



Strongly correlated electron systems
(superconductors)
and
Neutron scattering
-view from a neutron instrumental scientist-

J-PARC Center, JAEA

Masatoshi Arai

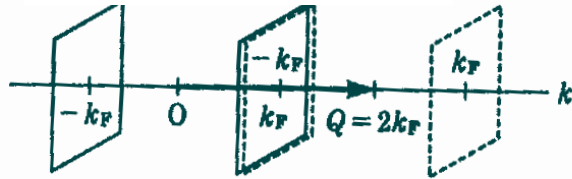




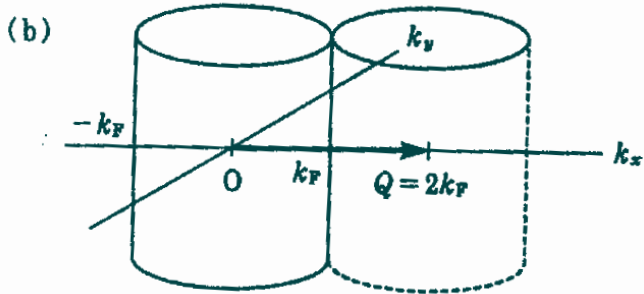
*J-PARC / Materials Life Science Facility
(the world class neutron/muon facility)*

Importance of the dimensionality of the electron system

(a) 1D Fermi Surface



2D Fermi Surface



Periodicity of electron system creates Fermi surface **nesting** and **gap formation**

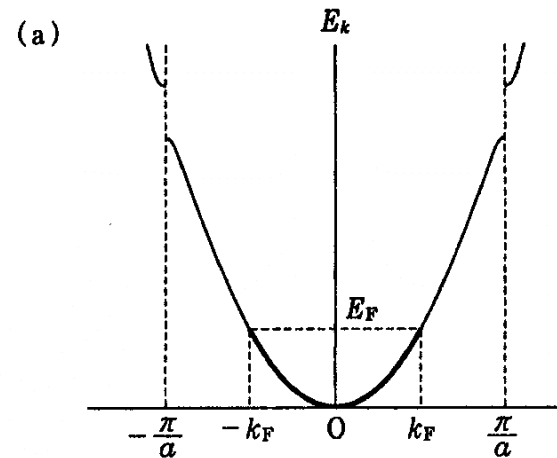


System's energy decreases !

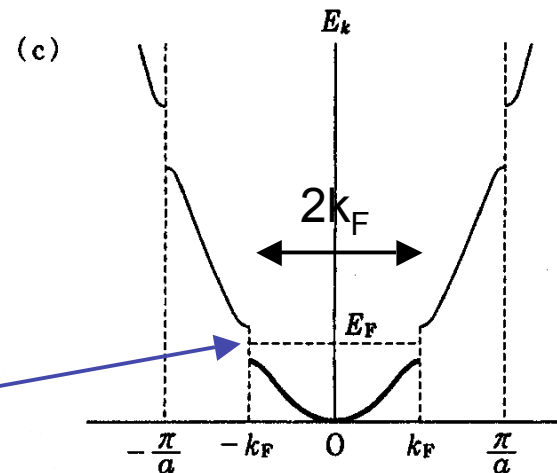
$$2\Delta(0) = 3.5k_B T_P^{MF}$$

It is the same as BCS

Band gap at lattice periodicity



Band gap at electron periodicity at E_F



2electrons in a unit cell -> insulator

Density response function (polarization susceptibility)

$$\chi(Q) = \frac{1}{V} \sum_k \frac{f_{k+Q} - f_k}{E_k - E_{k-Q}}$$

Singularity strength is dominated by the size of the nesting surface at E_F

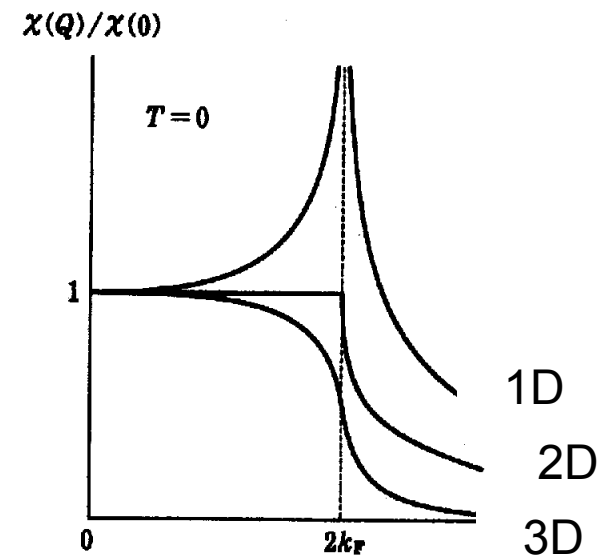
For 1D system

$$\chi(Q) = \frac{2m}{\pi \hbar^2 Q} \ln \left| \frac{Q + 2k_F}{Q - 2k_F} \right|$$

