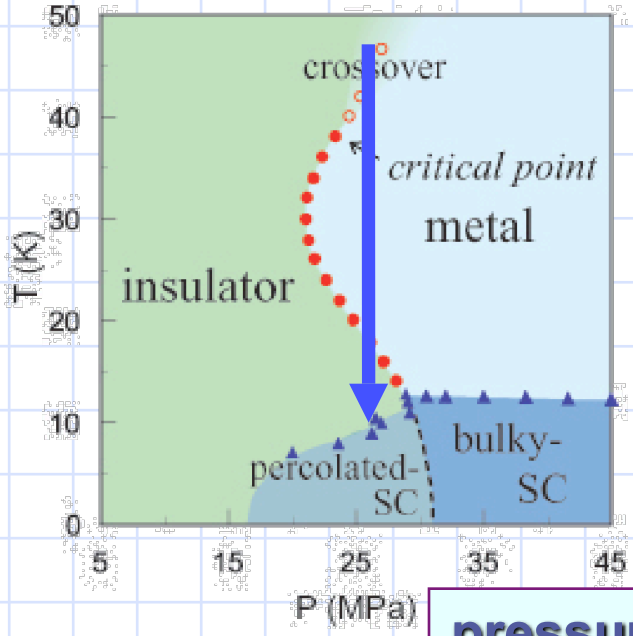




t′/t =0.8

Kanoda group

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

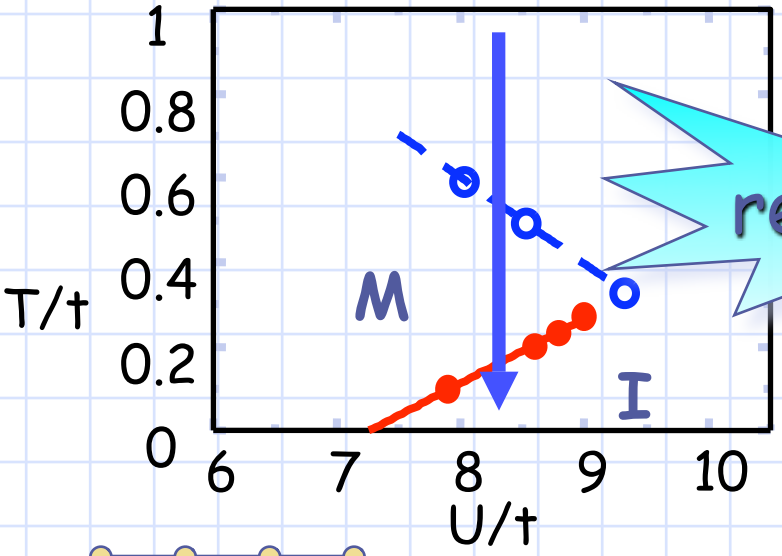


pressure

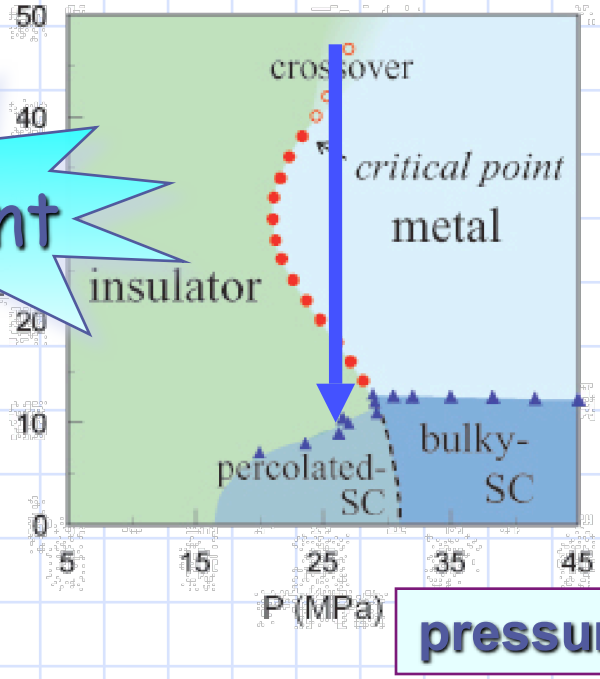
Phase diagram

Kanoda group

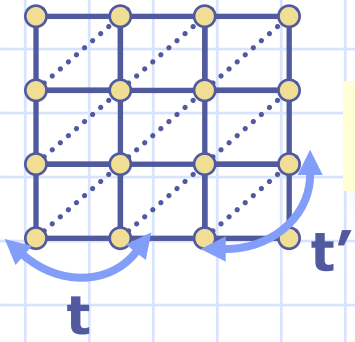
κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



reentrant



pressure

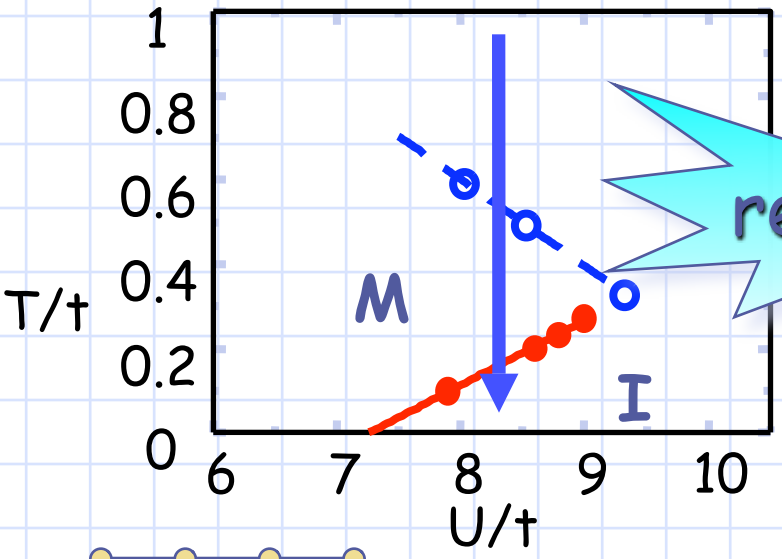


t'/t =0.8

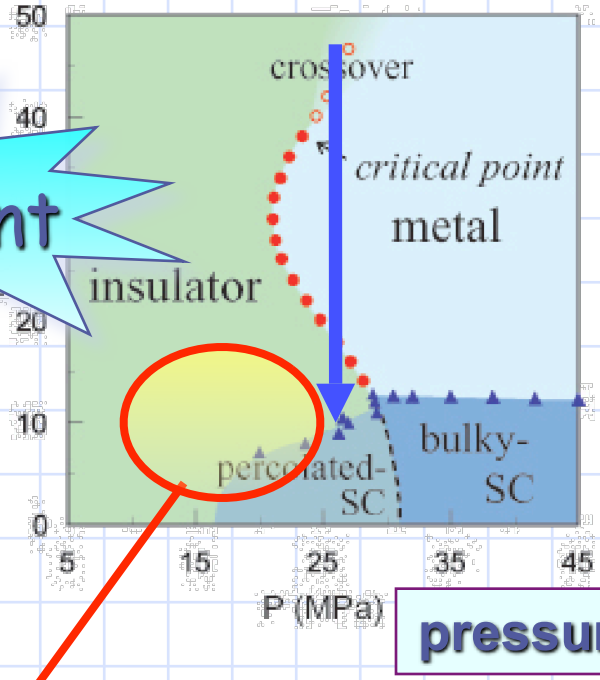
Phase diagram

Kanoda group

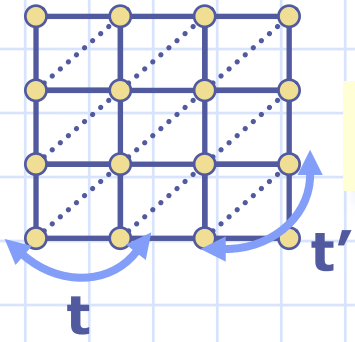
κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



reentrant



pressure



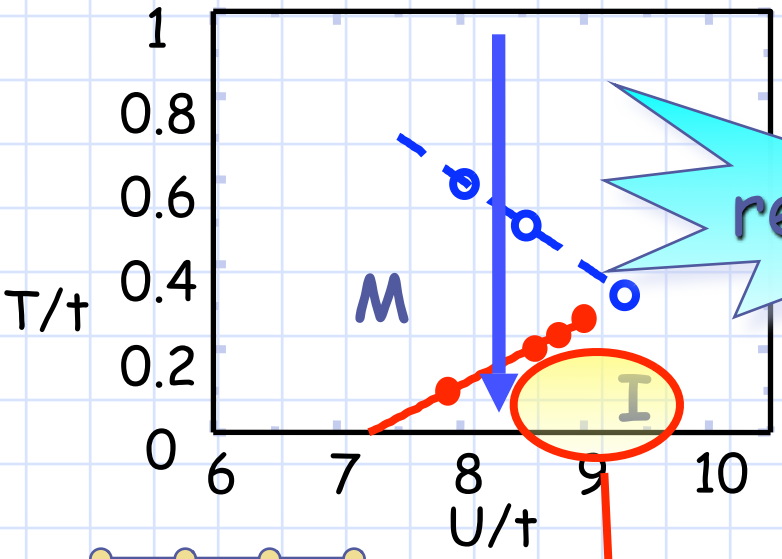
t'/t =0.8

Magnetic order

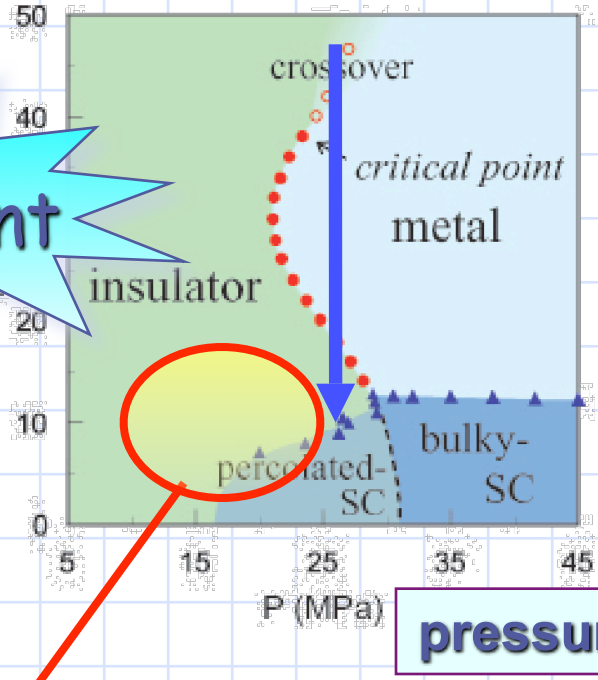
Phase diagram

Kanoda group

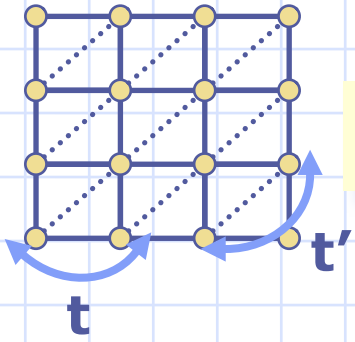
κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



reentrant



pressure



t'/t =0.8

?

