EXOTIC PHASES OF FRUSTRATED SYSTEMS

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Superclean materials/systems

- Superclean materials/systems provide a chance of novel exotic phases otherwise masked by disorders
- Frustrated systems are a good play ground where various exotic quantum phases are realized
- Examples of novel exotic phases include
  (1) spin liquid, also paramagnetic insulating phase
  (2) hidden order (multipole orders …)
- Superclean materials/systems are a good starting point to investigate impurity effects
  -- impurities are interesting, because their effects provide information on bulk properties

Main Achievements in PSM Project

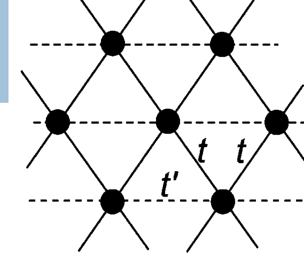
- Mott metal-insulator transition and exotic 1D spin correlation in Kagome Hubbard model
  [Ohashi, Kawakami, and Tsunetsugu, PRL 97, 066401 (2006)]
- ✔ Reentrant metal-insulator transition in the Hubbard model on anisotropic triangular lattice
  [Ohashi, Momoi, Tsunetsugu, and Kawakami, PRL 100, 076402 (2008)]
- Dislocations and vortices in Pair-Density-Wave superconductors
  [Agterberg and Tsunetsugu, Nature Phys. 4, 639 (2008)]
- Spin nematic order in S=1 bilinear-biquadratic model
  [Tsunetsugu and Arikawa, J. Phys. Soc. Jpn. 75, 083701 (2006)]
- ✔ Magnon-pair condensation and spin nematic state in frustrated spin system including ferromagnetic exchanges
  [Tsunetsugu and Zhitomirsky, in preparation]
- Impurity effects in spin nematic state
  [Takano and Tsunetsugu, in preparation]

Mott Transition in Anisotropic Triangular-Lattice Hubbard Model

- Phase Boundary Topology
- Heavy Quasiparticles

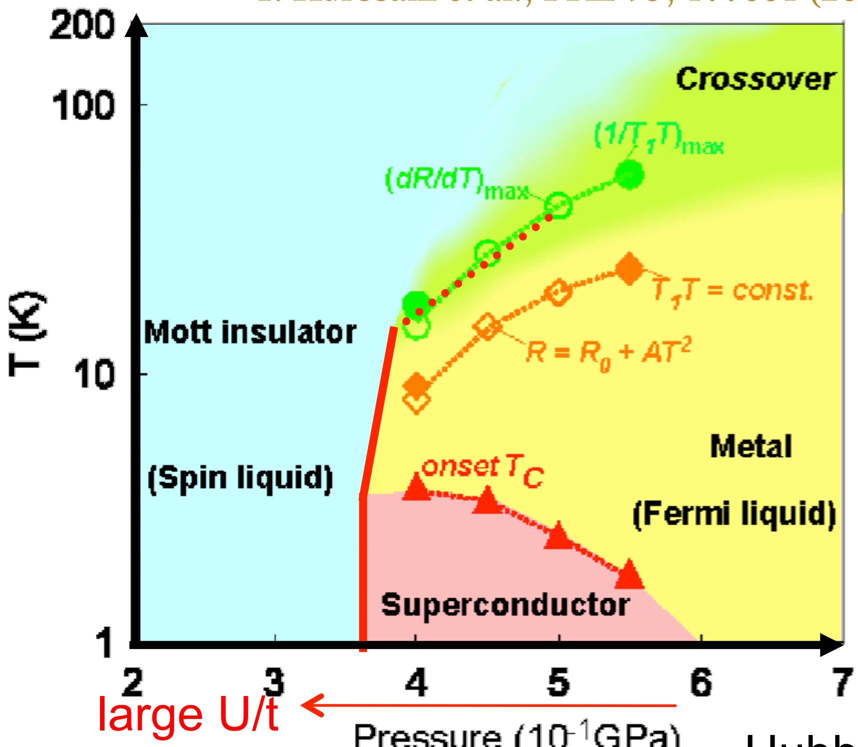
[Ohashi, Momoi, Tsunetsugu, and Kawakami, PRL **100**, 076402 (2008)]