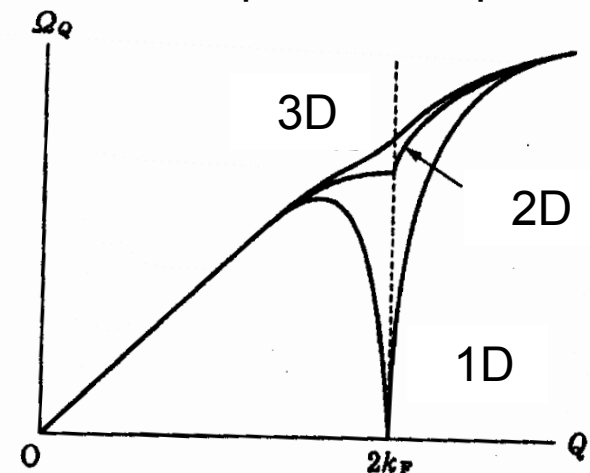
$$\chi(2k_F) = \frac{D_F}{N} \ln \frac{1.14 E_B}{k_B T}$$

In case for 1D,
Peierls transition always occurs
(metal- insulator transition)

Anomaly at $2k_F$ for electron system \Rightarrow **CDW**

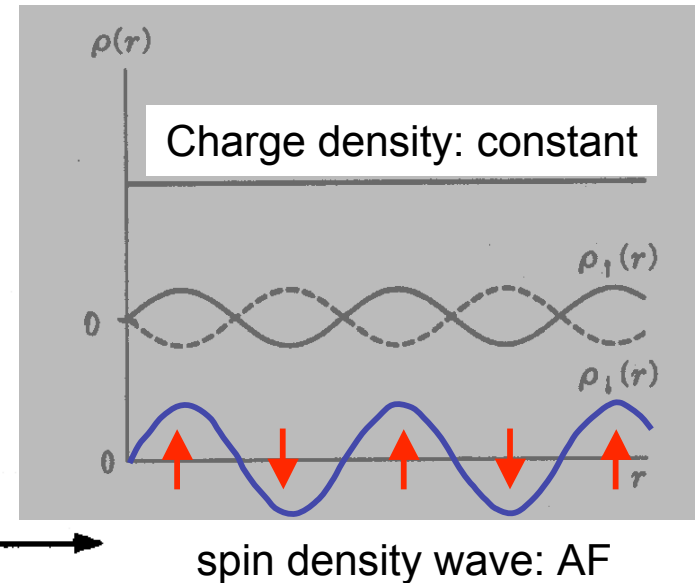
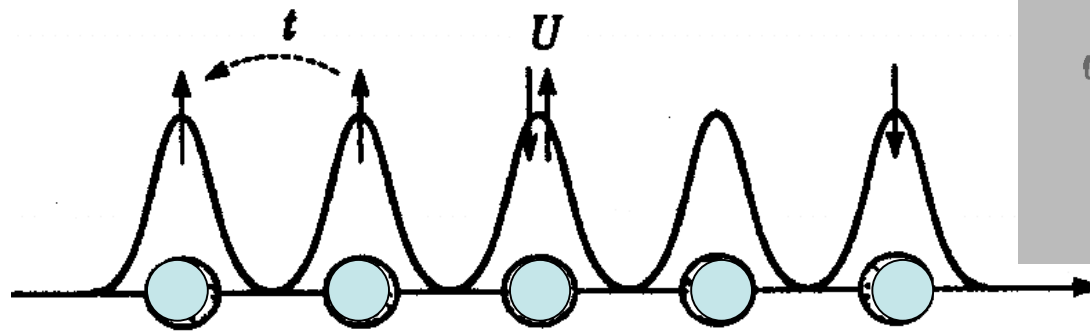