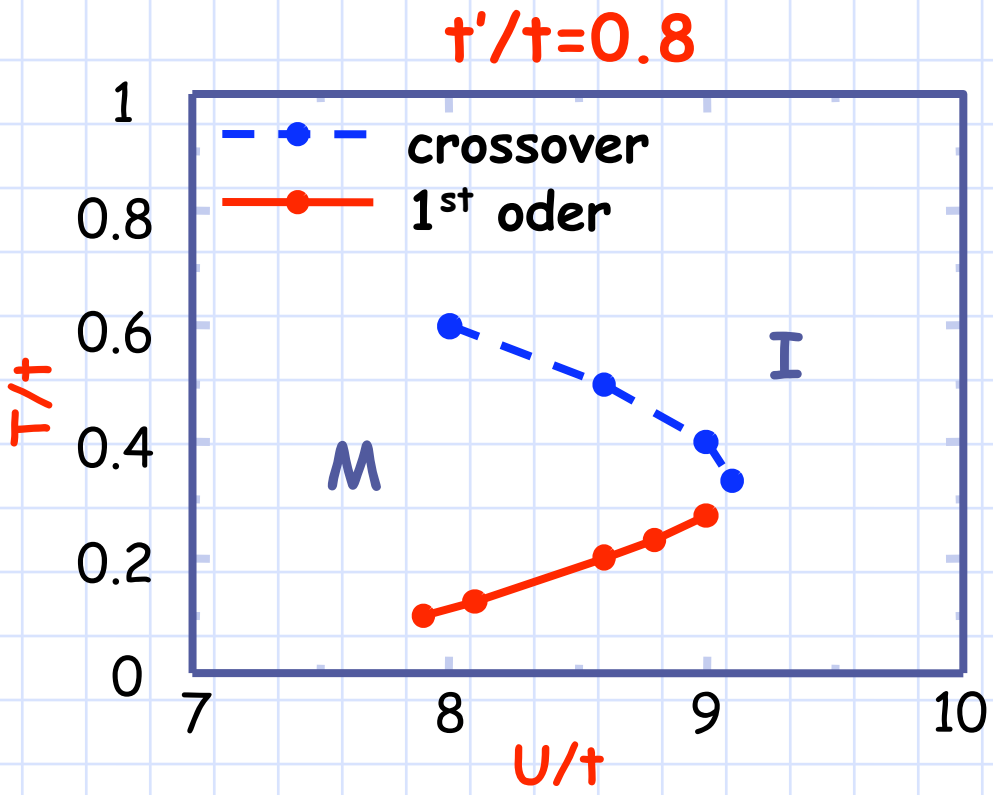
Magnetic order

YKIS 07
Kyoto
November 14, 2007

Magnetic instability

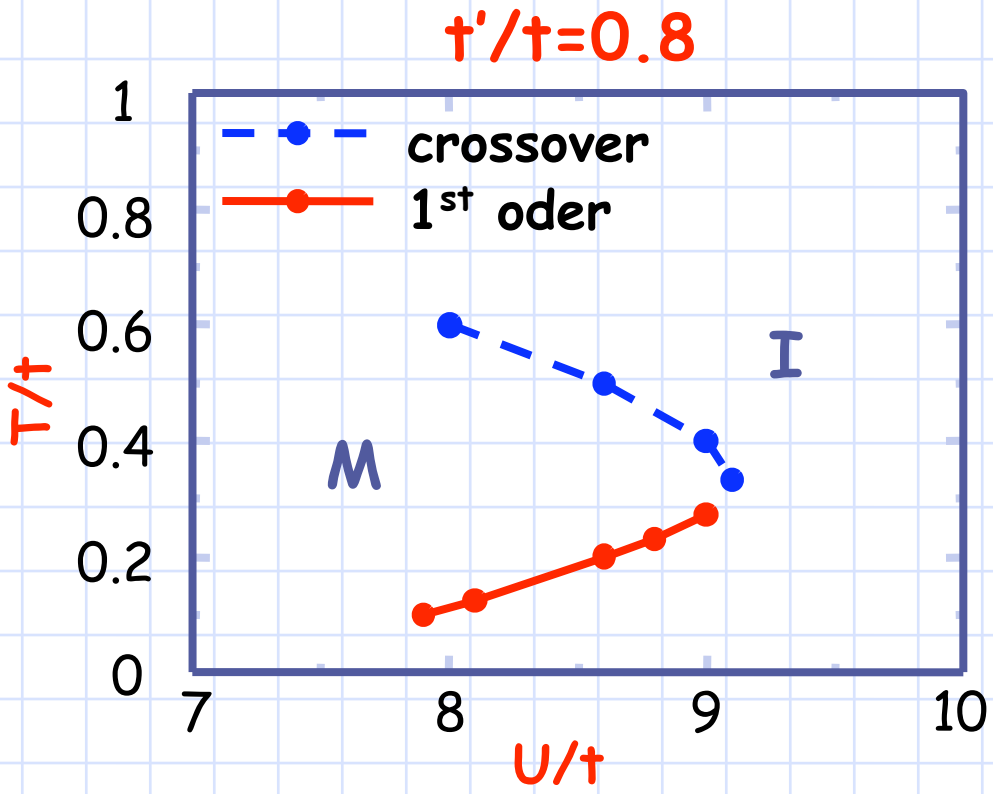
Magnetic instability

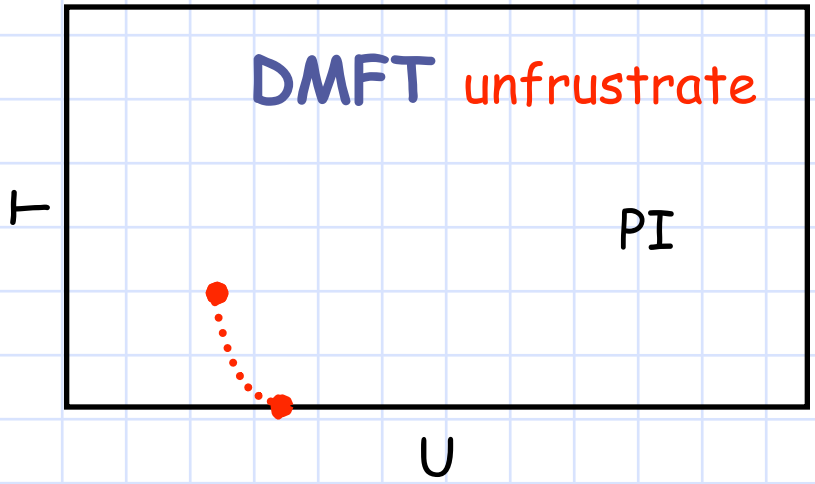
Cellular-DMFT → ordering at finite T



Magnetic instability

Cellular-DMFT → ordering at finite T

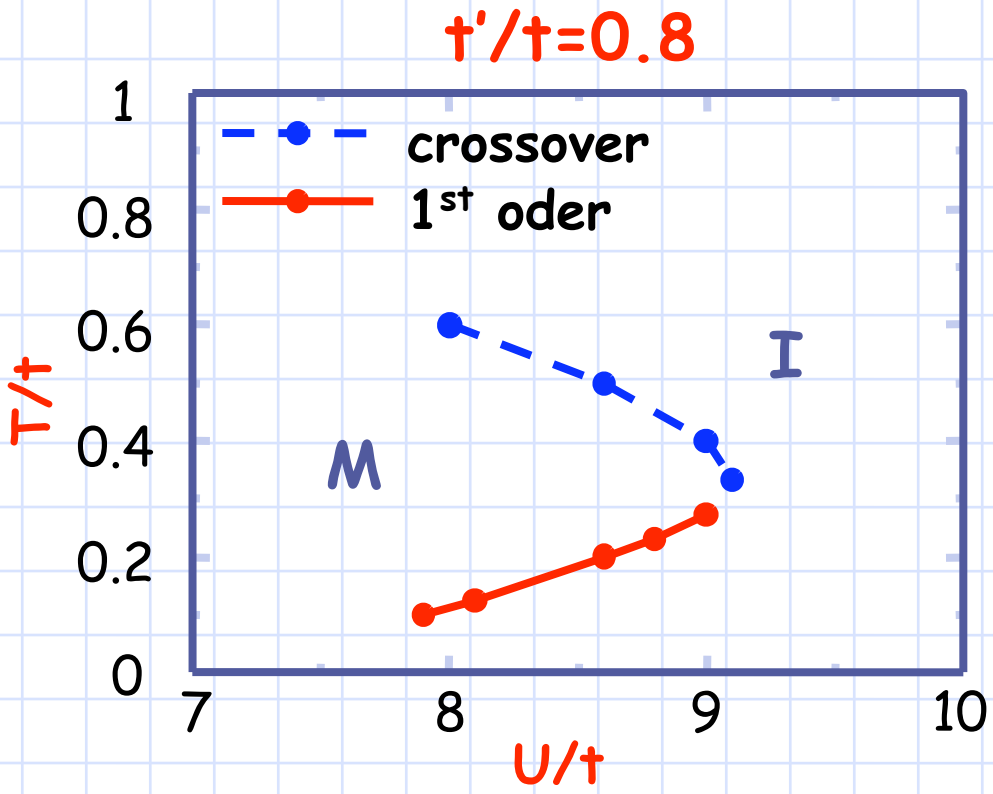


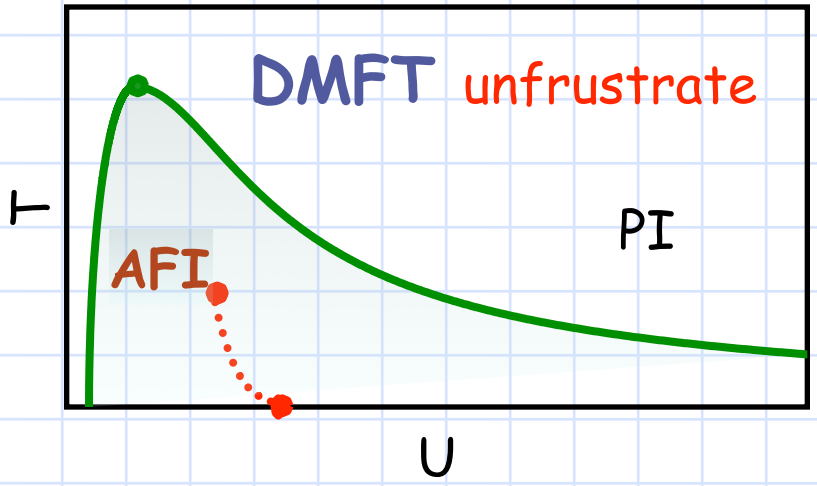


Georges et al. RMP 68, 13 (1996)
Zitzler et al. PRL 93 016406 (2004)

Magnetic instability

Cellular-DMFT → ordering at finite T



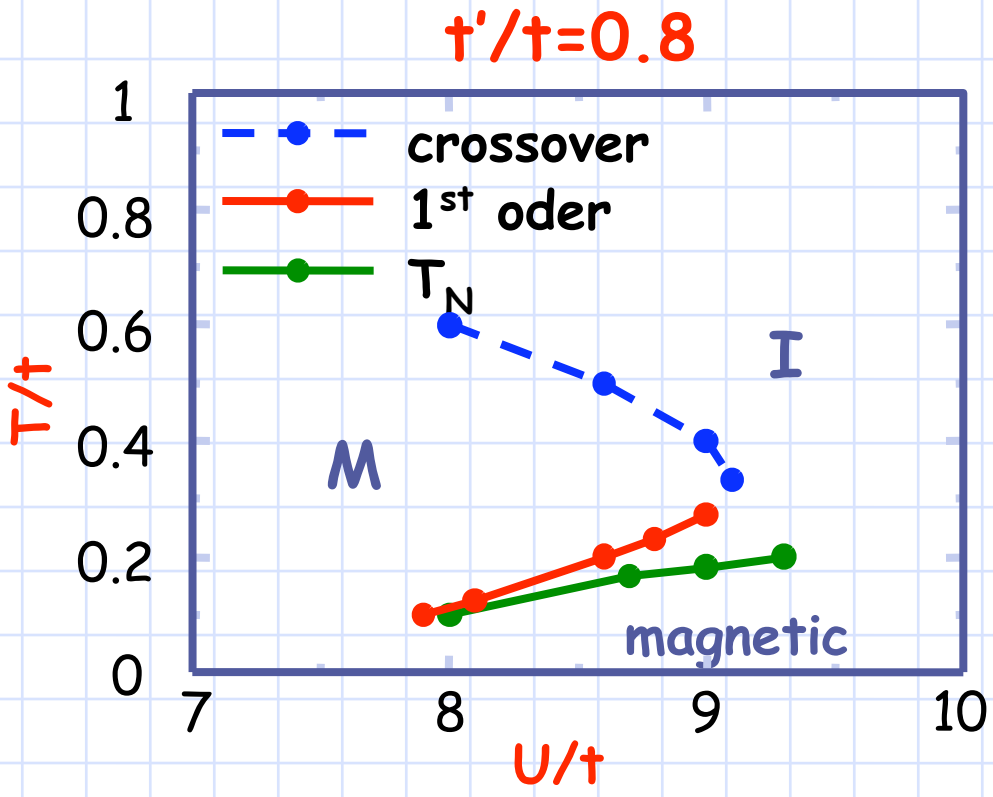


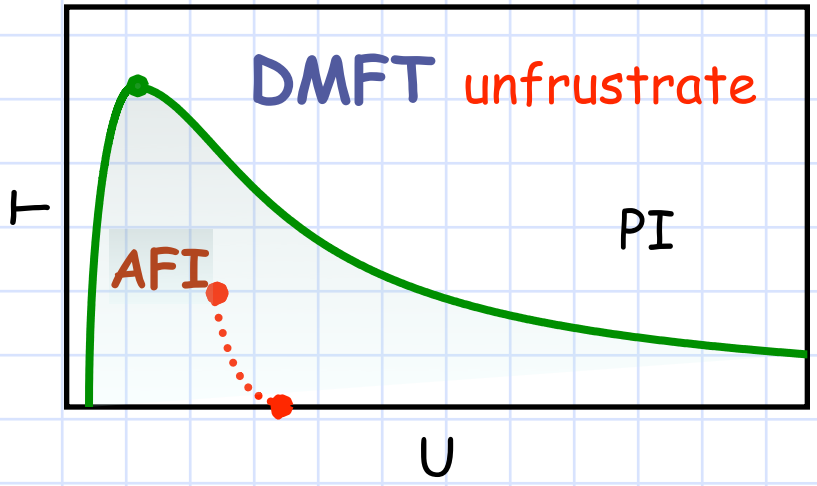
Georges et al. RMP 68, 13 (1996)
Zitzler et al. PRL 93 016406 (2004)

Mott transition disappears

Magnetic instability

Cellular-DMFT → ordering at finite T





Georges et al. RMP 68, 13 (1996)
Zitzler et al. PRL 93 016406 (2004)

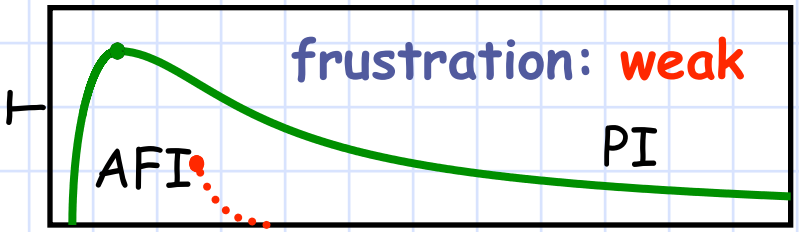
Mott transition disappears

Frustration: Mott transition survives !

Frustration ∞ dimensions

DMFT: frustrated Bethe lattice

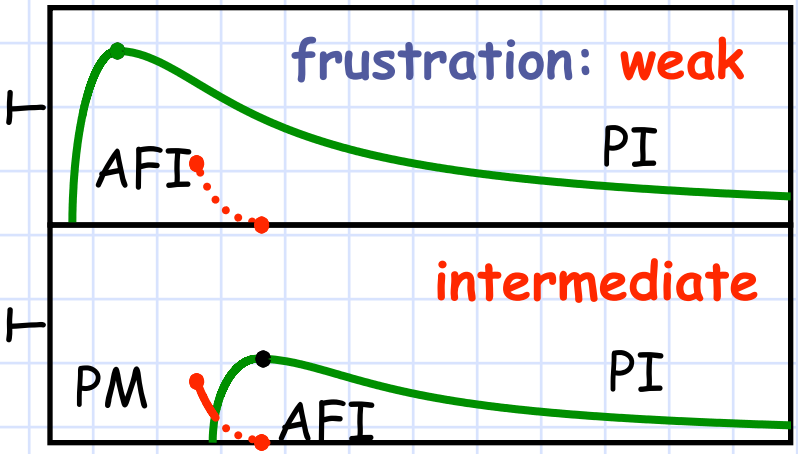
Zitzler et al. Phys. Rev. Lett. 93 016406



Frustration ∞ dimensions

DMFT: frustrated Bethe lattice

Zitzler et al. Phys. Rev. Lett. 93 016406



Frustration ∞ dimensions

DMFT: frustrated Bethe lattice

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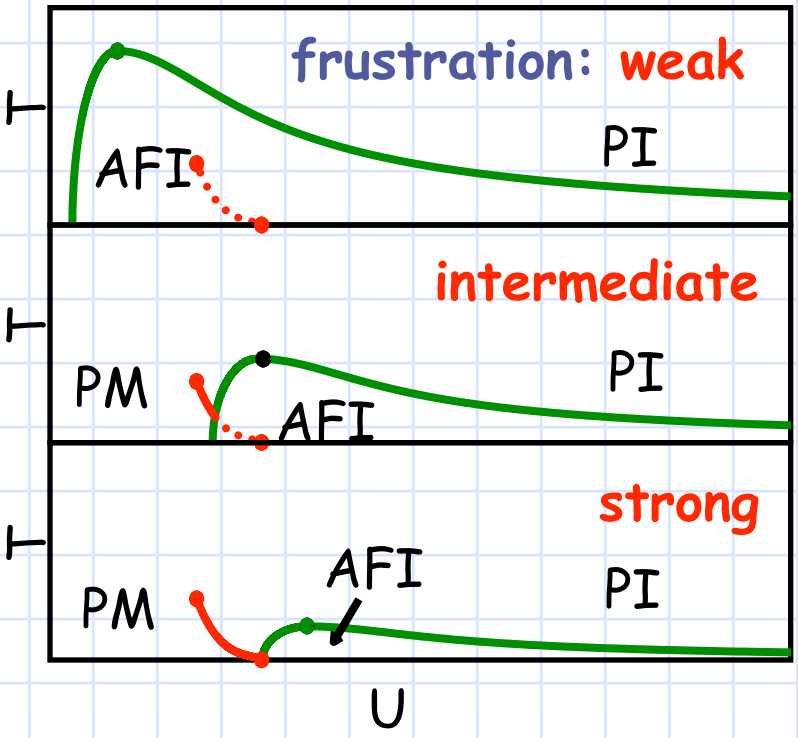