Mott transition in κ-type organic materials

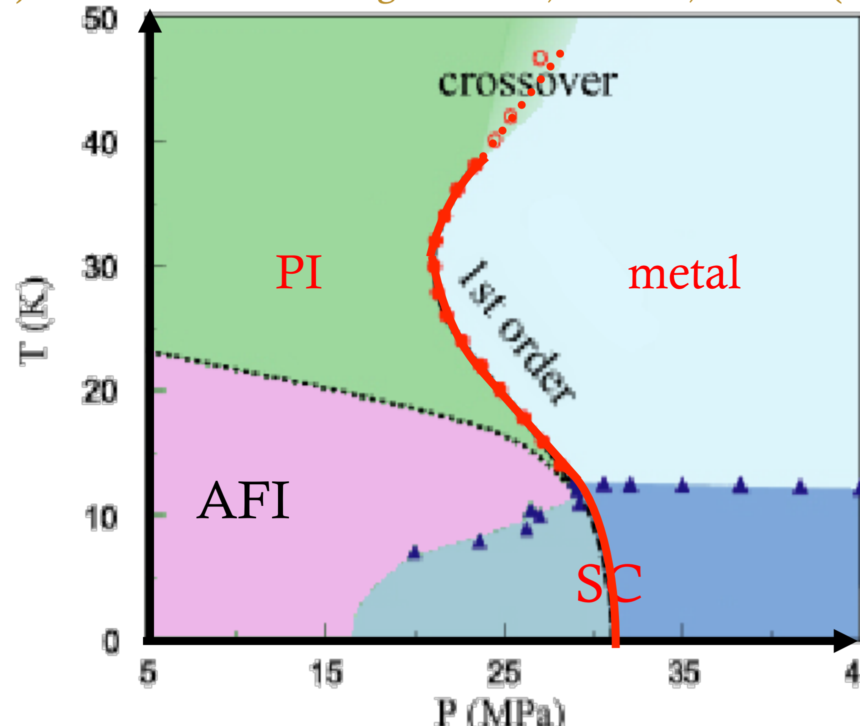


The shape of metal-insulator transition line is quite different between strongly frustrated system and less frustrated systems.

STRONG frustration
nearly perfect regular triangle
κ-$(ET)_2$-$Cu_2(CN)_3$ t'/t=1.06
Y. Kurosaki et al., PRL 95, 177001 (2005)



MODERATE frustration
distorted towards square
κ-$(ET)_2$-Cu$[N(CN)_2]$Cl t'/t=0.75
F. Kagawa et al., PRB 69, 064511 (2004)



Hubbard model

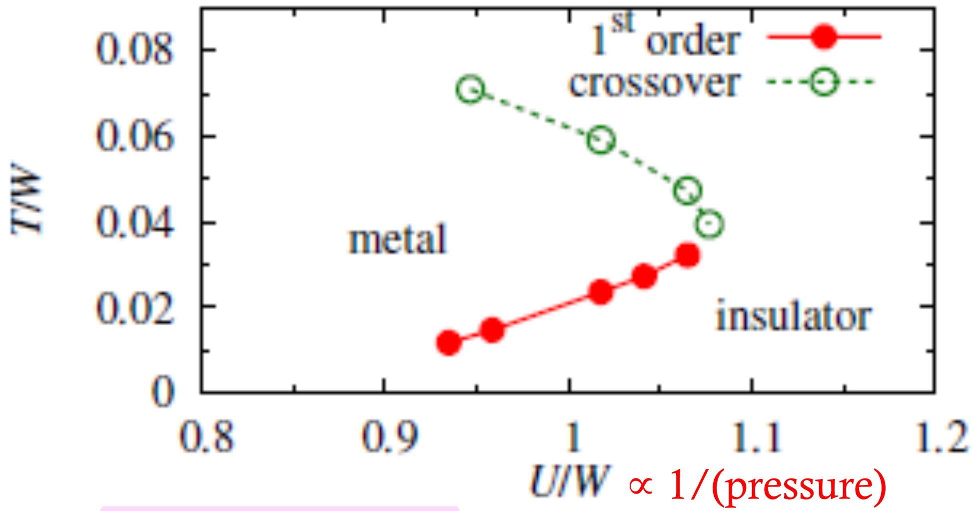
$$H = \sum_{\langle i,j\rangle,\sigma} \left(t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \mathrm{H.\,c.}\right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

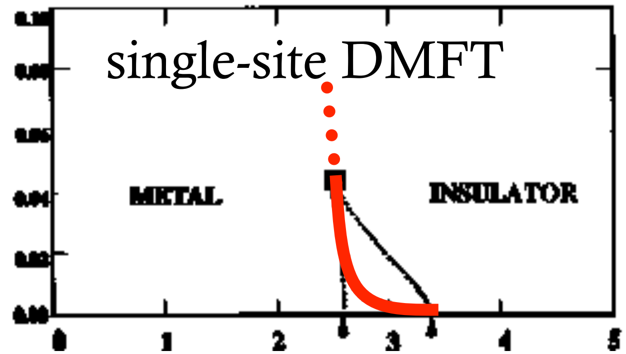
Insulator-metal-insulator reentrant transitions

U-T Phase Diagram (cluster dynamical mean-field theory)

$t'/t=0.8$ band width: W=8.45t

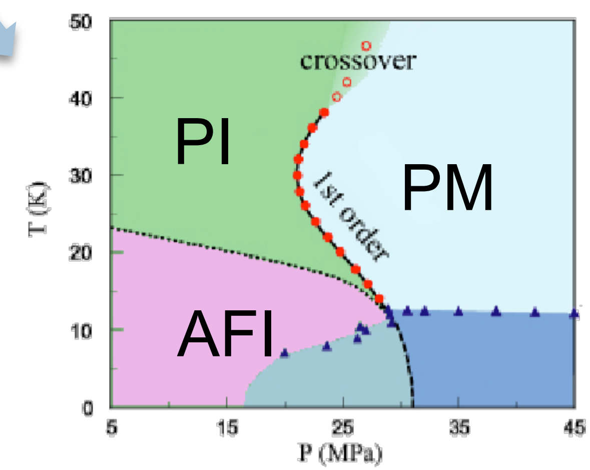
short-range spatial correlations are essential