Kohn anomaly at $2K_F$
in the phonon dispersion



Correlated electron system and Hubbard model

Transfer integral: t On site Coulomb: U



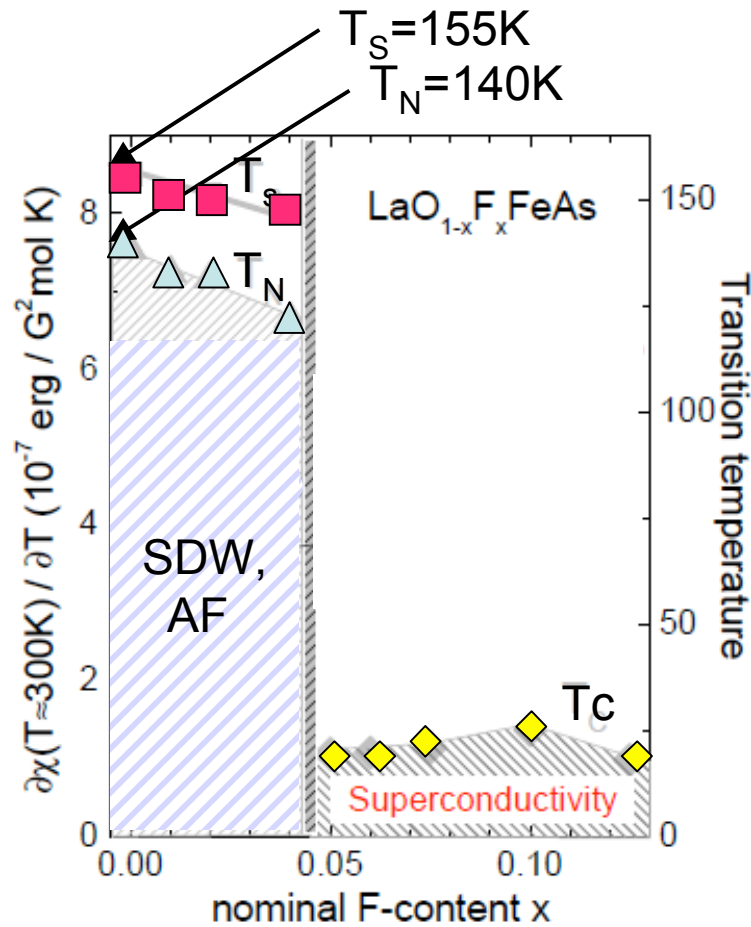
$$\chi_S(Q) = \frac{g\mu_B \chi(Q)}{1 - \frac{1}{2}U\chi(Q)}$$

Spin susceptibility has an anomaly at a finite T

There is always a temperature where $Uc(Q)/2=1$, because of the character of $c(Q)$

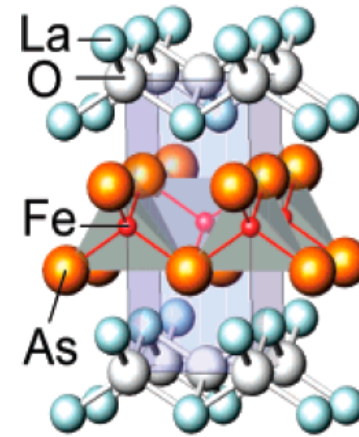
\Rightarrow **2- k_F -SDW is created if there is U (electron correlation) under nesting condition.**

2D - SDW from LaFeAsO



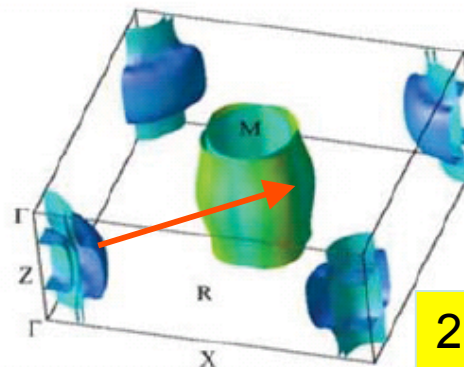
electron concentration

R. Klingeler, et al., cond-mat 2008



2D nature in the electronic states

$\text{LaFeAsO}_{1-x}\text{F}_x$ $T_C \sim 26\text{K}$ Kamihara, Hosono et al. J. Am. Chem. Soc. 130, 3296 (2008).



2D-Fermi surface
 Γ ; hole like cylinder,
 M; electron like cylinder

2D - Fermi surface nesting
 2D-SDW, SC

5-orbitals ($d(Z^2-R^2)$, $d(XZ)$, $d(YZ)$, $d(X^2-Y^2)$, $d(XY)$) of 3d states have contribution
 It is not a Mott insulator ($U \sim 1\text{eV}$)

D.J. Singh and M.H. Du, Phys. Rev. Lett. 100, 237003 (2008).