Frustration ∞ dimensions

DMFT: frustrated Bethe lattice

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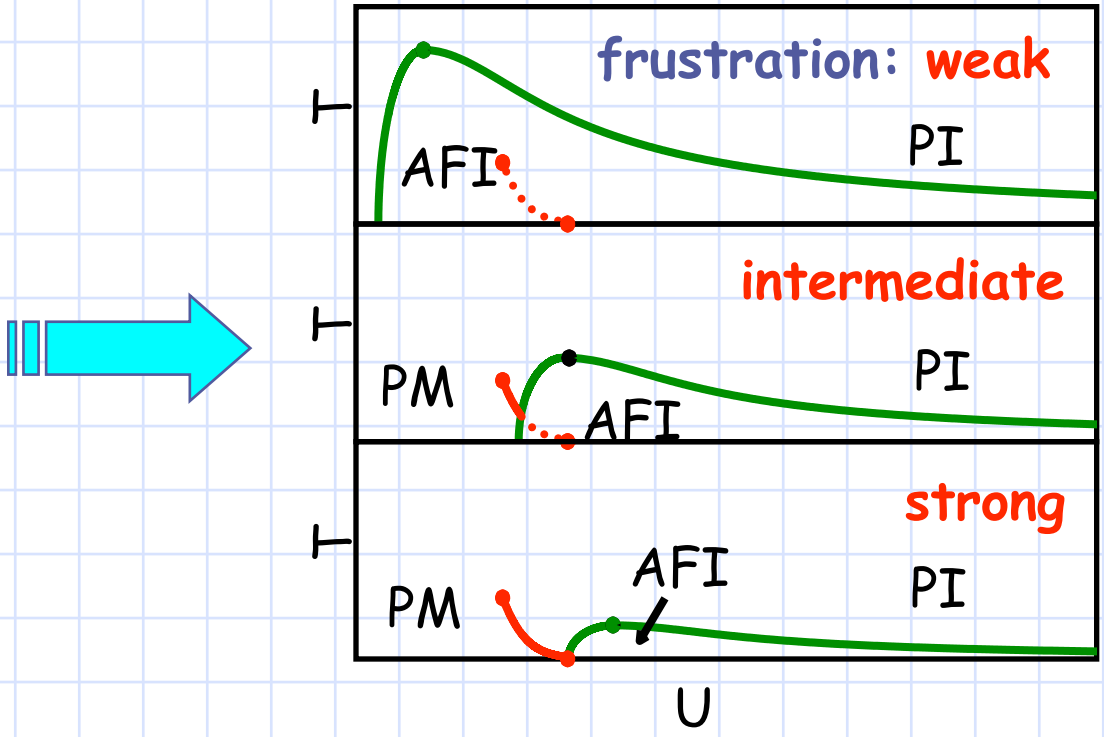
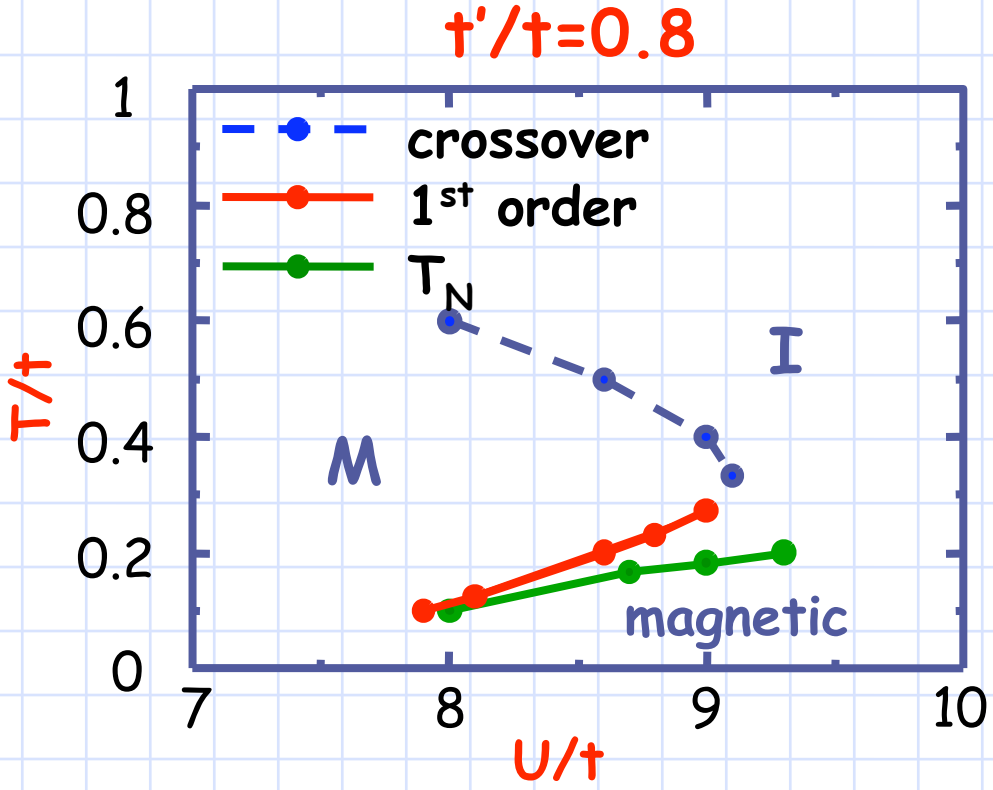


Comparison: frustrated systems in infinite dimensions

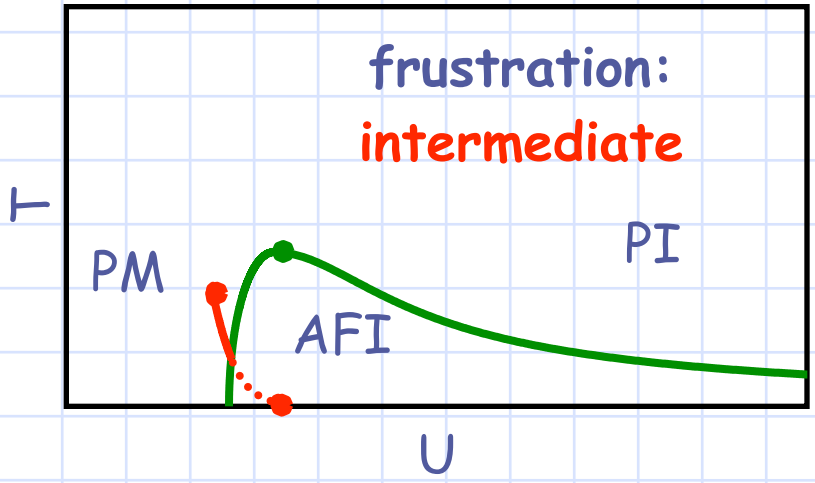


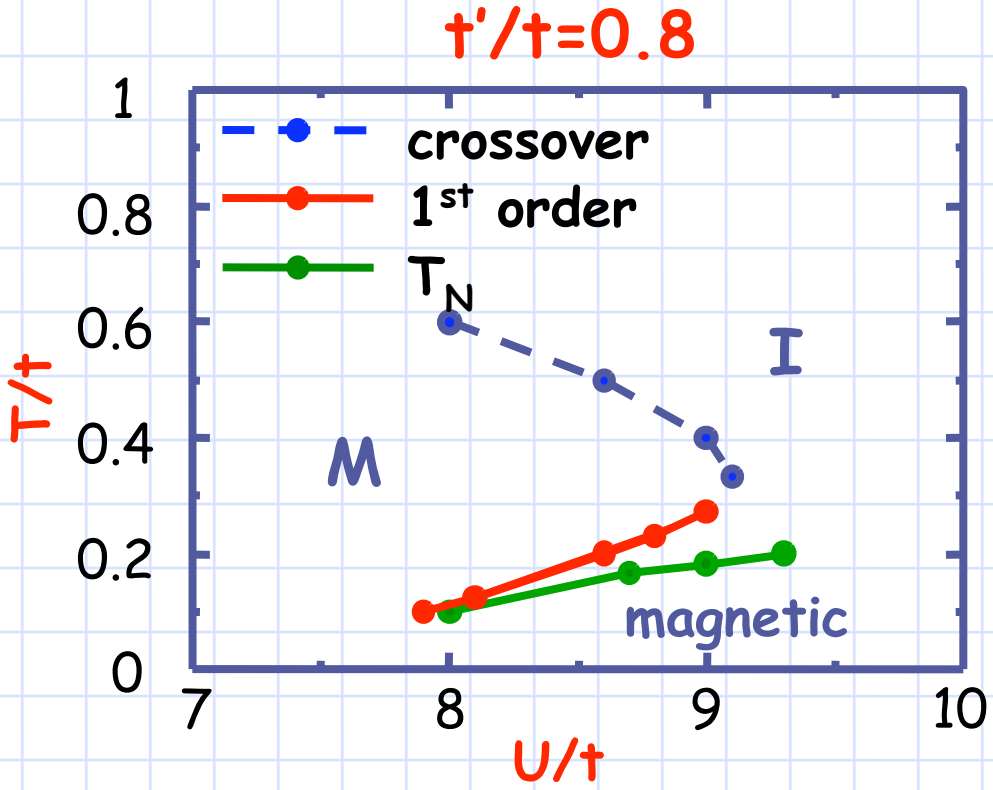
Cellular-DMFT

Comparison: frustrated systems in infinite dimensions

DMFT: frustrated Bethe lattice

Zitzler et al. PRL 93 016406 (2004)



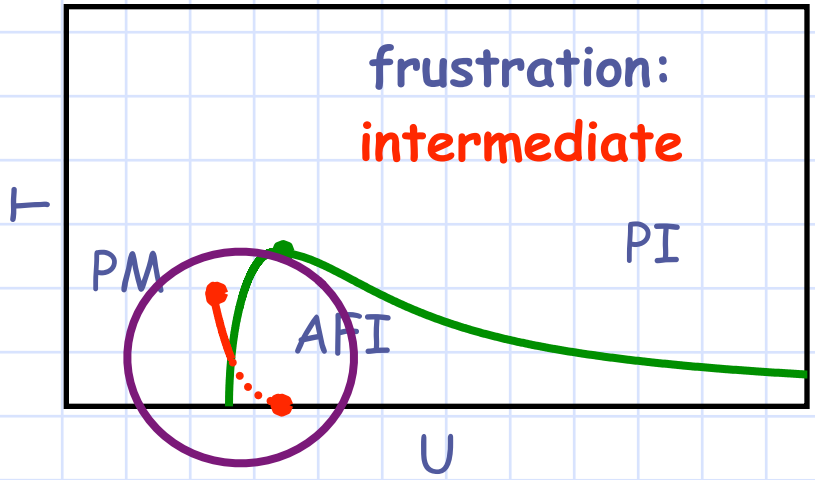


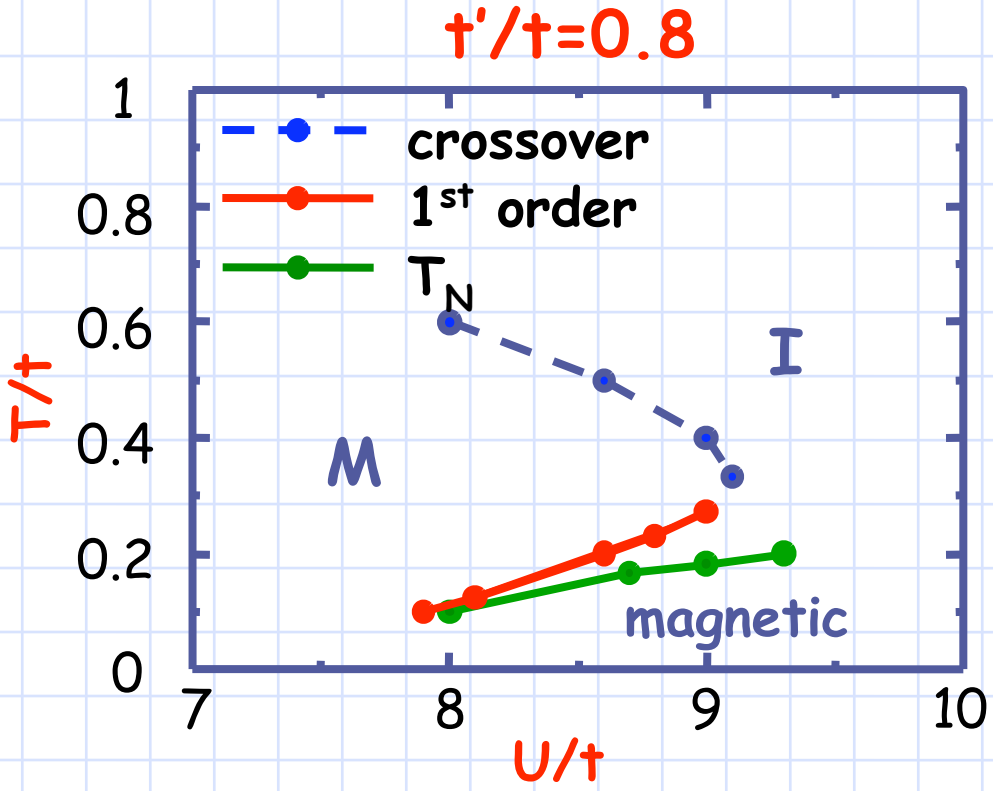
Cellular-DMFT

Comparison: frustrated systems in infinite dimensions

DMFT: frustrated Bethe lattice

Zitzler et al. PRL 93 016406 (2004)



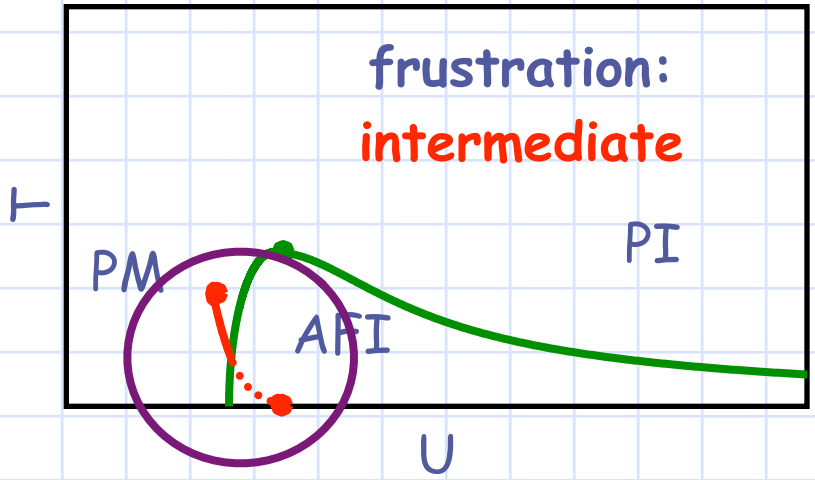


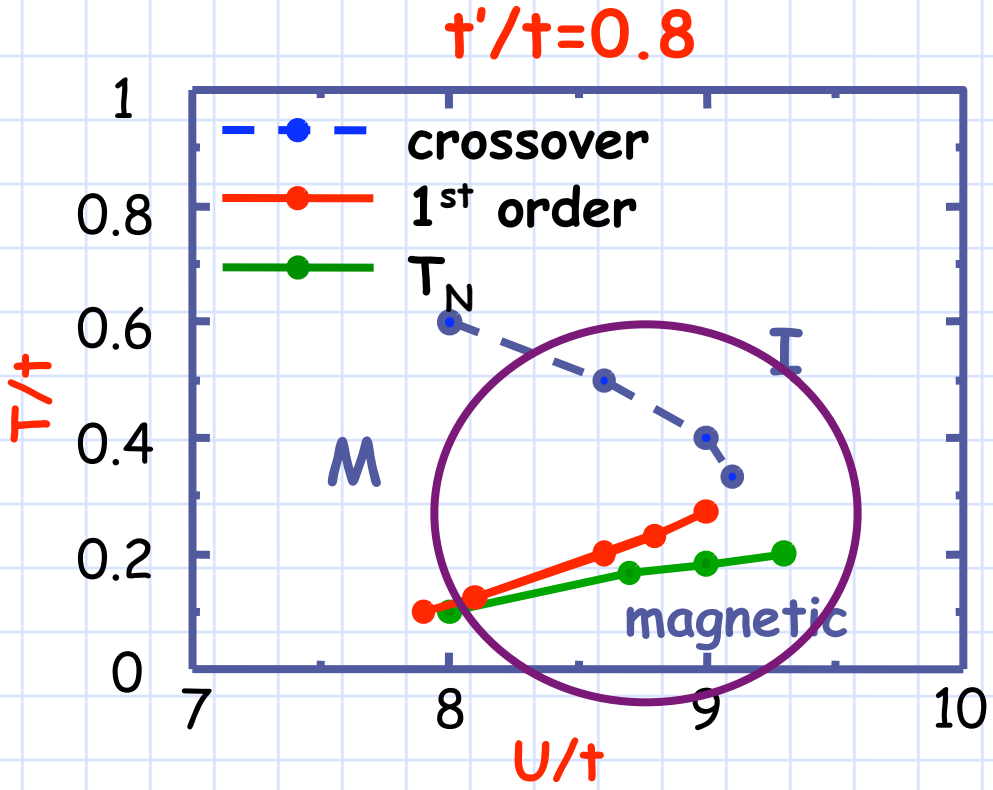
Cellular-DMFT

Comparison: frustrated systems in infinite dimensions

DMFT: frustrated Bethe lattice

Zitzler et al. PRL 93 016406 (2004)