Reentrant !!

consistent



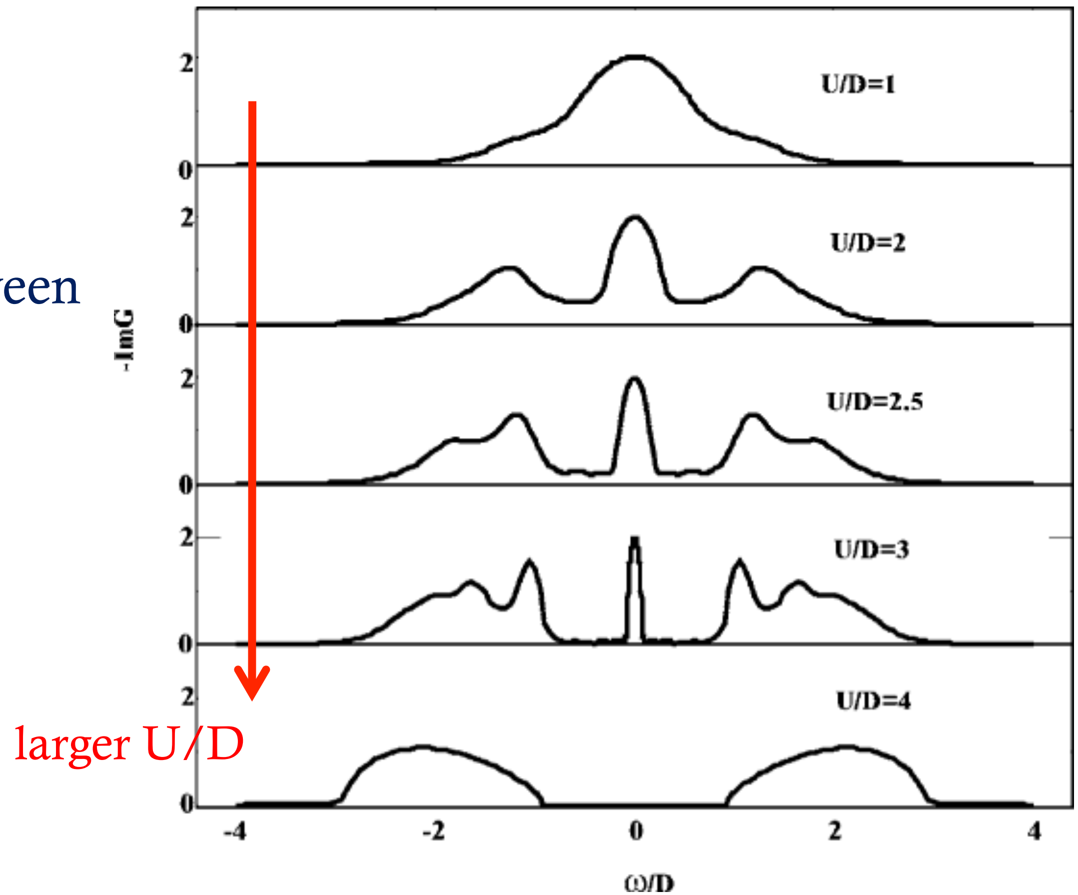
large U/t ←

Determined from the double occupancy data, the phase diagram shows a reentrant behavior of metal-insulator transition/ crossover.
This is qualitatively consistent with the experiment on κ-$(ET)_2$-Cu$[N(CN)_2]$Cl.

Mott transition – single site DMFT picture

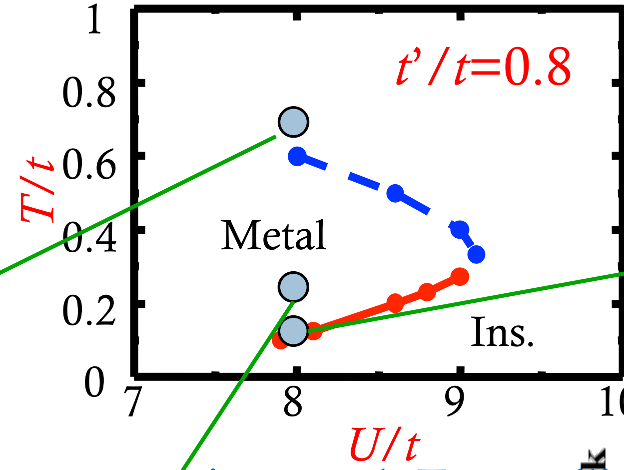
Mott transition is driven by transfer of spectral weight between high-energy Mott band and low-energy quasiparticle band