Structural Phase transition at 155K
 (Tetragonal → Monoclinic)
 and
 3D-Anti-Ferromagnetic Long range order below 140K
 (Cruz et al. Nature 2008)

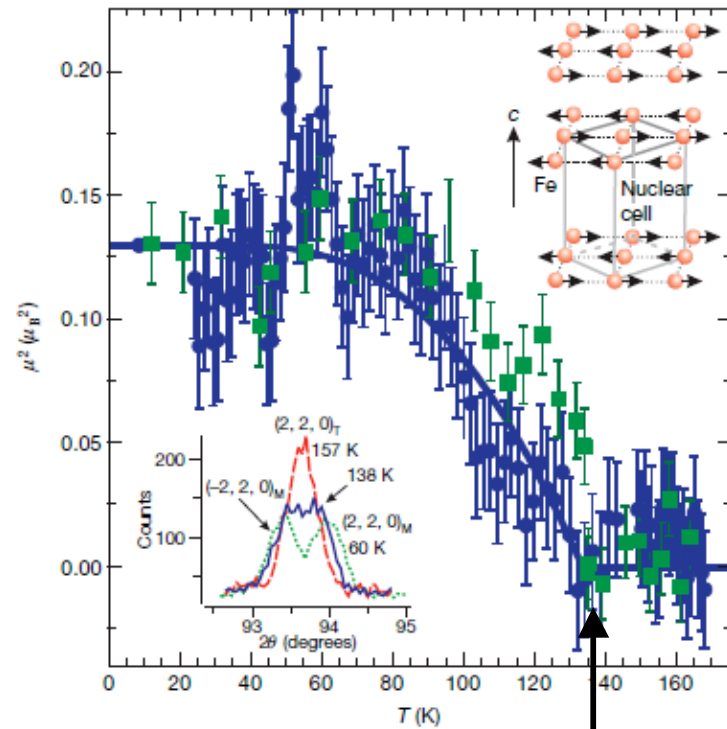
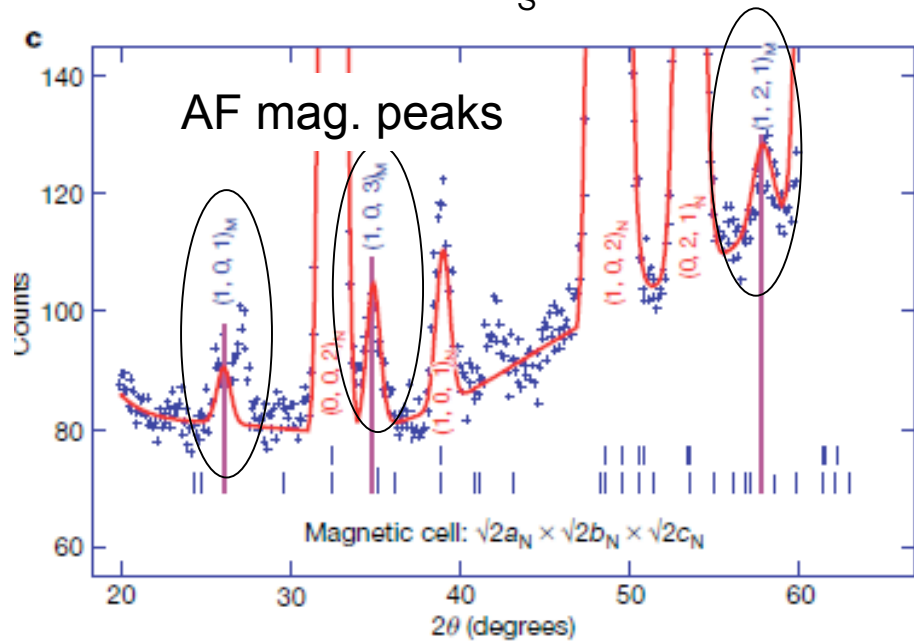
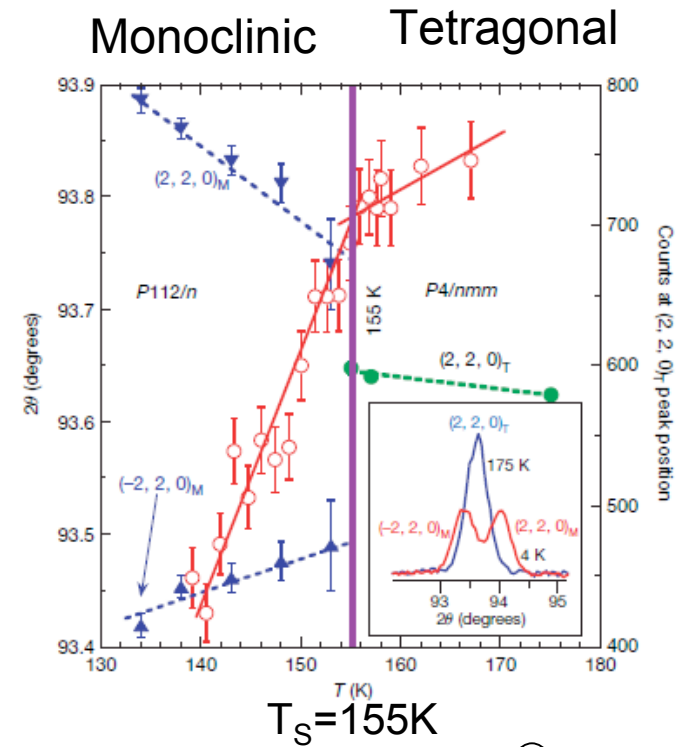