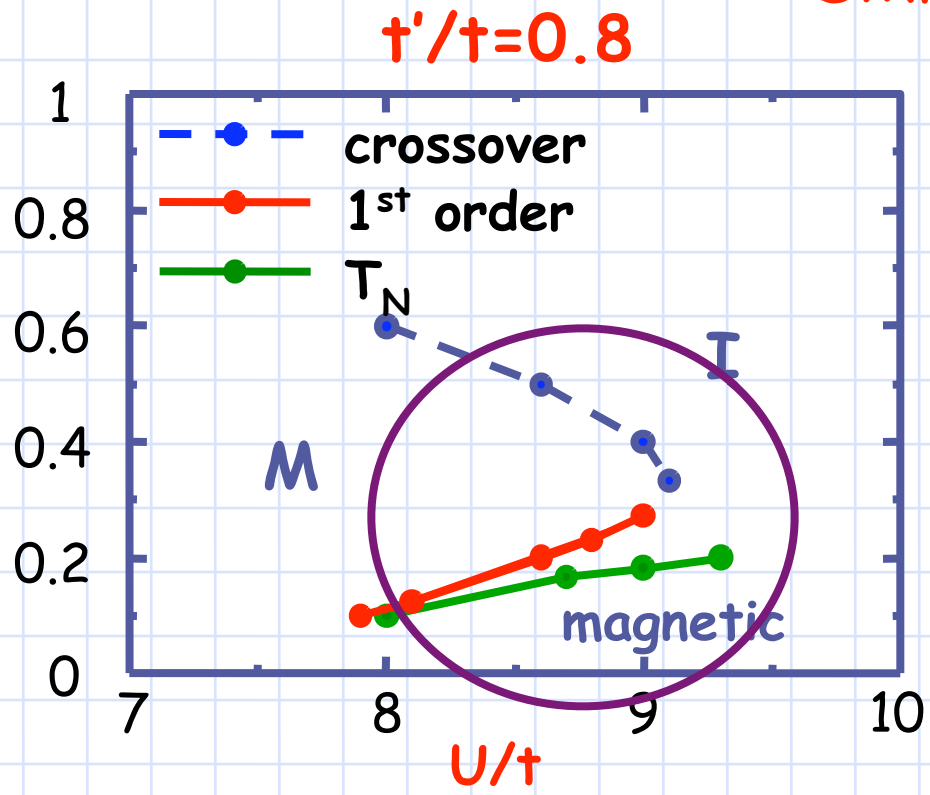


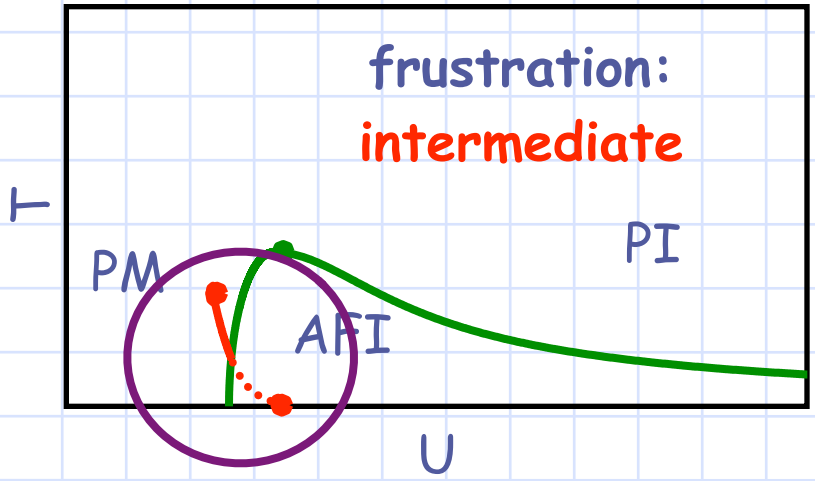
Cellular-DMFT

Comparison: frustrated systems in infinite dimensions

DMFT: frustrated Bethe lattice

Zitzler et al. PRL 93 016406 (2004)





Cellular-DMFT

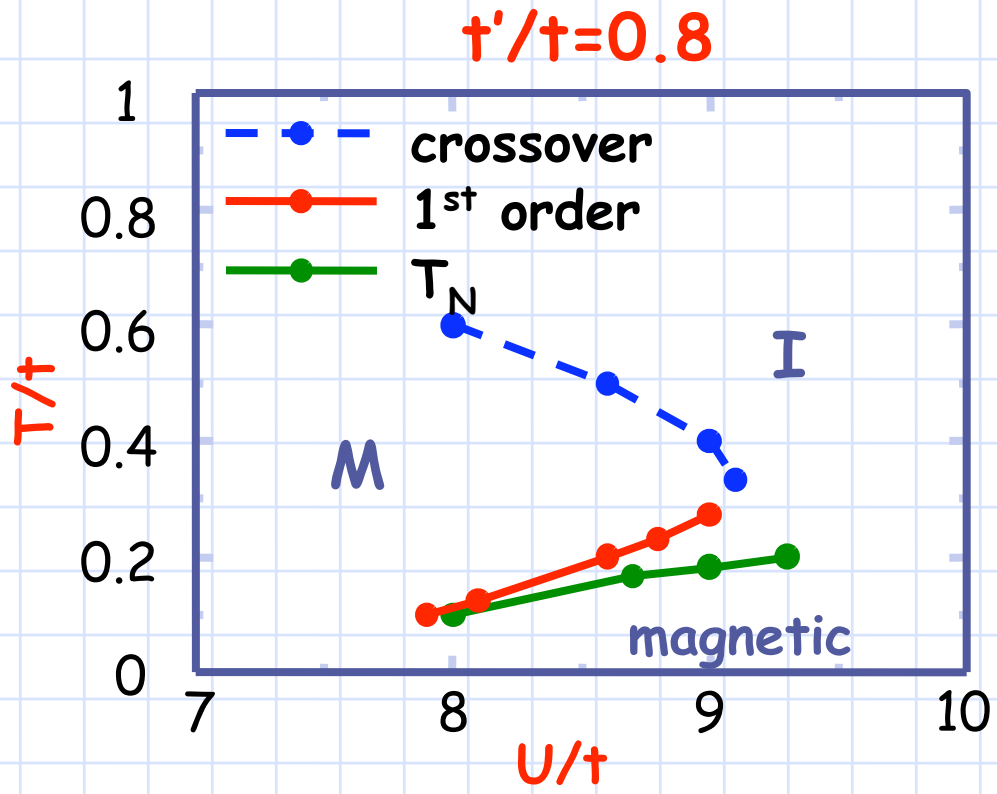
Spatial fluctuations

change in U_c critical line

nonmag. insulator

Comparison with organics

Cellular-DMFT → order at finite T

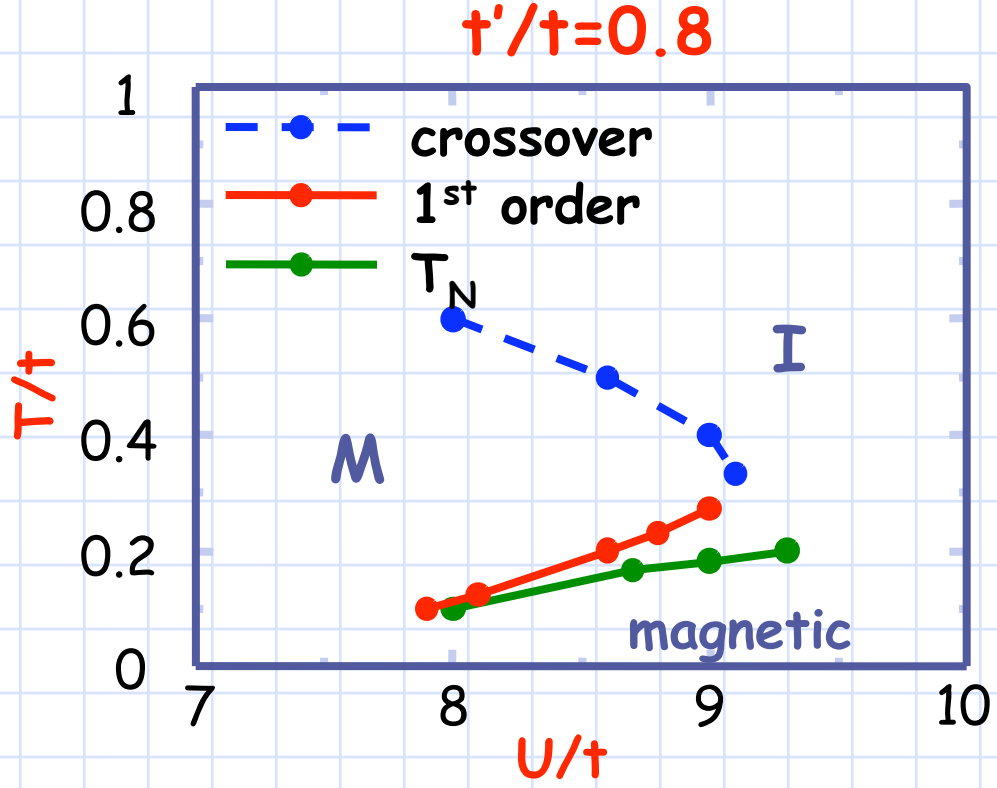


Comparison with organics

Cellular-DMFT →

- order at finite T
- stabilized by 3D

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

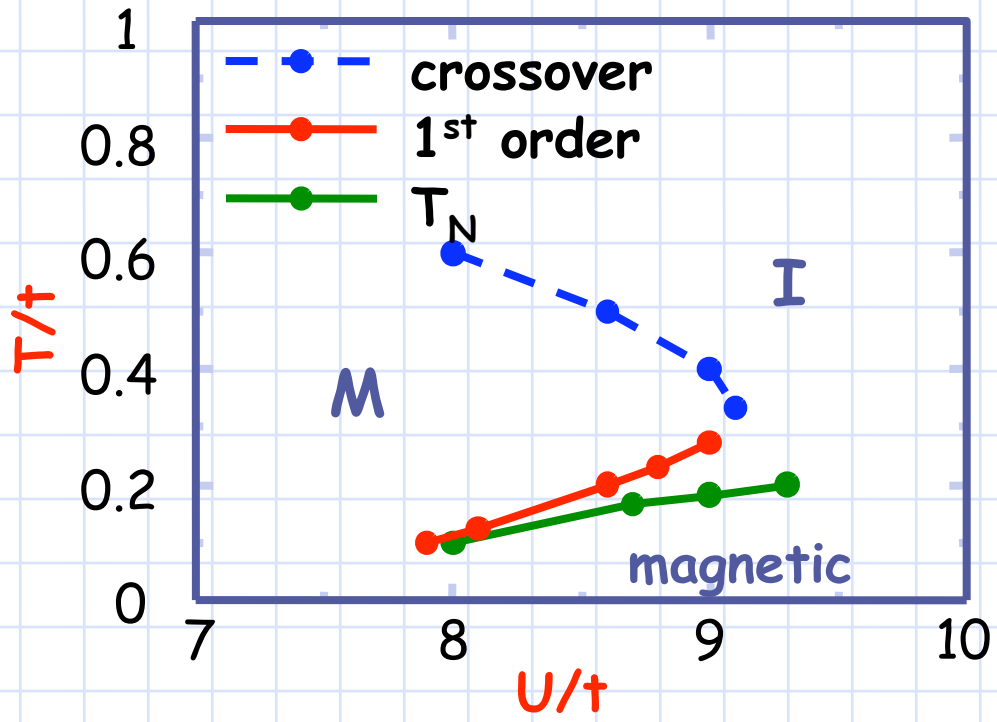


Comparison with organics

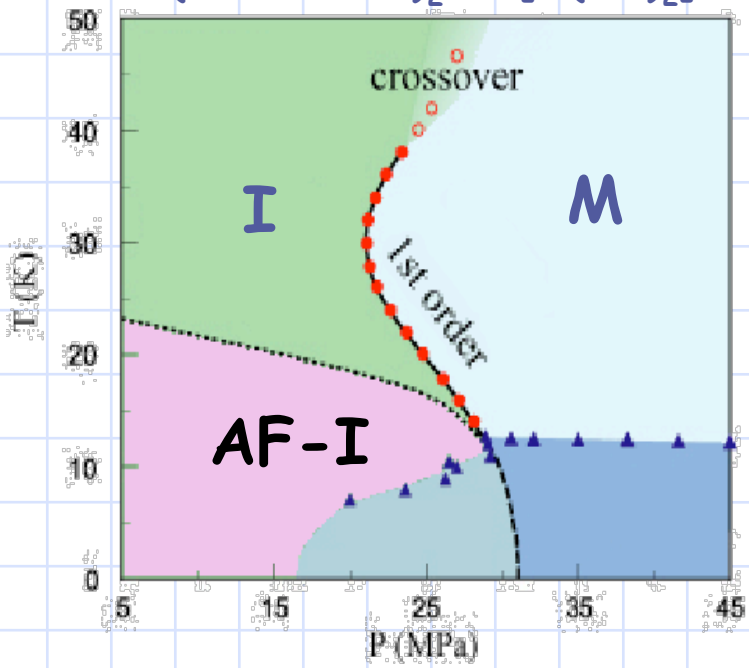
Cellular-DMFT →
- order at finite T
- stabilized by 3D

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

t'/t=0.8



κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

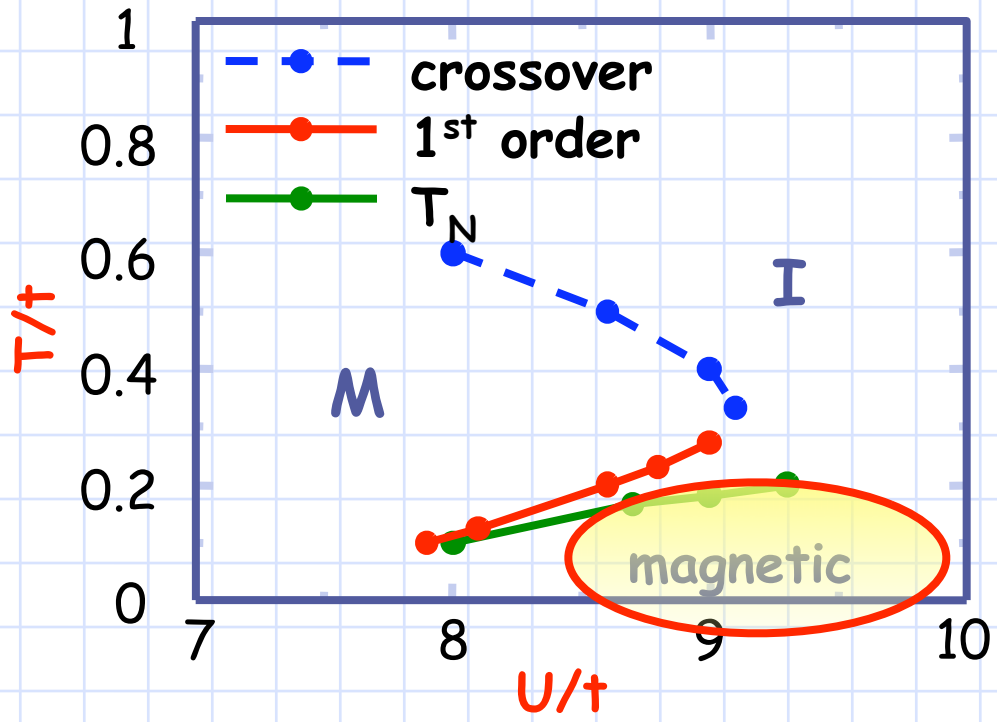


Comparison with organics

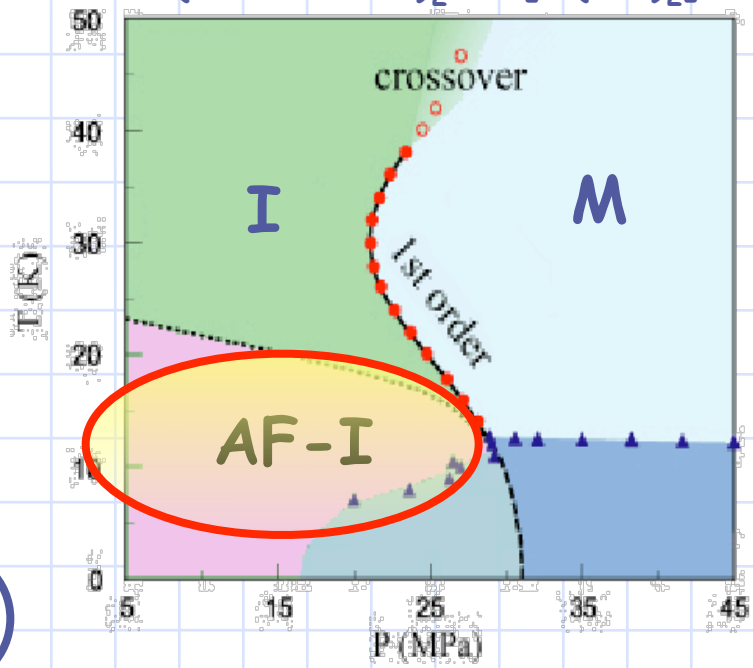
Cellular-DMFT →
- order at finite T
- stabilized by 3D

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

t'/t=0.8



κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



Consistent wit EXP.