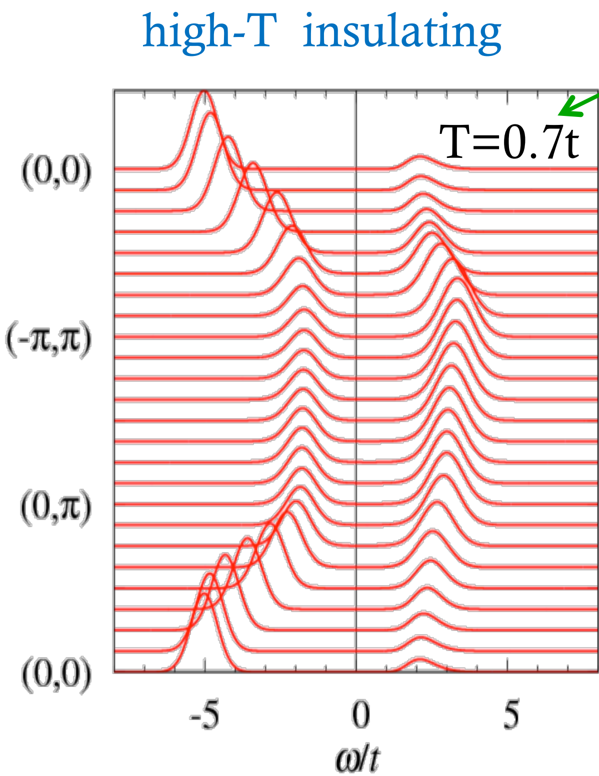
local electron spectral function $-\mathrm{Im}\, G$



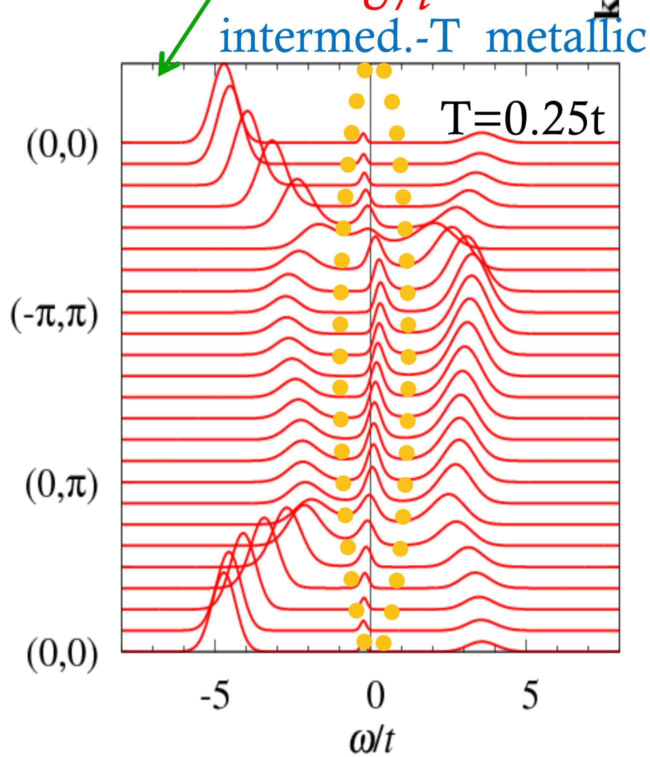
[Zhang, Rosenberg, and Kotliar, PRL, 1993]

Electron Spectral Function $A_k(\omega)$: reentrant behavior

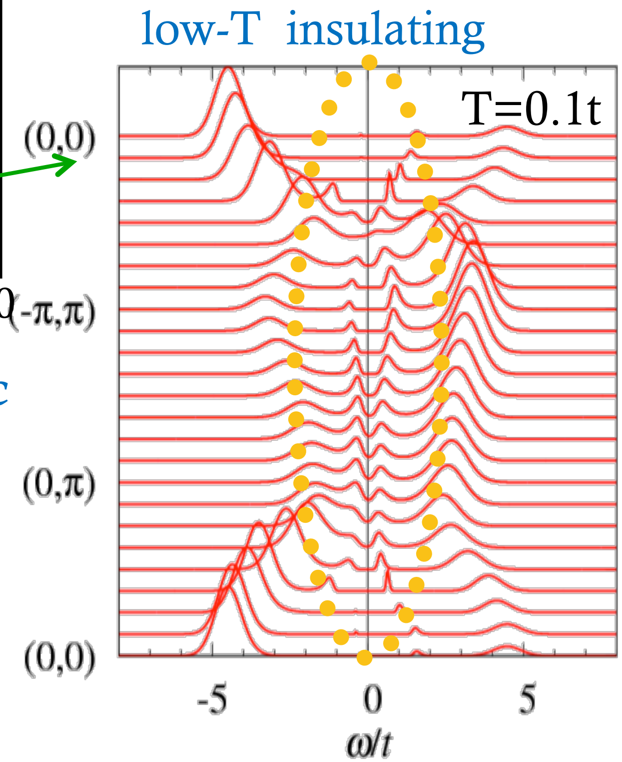




- no low-ω quasiparticles
- Hubbard gap



- sharp quasiparticle peaks appear inside the Mott gap



- quasiparticle peak splits
- different from high-T insulating phase

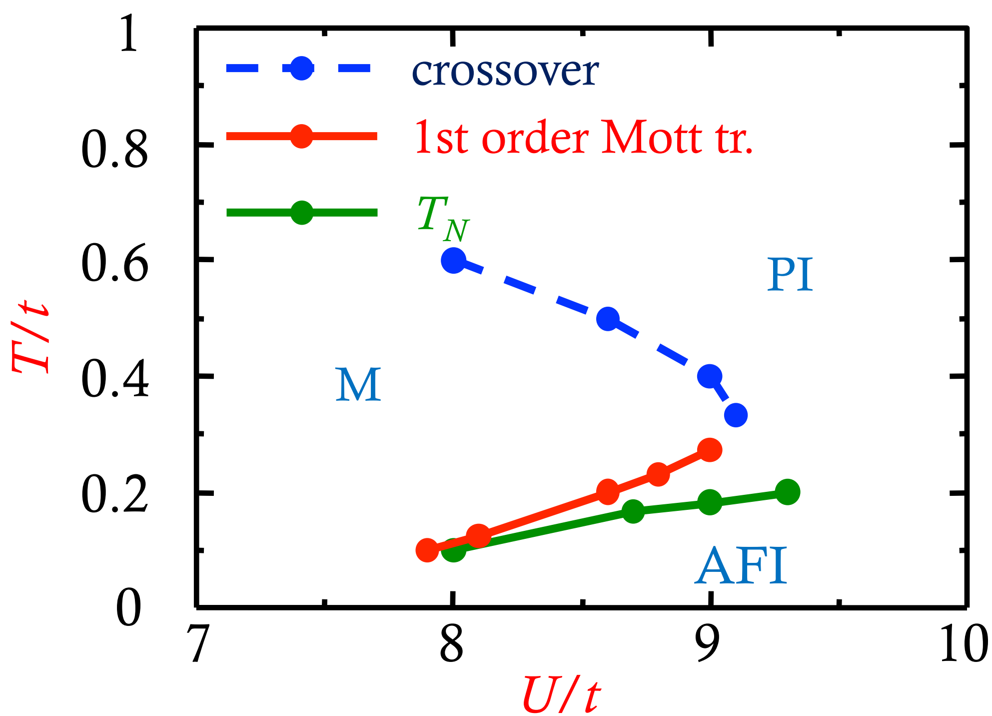
Magnetic order

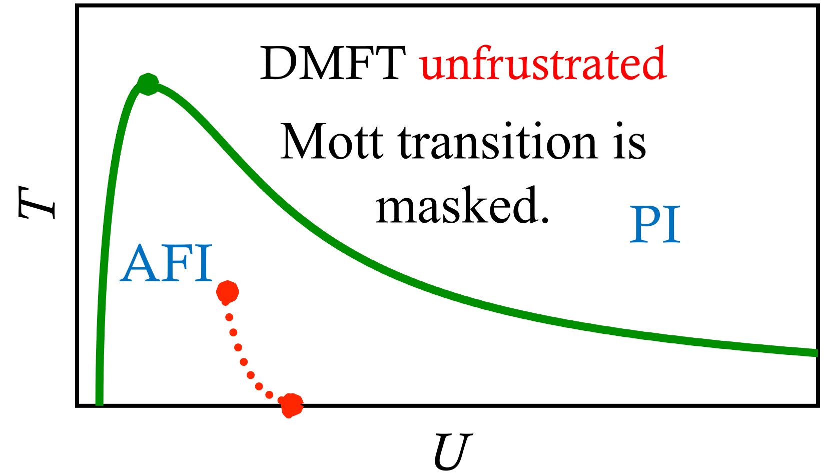
Cellular-DMFT → • magnetic LRO at T>0

weak 3-dim couplings stabilize LRO

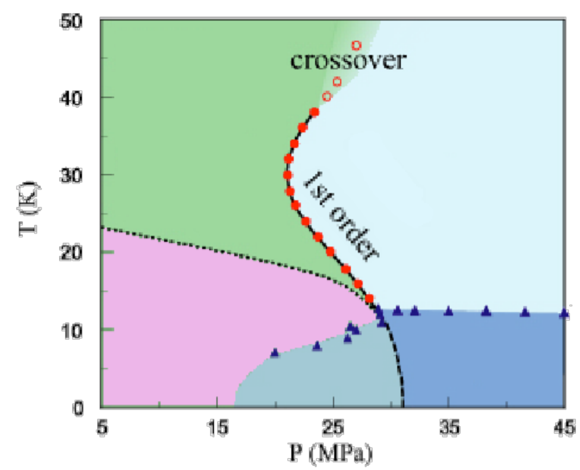
Georges et al. RMP 68, 13 (1996)
Zitzler et al. PRL 93 016406 (2004)

anisotropy: $t'/t=0.8$





consistent



Frustrated system:
Mott transition is NOT masked
Paramagnetic insulator phase exists