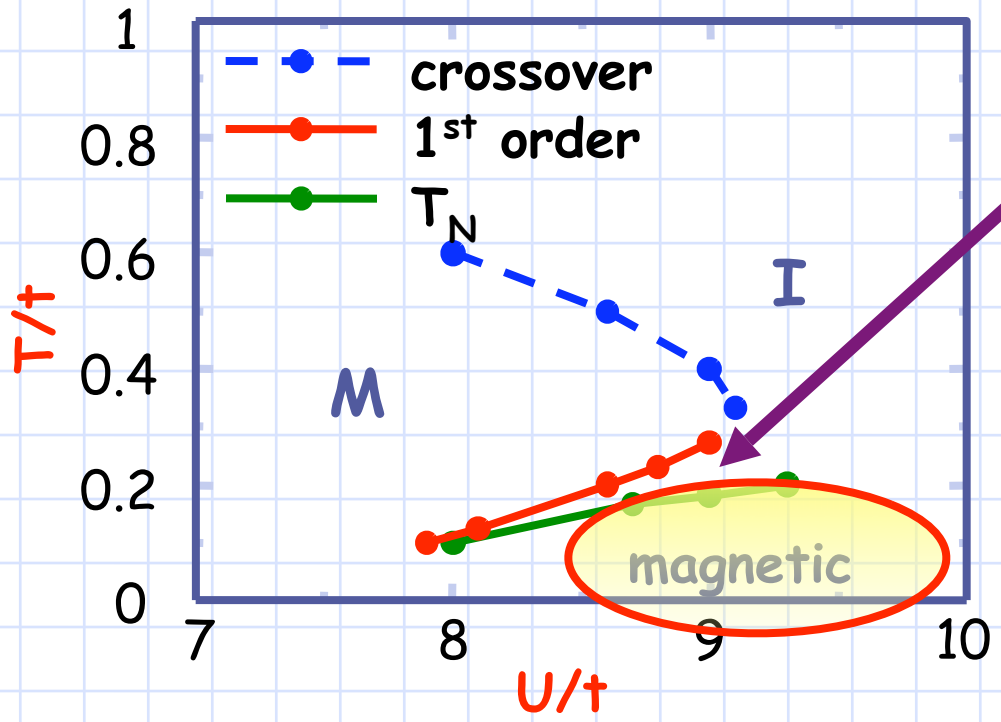
Comparison with organics

Nonmag insulator

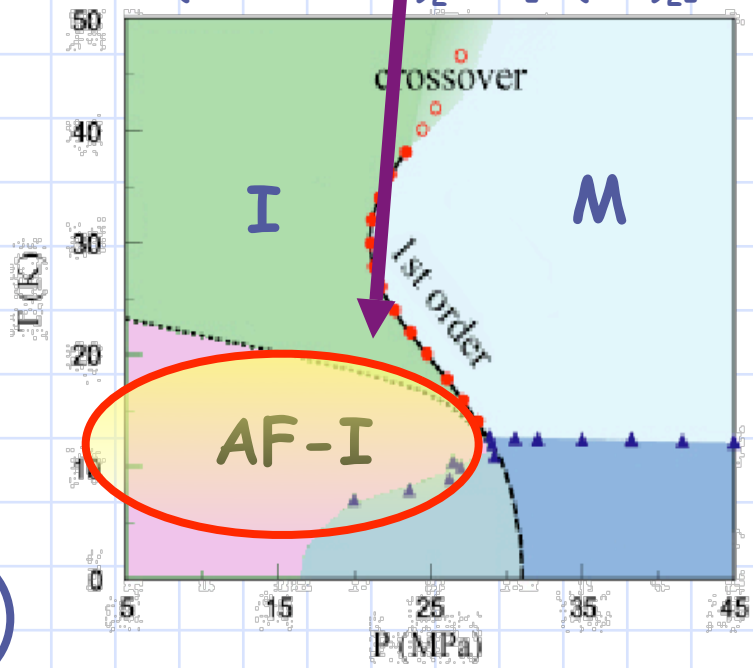
Cellular-DMFT →
- order at finite T
- stabilized by 3D

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

t'/t=0.8



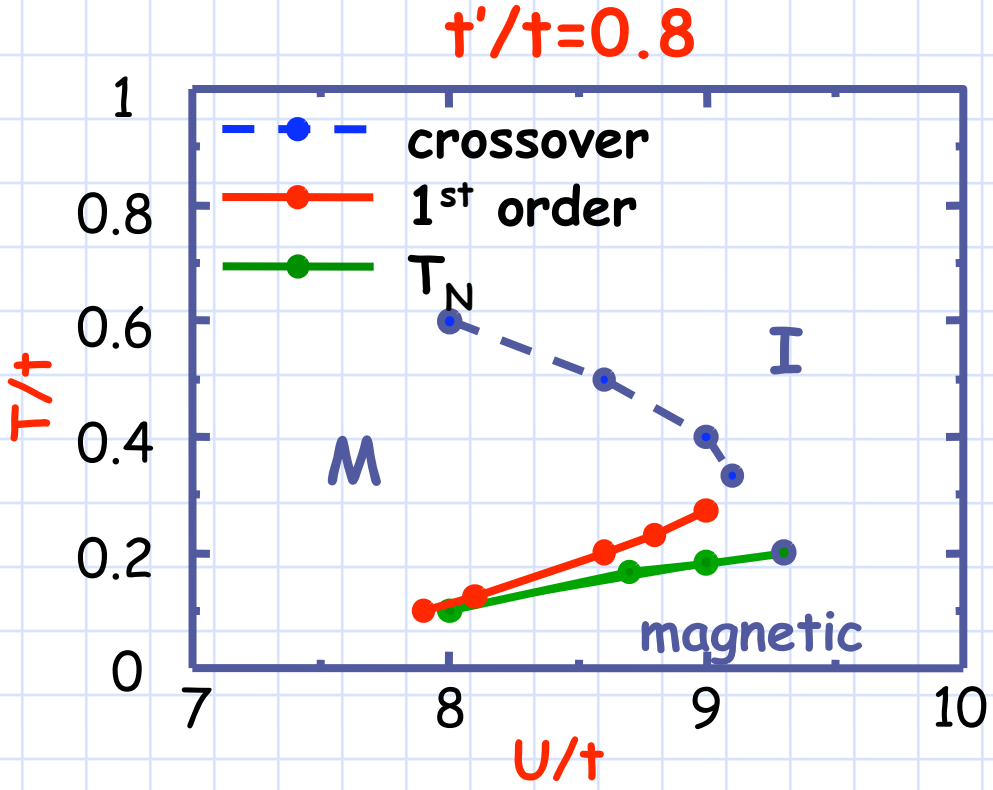
κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl



Consistent wit EXP.

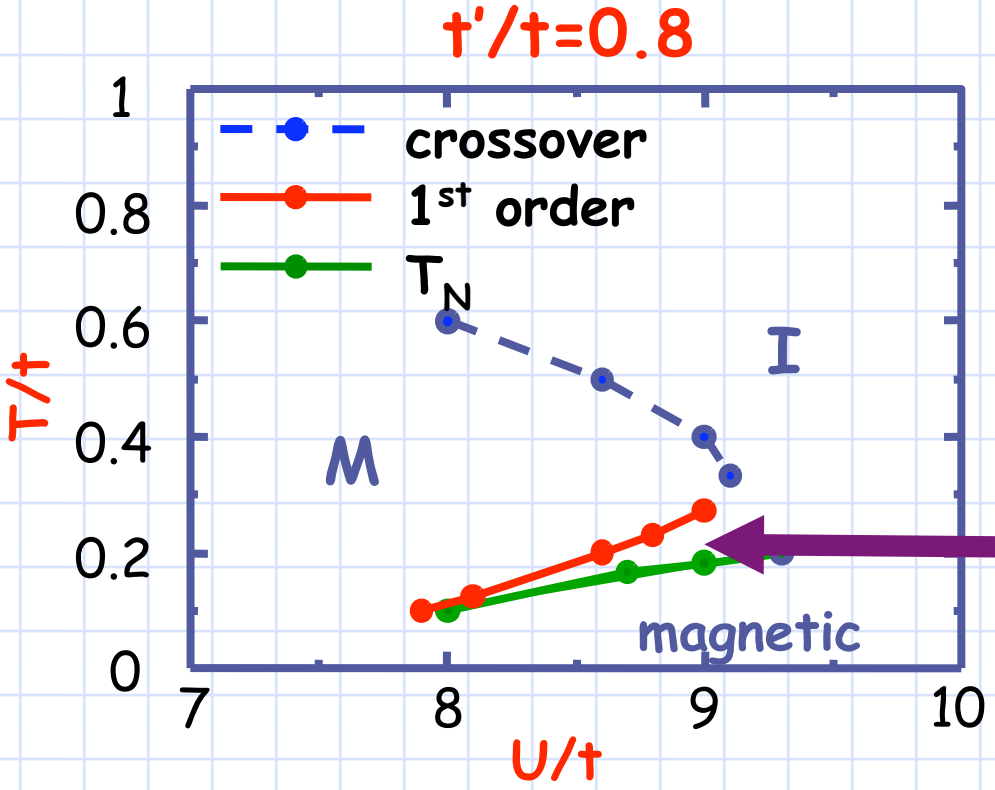
q-dependent susceptibility

Inherent in nonmagnetic insulator !

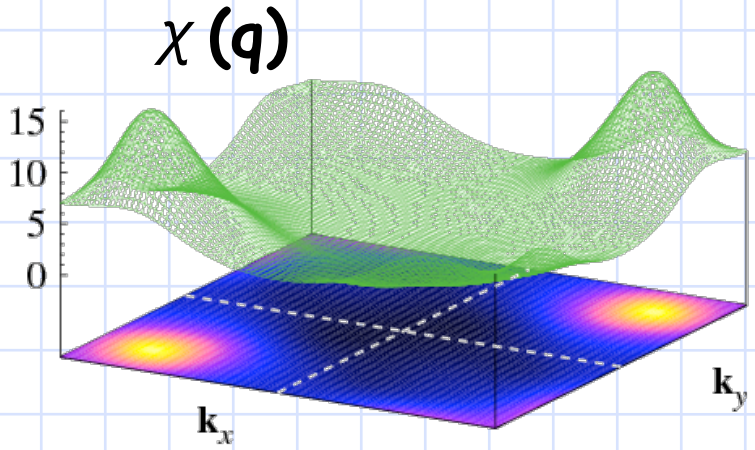


q-dependent susceptibility

Inherent in nonmagnetic insulator !



U/t=9, T/t=0.2



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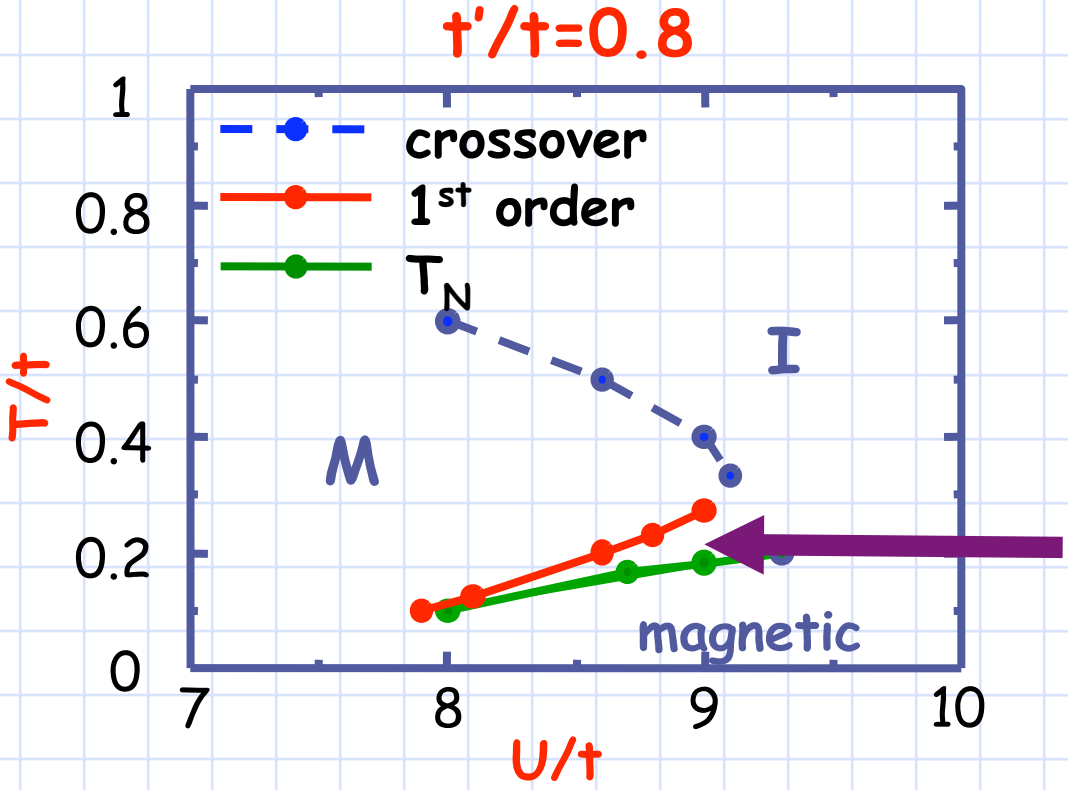
q-dependent susceptibility

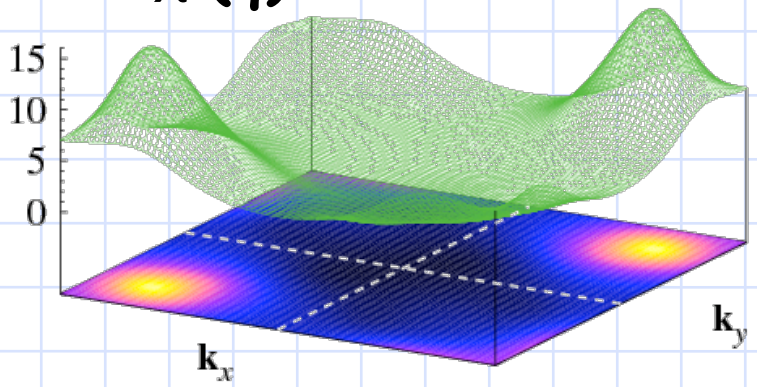
Inherent in nonmagnetic insulator !



U/t=9, T/t=0.2

Incommensurate

$\chi(q)$



- peak at $q \sim (0.75\pi, 0.75\pi)$
- not diverge

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Kyoto
November 14, 2007

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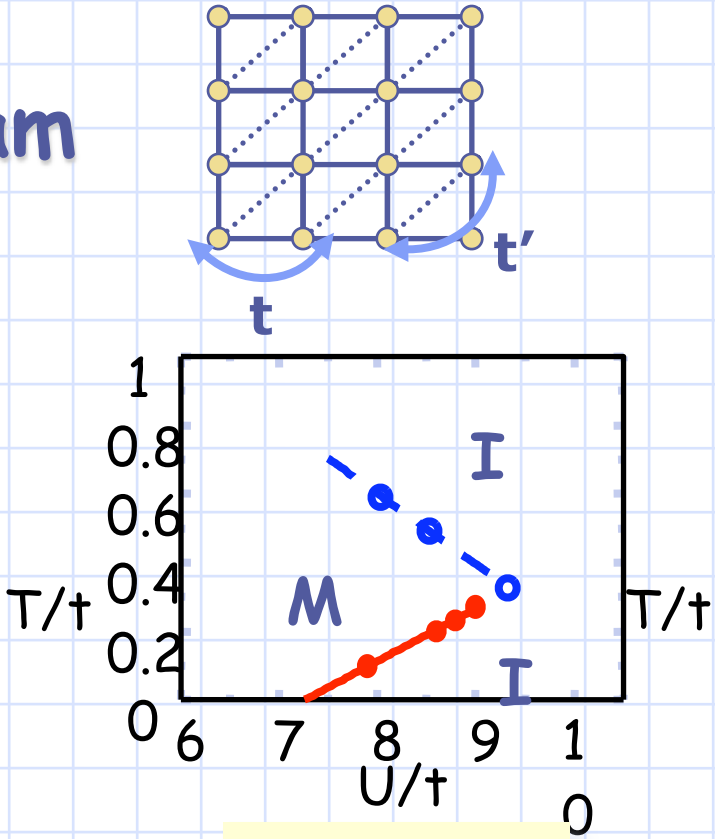
Kyoto
November 14, 2007

What happens ?