Magnon-pair BEC and spin-nematic state

- frustrated quantum spin system including ferromagnetic exchange interactions
- quasi-1D material $LiCuVO_4$ (S=1/2)

[Tsunetsugu and Zhitomirsky, in preparation]

Possibility of Spin Nematic Order

- Hidden non-”magnetic” order？
  spontaneous sym. breaking of spin rotation symmetry
  spin inversion and time reversal sym. are NOT broken

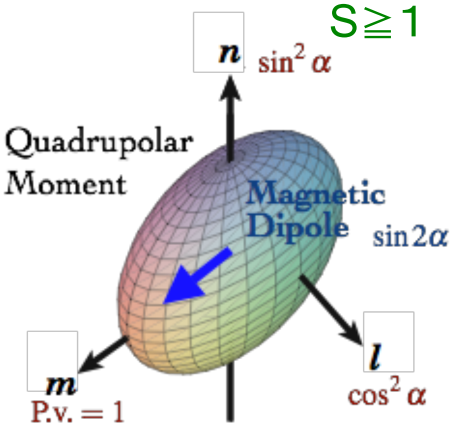
Blume, Chen&Levy...

Non-magnetic order: $\langle \mathbf{S} \rangle = \mathbf{0}$

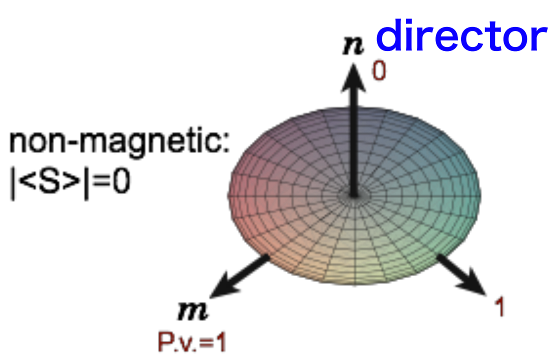
order parameter $Q_{\mu\nu} = \frac{1}{2}\langle S_i^\mu S_j^\nu + S_i^\nu S_j^\mu \rangle - \frac{1}{3}\delta_{\mu\nu}\langle \vec{S}_i \cdot \vec{S}_j \rangle$

anisotropy of spin fluctuations

S≧1

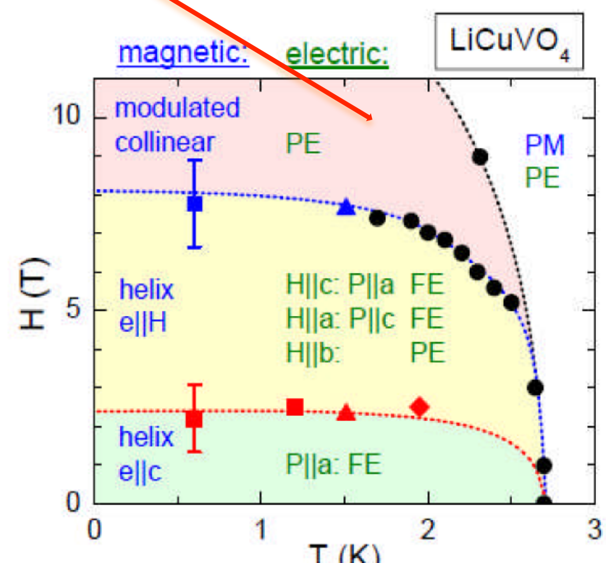


$$\sum_\mu Q_{\mu\mu} = S(S+1)$$



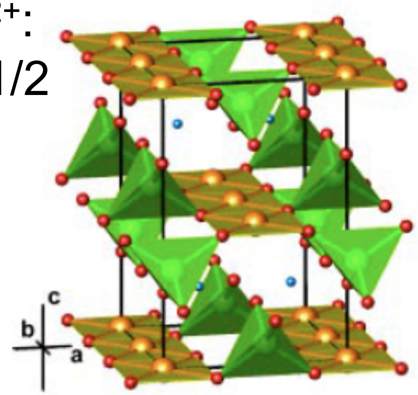
$LiCuVO_4$

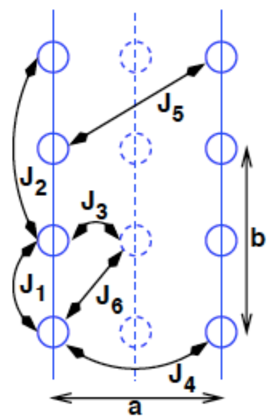
- quasi-1D frustrated magnet $LiCuVO_4$ in strong magnetic field
  - $|H| < H_{c1}$ helical state at low temperatures
  - $H_{c1} < |H| < H_{c2}$ NO magnetic LRO, mysterious state
- spin nematic phase?:
  $<S_i^a S_j^b + S_i^b S_i^a> - (1/2)\delta_{ab} <\mathbf{S}_i^\perp \cdot \mathbf{S}_i^\perp>$
- take into account interchain couplings (2D / 3D)