control frustration

by changing t'/t

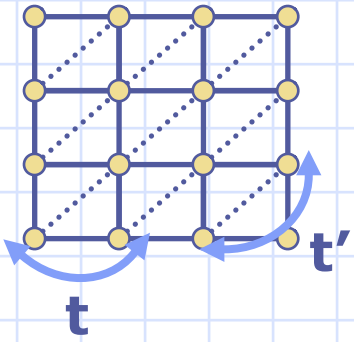
Phase diagram

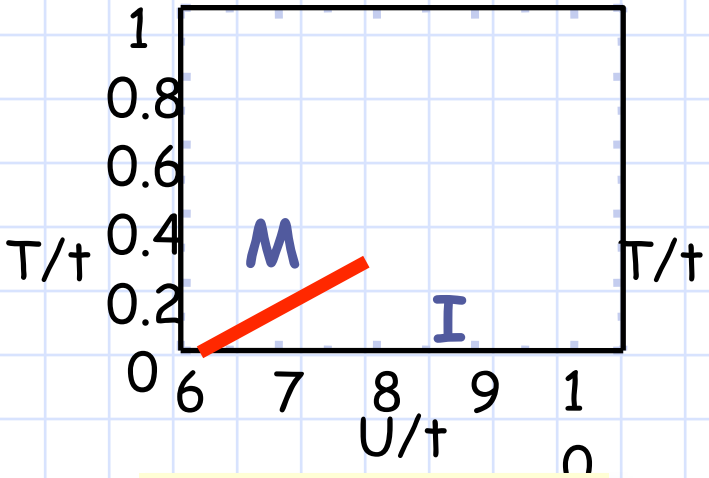


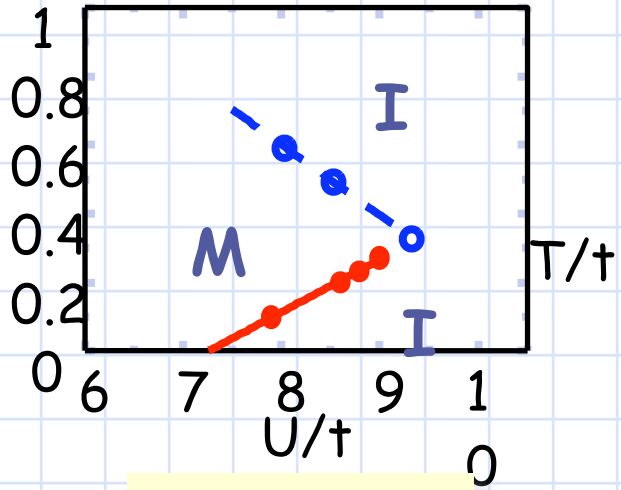
t'/t =0.8

Intermediate

Phase diagram







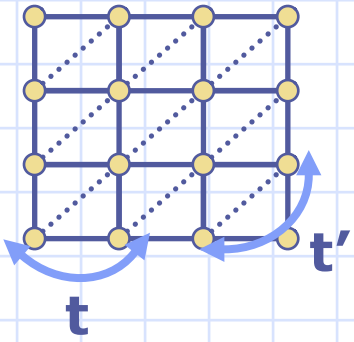
smaller t'/t

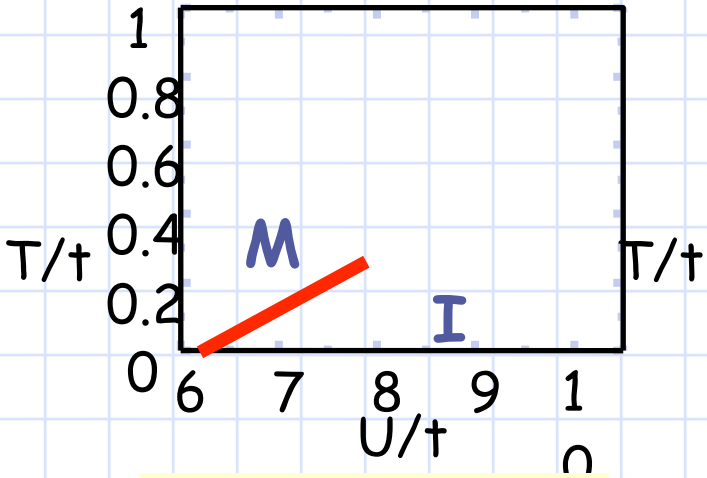
t'/t =0.8

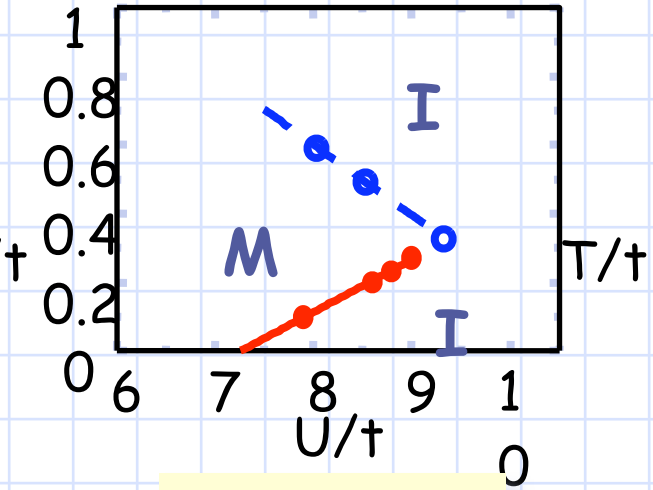
Weak frustration

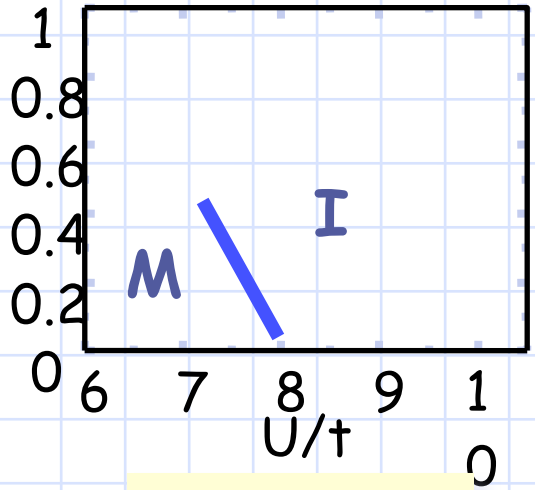
Intermediate

Phase diagram









smaller t'/t

t'/t =0.8

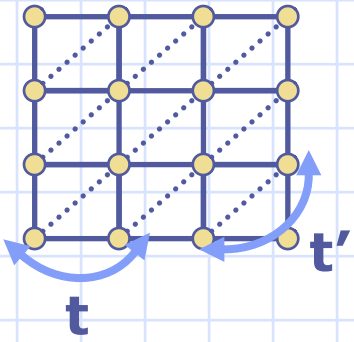
t'/t =1

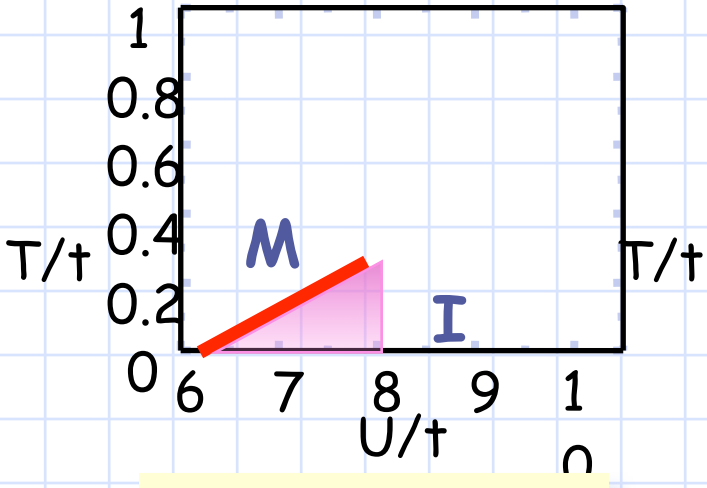
Weak frustration

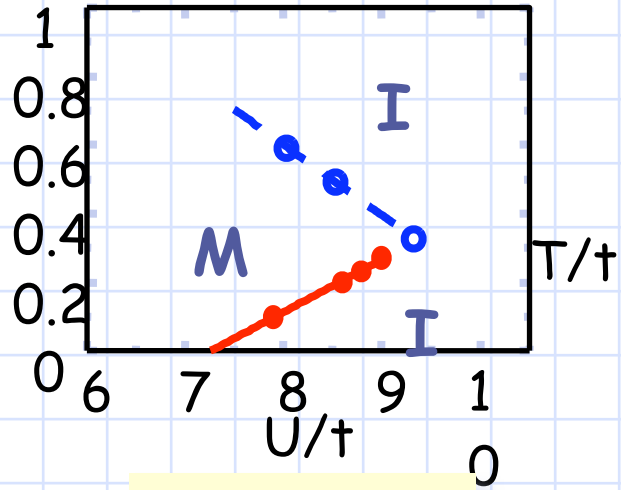
Intermediate

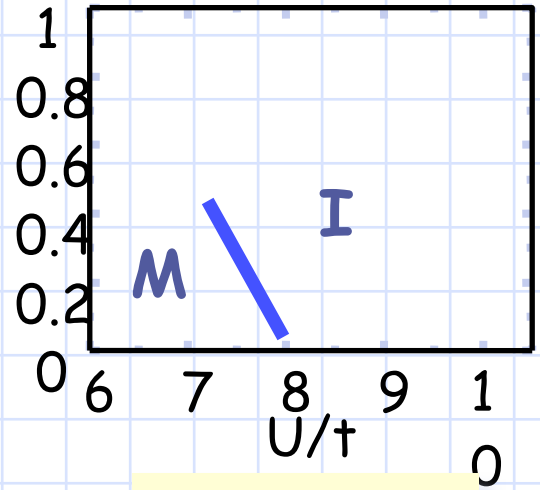
Strong frustration

Phase diagram









smaller t'/t

t'/t =0.8

t'/t =1

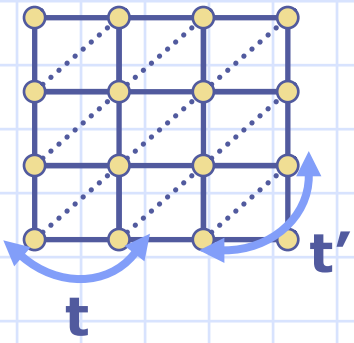
Weak frustration

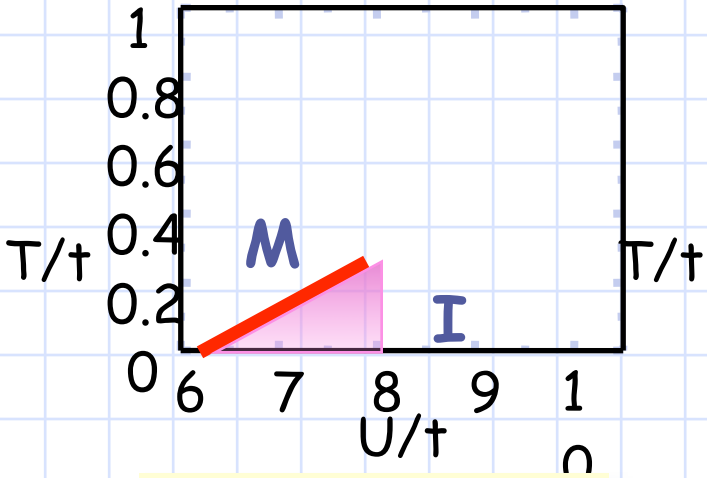
Intermediate

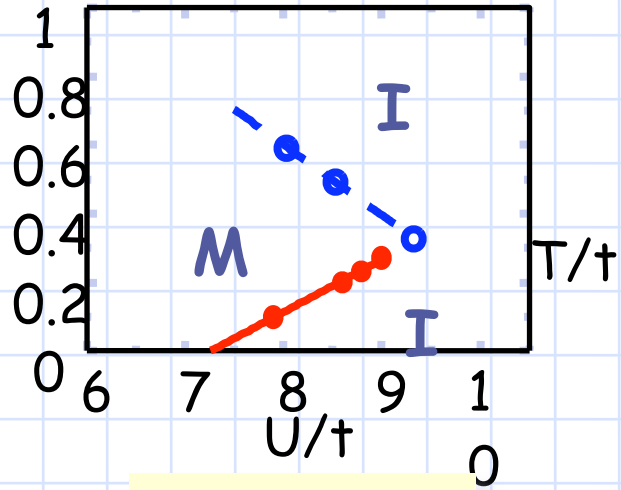
Strong frustration

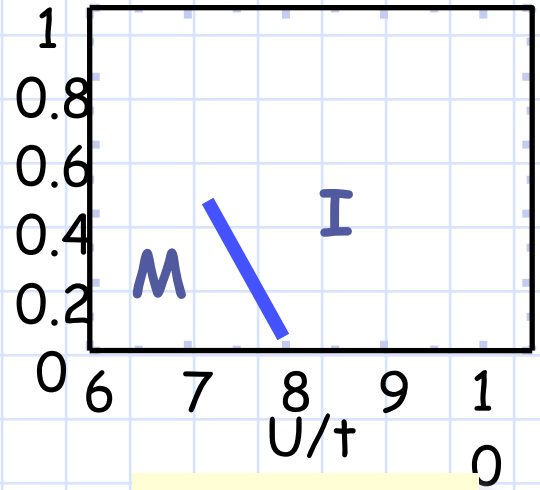
Magnetic order ?

Phase diagram









smaller t'/t

t'/t =0.8

t'/t =1

Weak frustration

Intermediate

Strong frustration

Magnetic order ?

Reentrant

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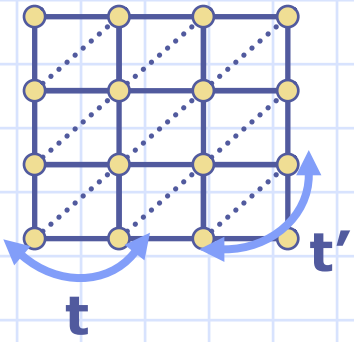
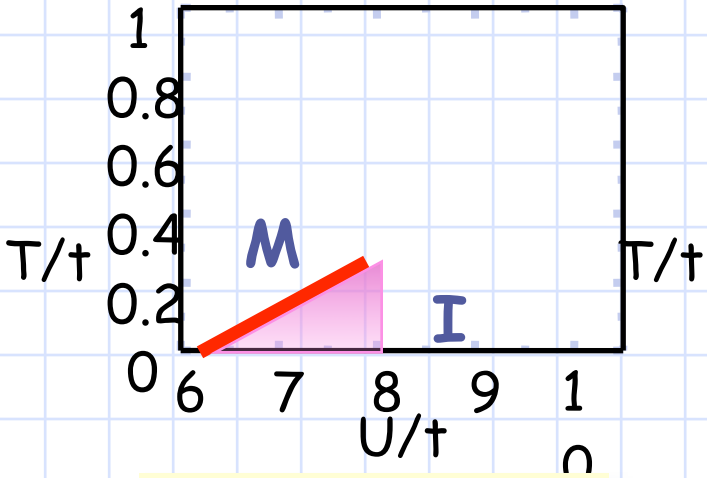
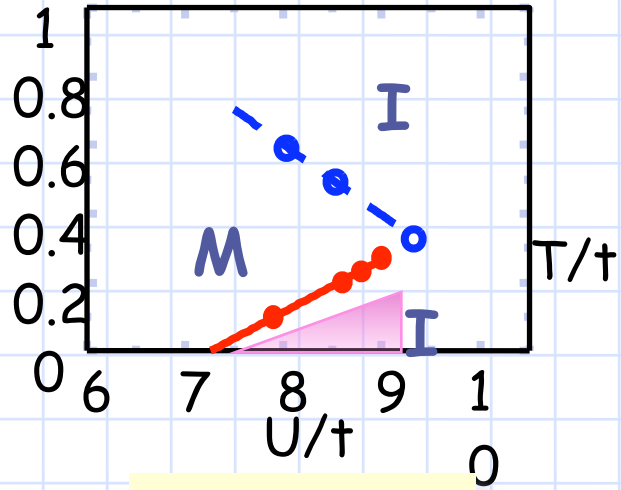
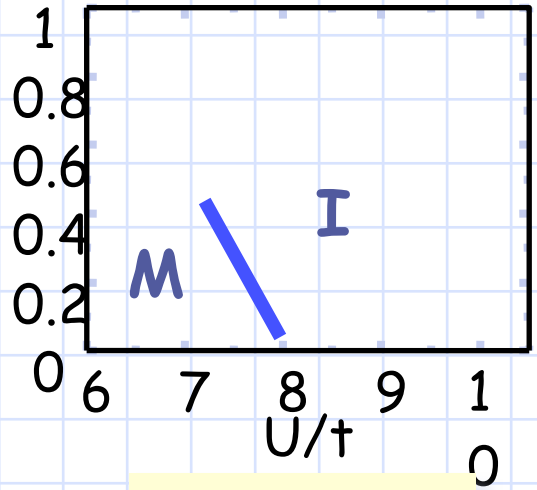
Phase diagram









smaller t'/t

t'/t =0.8

t'/t =1

Weak frustration

Intermediate

Strong frustration

Magnetic order ?

Reentrant

AF correlations at low T

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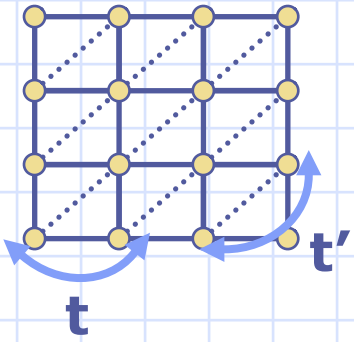
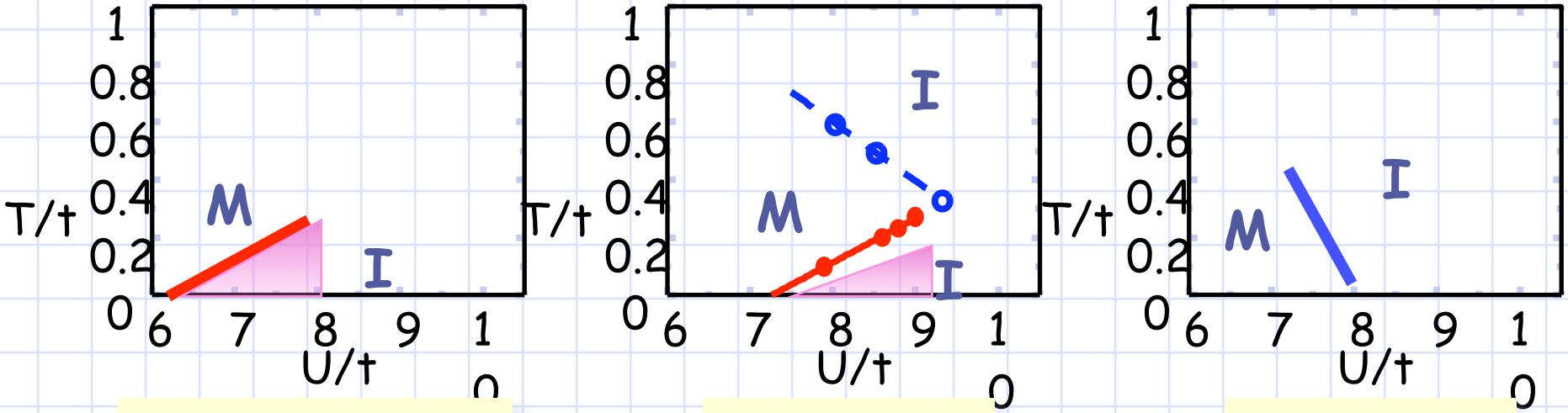
Phase diagram





smaller t'/t

t'/t =0.8

t'/t =1

Weak frustration

Magnetic order ?

Intermediate

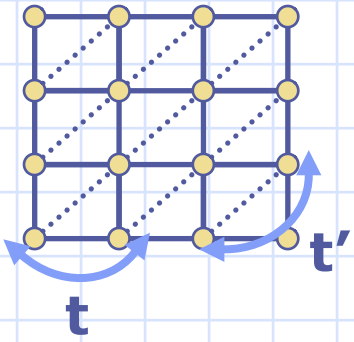
Reentrant

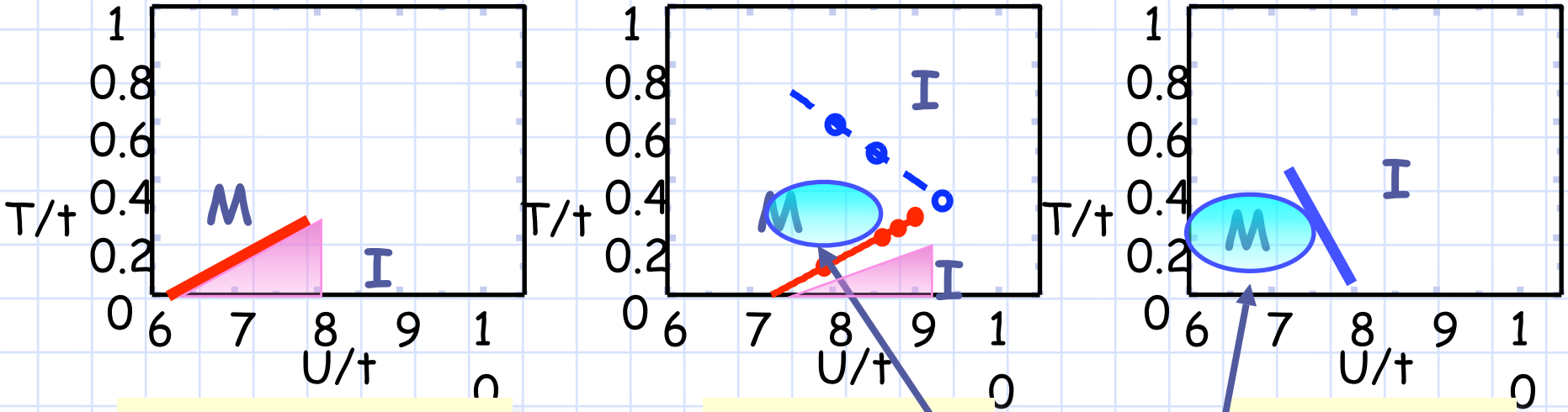
AF correlations at low T

Strong frustration

Non-monotonic T-dependence

Phase diagram





smaller t'/t

t'/t =0.8

t'/t =1

Weak frustration

Intermediate

Strong frustration

Magnetic order ?

Reentrant

AF correlations at low T

Non-monotonic T-dependence

Frustration-induced heavy electrons

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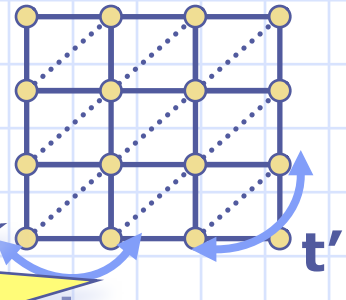
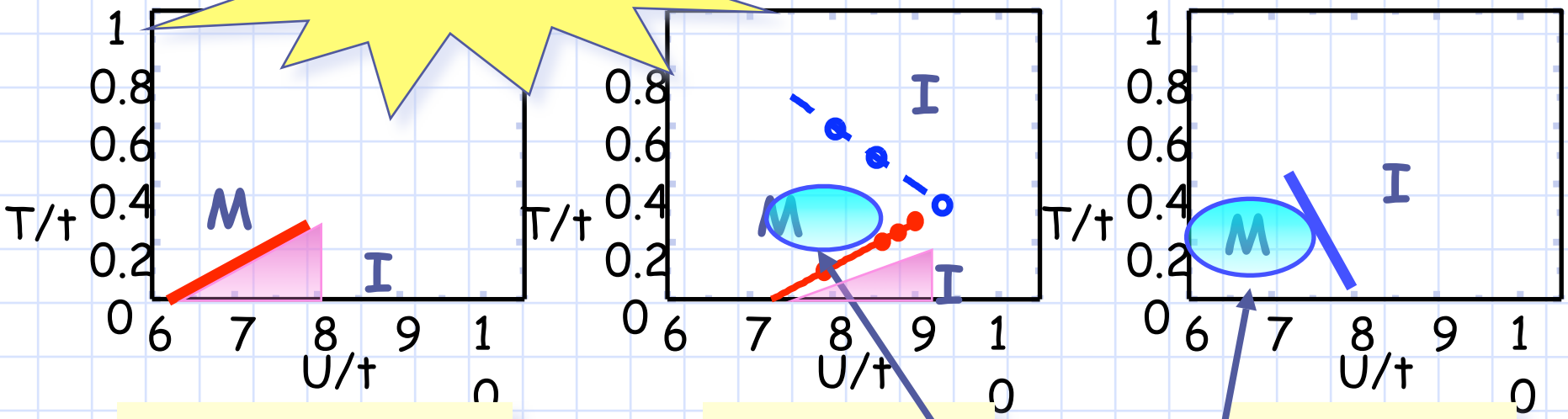
Phase diagram



Universal feature



smaller t′/t

t′/t =0.8

t′/t =1

Weak frustration

Intermediate

Strong frustration

Magnetic order ?

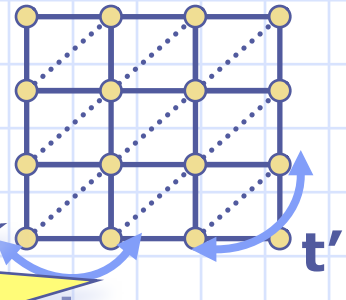
Reentrant

AF correlations at low T

Non-monotonic T-dependence

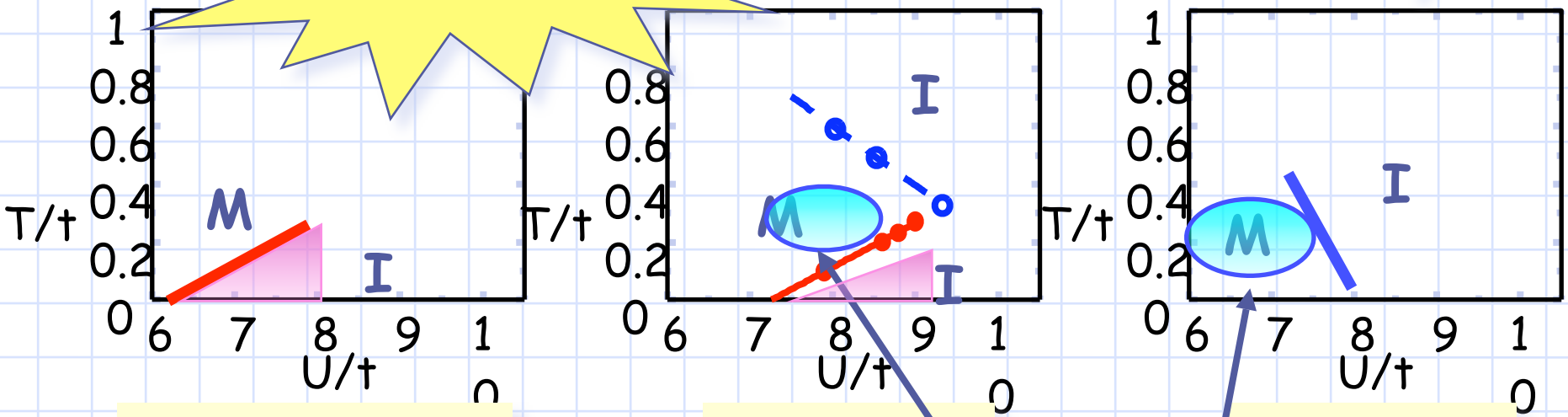
Frustration-induced heavy electrons

Phase diagram



Universal feature

Similar to Kagome



smaller t'/t

t'/t =0.8

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Weak frustration

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Strong frustration

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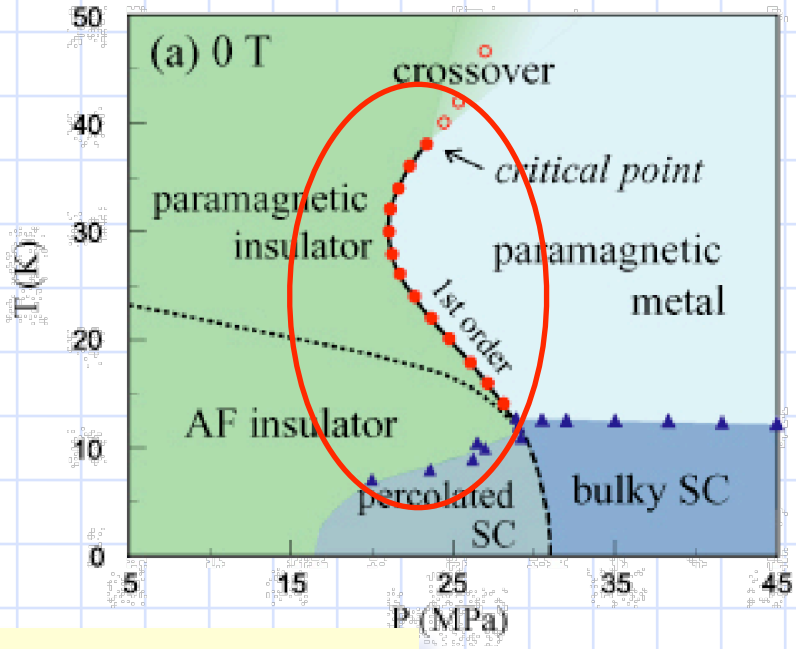
Frustration-induced heavy electrons

κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

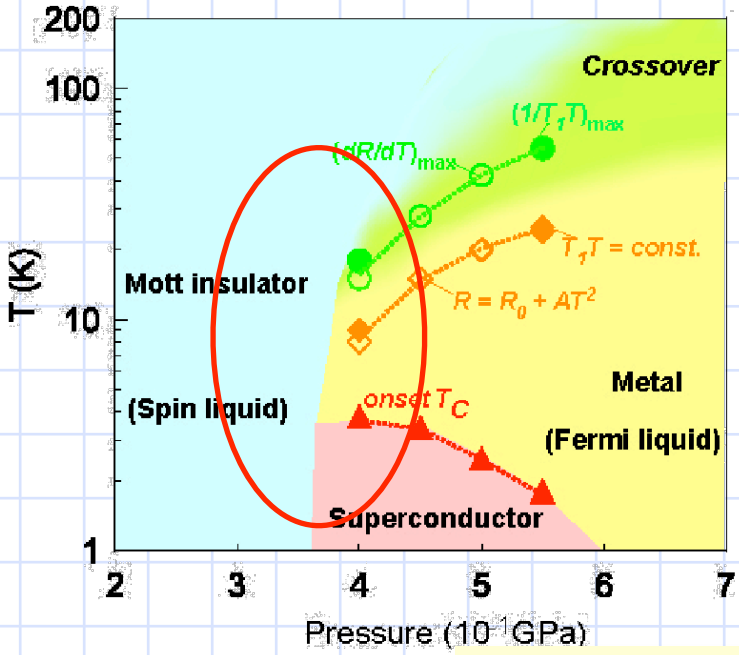
F. Kagawa et al., PRB 69, 064511 (2004)