(Schrettle et al. 2007)

Cu^{2+}:
S=1/2





Exchange parameters

(Enderle et al, 2005)

	Method	$i = 1$	2	3	4	5	6
$R_i J_i$	neutron scattering	−1.6(2)	5.59(8)	−0.014(10)	0.01(3)	−0.40(8)	0.08(4)
$R_i J_i$	neutron scattering	−1.6(2)	5.60(8)	−0.015(9)	–	−0.37(5)	0.08(4)
J_i	high-T series fit to χ	−1.6	3.87(2)	−0.015	–	−0.37	0.08
J_i	$N = 16$-ring fit to χ	−1.8	4.3	–	–	–	–
J_i	LDA/TB	−3	6.1	0.11	0.79	0.06	0.02
t_i	LDA/TB	−74	−83	11	29	8	−5

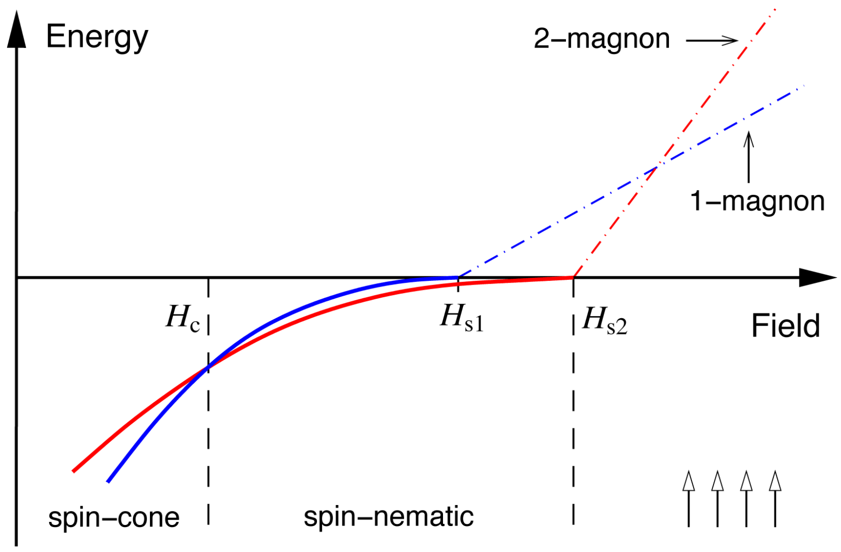
Energetics near saturation field

magnons: ↓ spins in the ↑ spin background ➔ bosons

spin nematic order parameter $Q_{ab} \Leftrightarrow \langle S^- S^- \rangle \Leftrightarrow \langle a^\dagger a^\dagger \rangle$

magnon-pair BEC
~ BCS
(but bosonic, spinless)

E=0



(cf. Momoi
et al for 1D case)

H_{s1}=46.5 [T]

H_{s2}=47.1 [T]

for $LiCuVO_4$

Quasiparticle excitations

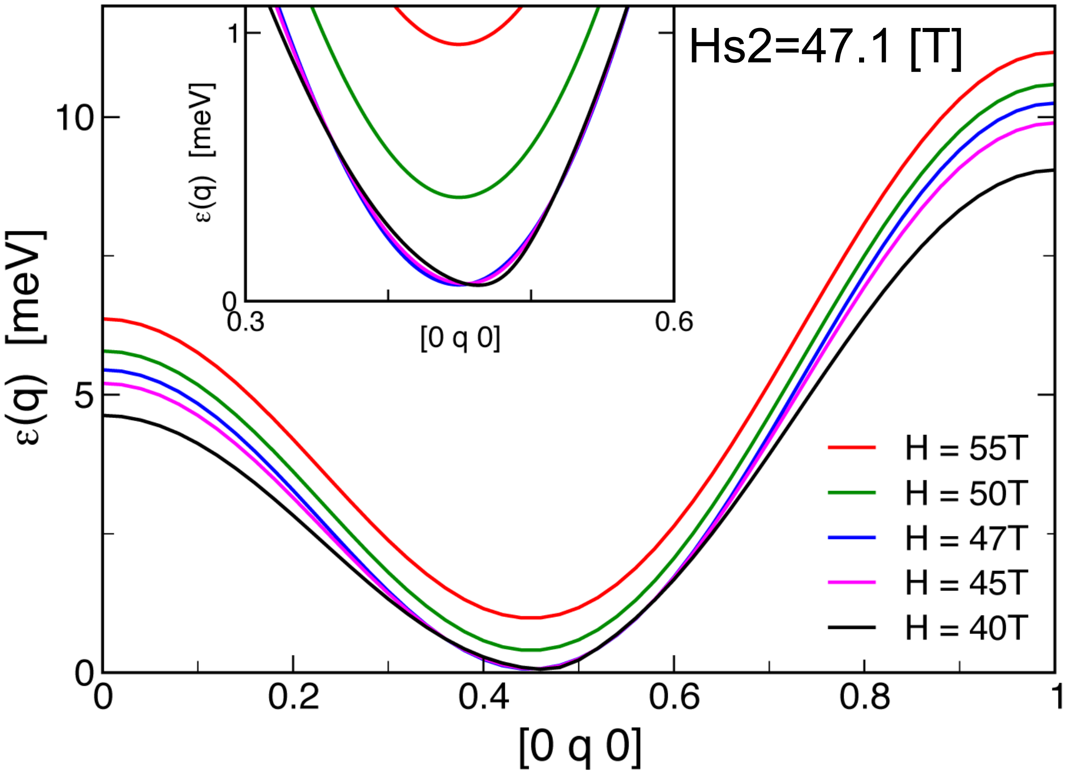
$$\varepsilon_{\mathbf{K}/2+\mathbf{q}} = \omega_{\mathbf{q}} - \sum_{\mathbf{r}} J(\mathbf{r})(\tfrac{1}{2} - n - n_{\mathbf{r}}) \sin \tfrac{1}{2}\mathbf{K}\mathbf{r} \, \sin \mathbf{q}\mathbf{r},$$

quasiparticle energy

$$\omega_{\mathbf{q}} = \sqrt{A_{\mathbf{q}}^2 - B_{\mathbf{q}}^2}\,, \quad B_{\mathbf{q}} = \sum_{\mathbf{r}} J(\mathbf{r}) \Delta_{\mathbf{r}} \cos \mathbf{q}\mathbf{r}\,,$$

$$A_{\mathbf{q}} = H - \sum_{\mathbf{r}} J(\mathbf{r})(\tfrac{1}{2} - n - n_{\mathbf{r}})(1 - \cos \tfrac{1}{2}\mathbf{K}\mathbf{r} \, \cos \mathbf{q}\mathbf{r}),$$

\+ gapless Goldstone mode (collective)



H-dependence

(completely polarized phase)
global shift of dispersion

(spin nematic phase)
gap essentially unchanged
~ 0.07 [meV]
w/ deformation of dispersion

⇒possible to check by experiments (eg, inelastic neutron scattering)

Another method of detecting spin nematic order

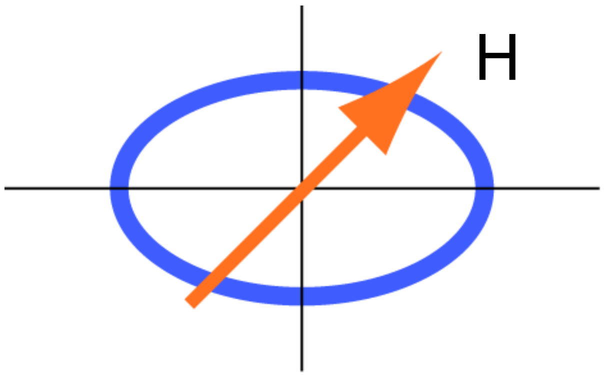
- indirect detection via coupling to magnetic dipole

  eg: nematic order parameter $Q_{\mu\nu}(\mathrm{k})\neq 0$

  → coupling $\mathrm{F}=\alpha\, H_\mu(\mathrm{k}=0)\, M_\nu(-\mathrm{k})\, Q_{\mu\nu}(\mathrm{k})$

  → induced transv. field $H_\nu(\mathrm{k})= \alpha\, H_\mu(\mathrm{k}=0)\, Q_{\mu\nu}(\mathrm{k})$

Apply H_μ and check if one can detect $M_\nu(-\mathrm{k})$



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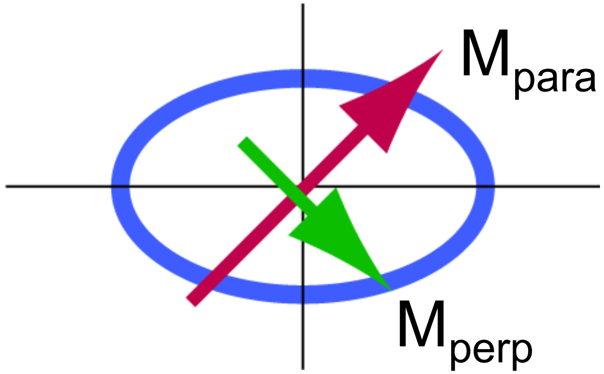

$$\langle S_i^x S_j^x\rangle - \langle S_i^y S_j^y\rangle \neq 0$$

Short summary

(1) Half-filled Hubbard model on anisotropic triangular lattice (t-t'-U)
•reentrant metal-insulator transition/crossover is reproduced
by cluster DMFT calculation
•high-T M-I crossover – driven by large entropy in frustrated insulating phase
•low-T M-I transition -- driven by spin fluctuations
•intermediate metallic phase – heavy quasiparticles inside Mott gap

(2) Spin nematic state in S=1/2 spin system in magnetic field
•magnon-pair BEC in frustrated spin system
including ferromagnetic couplings near saturation magnetic field
•coherent state and correlation functions
•quasiparticle excitations – finite energy gap and H-dependence
•methods of detecting spin nematic order