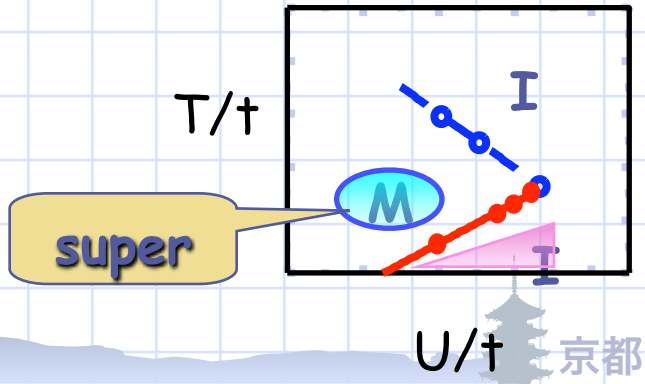
t'/t =0.75

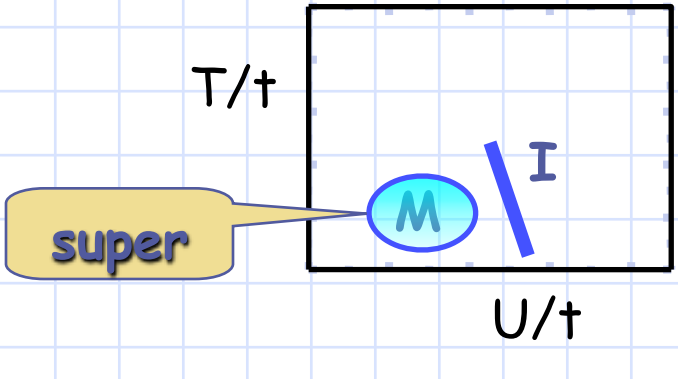
κ-(BEDT-TTF)$_2$-Cu$_2$(CN)$_3$

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



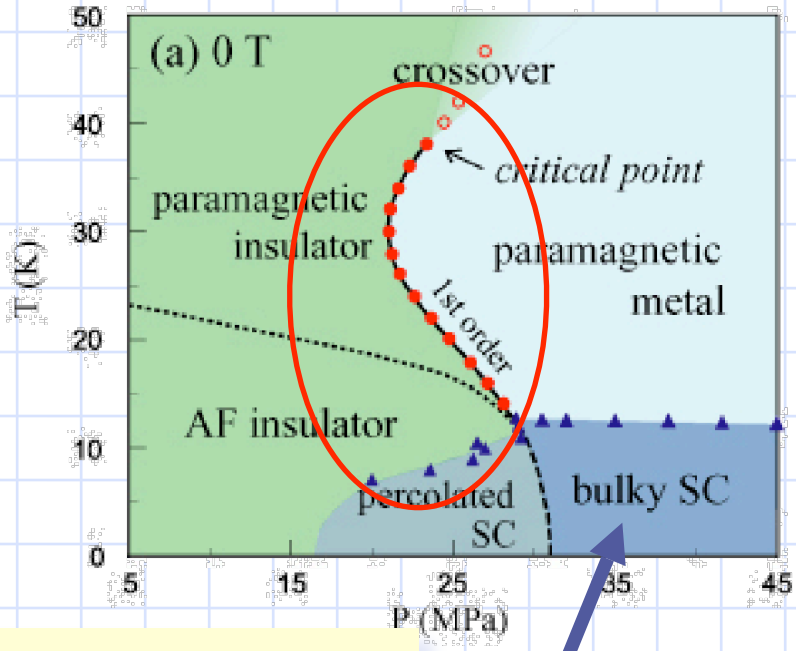
t'/t =1.06





κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

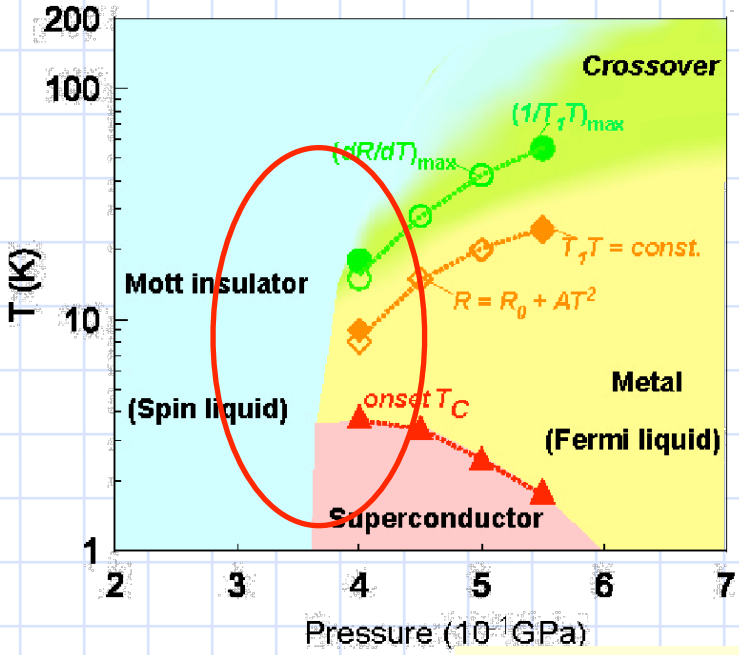
F. Kagawa et al., PRB 69, 064511 (2004)



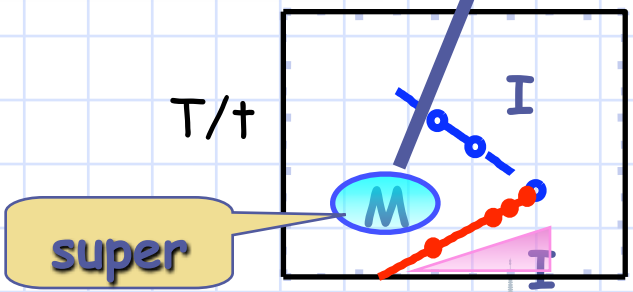
t'/t =0.75

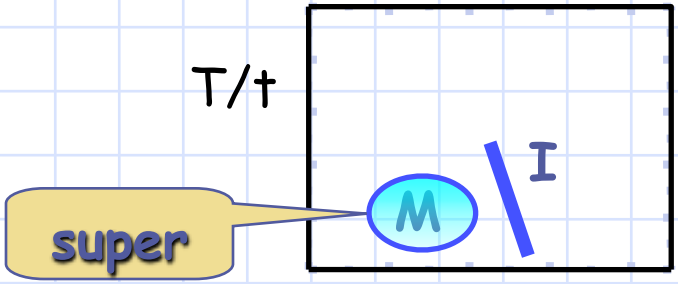
κ-(BEDT-TTF)$_2$-Cu$_2$(CN)$_3$

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



t'/t =1.06





κ-(BEDT-TTF)$_2$-Cu[N(CN)$_2$]Cl

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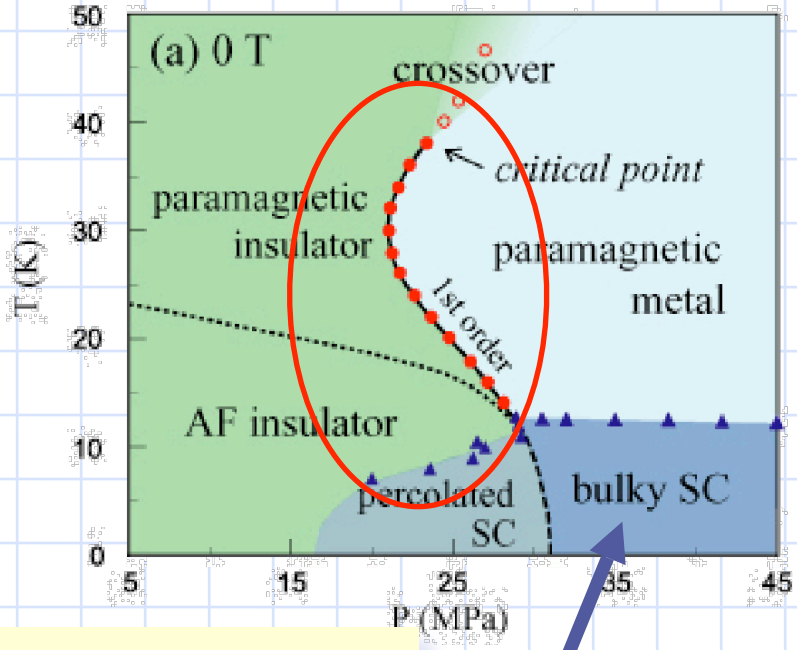
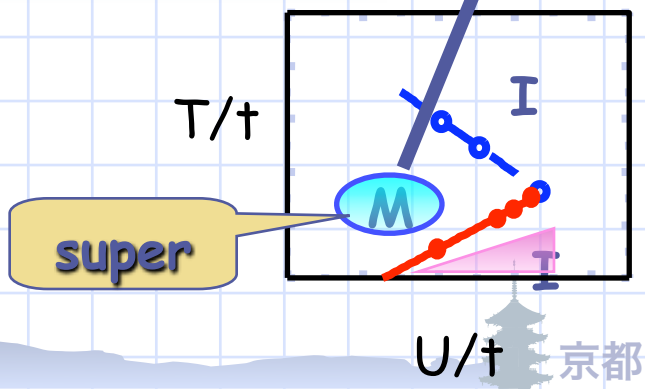
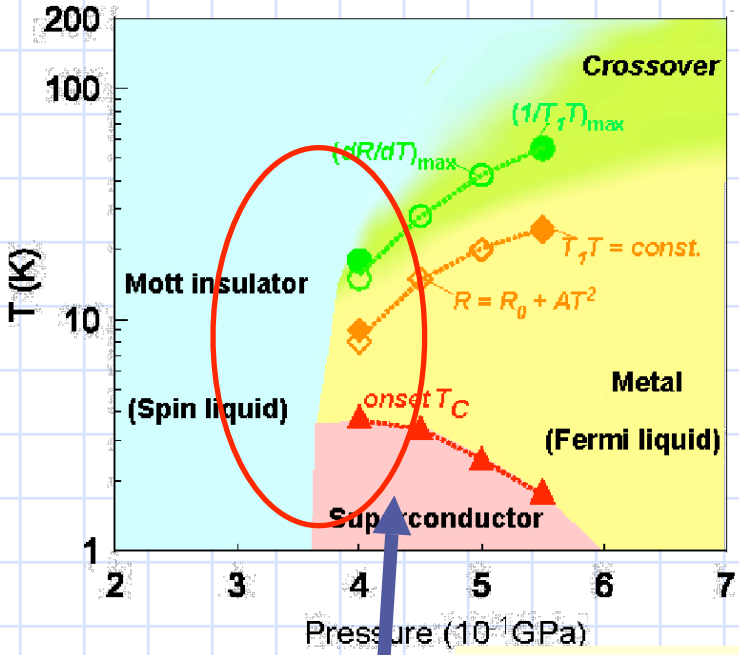


t'/t =0.75

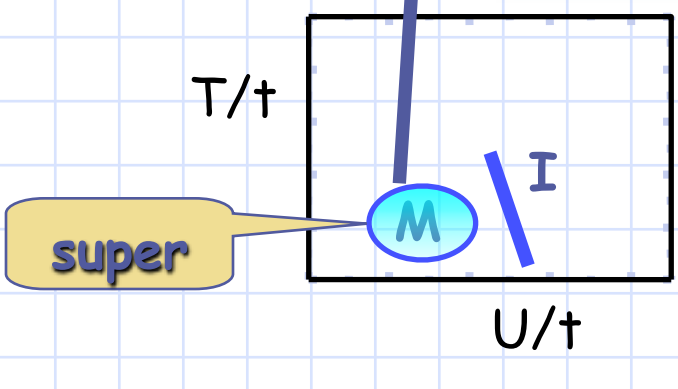


κ-(BEDT-TTF)$_2$-Cu$_2$(CN)$_3$

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



t'/t =1.06

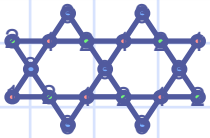


Summary

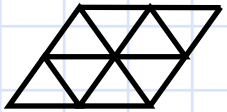
Mott transitions: frustrated systems

Hubbard model

Kagome



Triangular



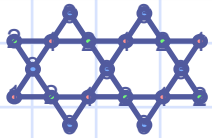
Anomalous behavior near MIT (finite T)

Summary

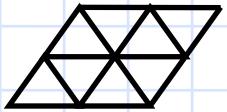
Mott transitions: frustrated systems

Hubbard model

Kagome



Triangular



Anomalous behavior near MIT (finite T)

1. Strong frustration

   Frustration-induced heavy electrons

2. Intermediate frustration

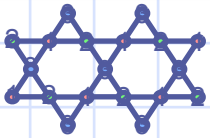
   Reentrant behavior

Summary

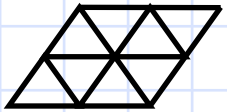
Mott transitions: frustrated systems

Hubbard model

Kagome



Triangular



Anomalous behavior near MIT (finite T)

Common

1. Strong frustration

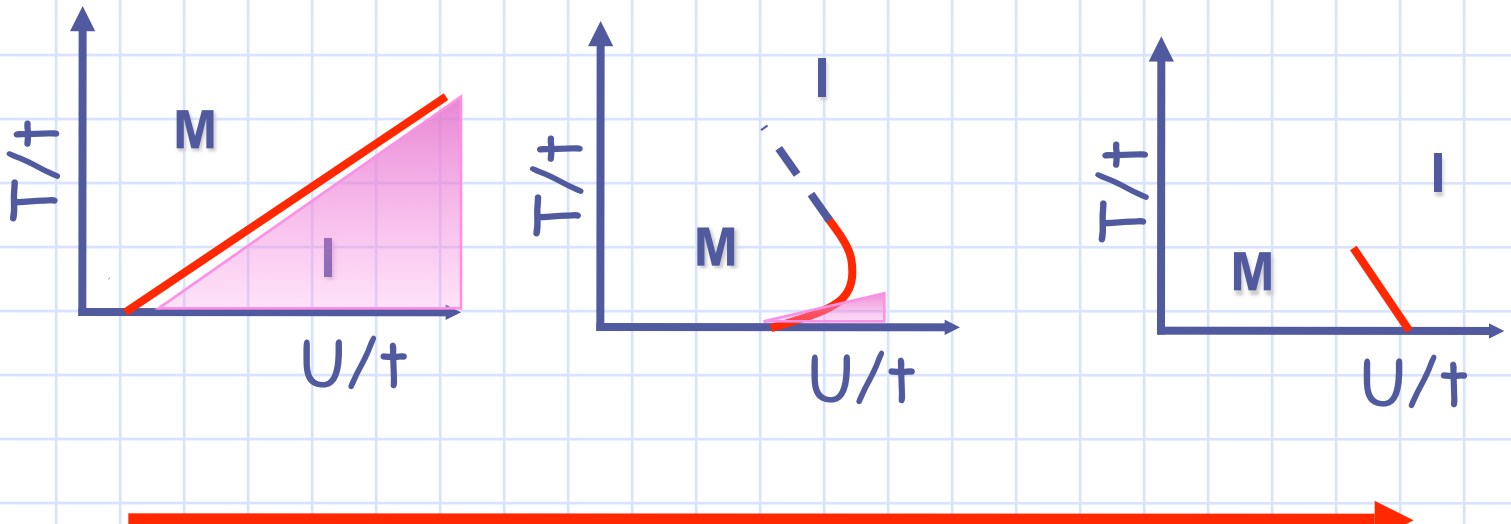
   Frustration-induced heavy electrons

2. Intermediate frustration

   Reentrant behavior

Generic features !?

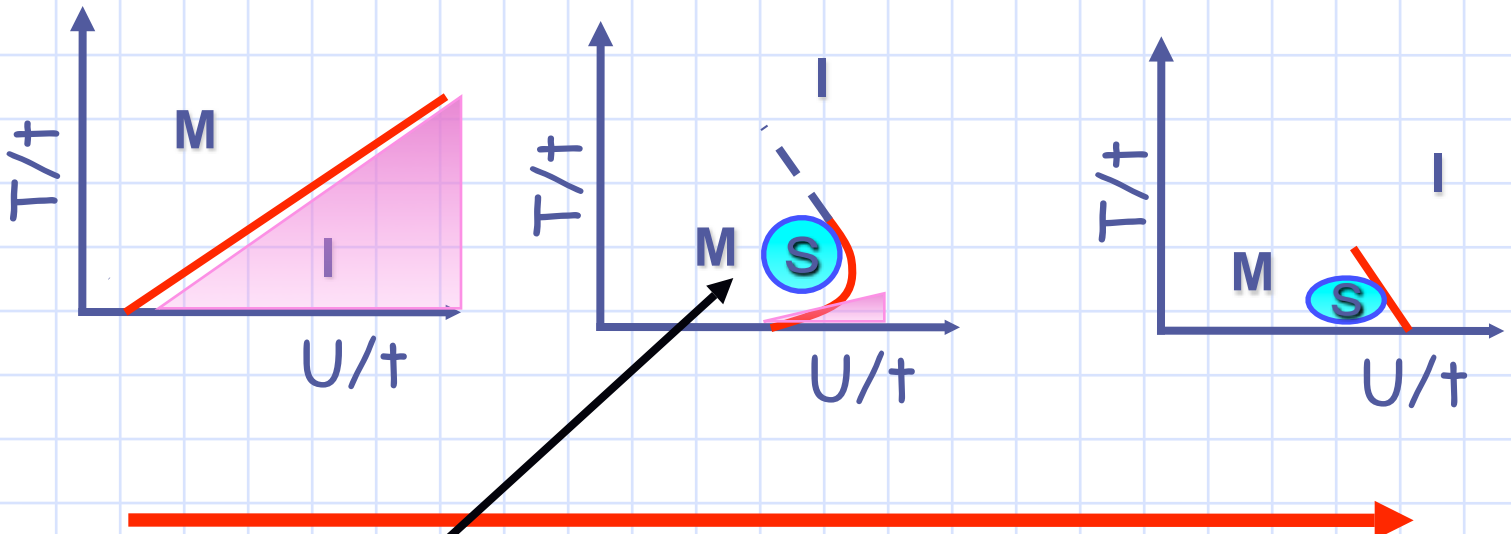
correlations
frustration
Quantum fluctuations



Frustration

Generic features !?

correlations
frustration
Quantum fluctuations



Moderately
high Tc

YKIS 07
Kyoto
November 14, 2007

Thank you for your attention !