Figure 4 | Temperature dependence of the order parameter at

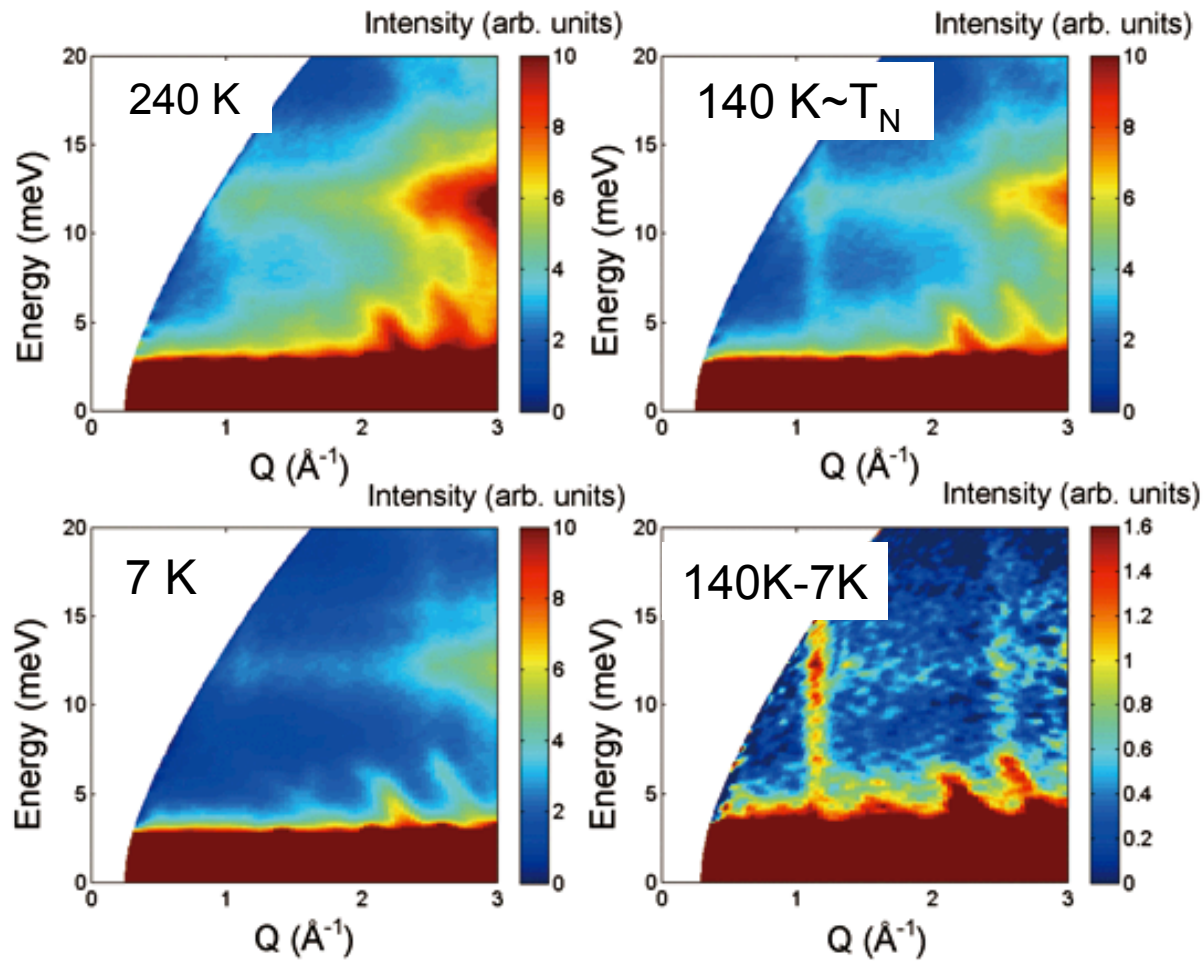
$T_N = 140\text{K}$

(AF points; $(101)_M$, $(103)_M$, $(121)_M$)



Inelastic Neutron Scattering from a powder sample (LaFeAsO)

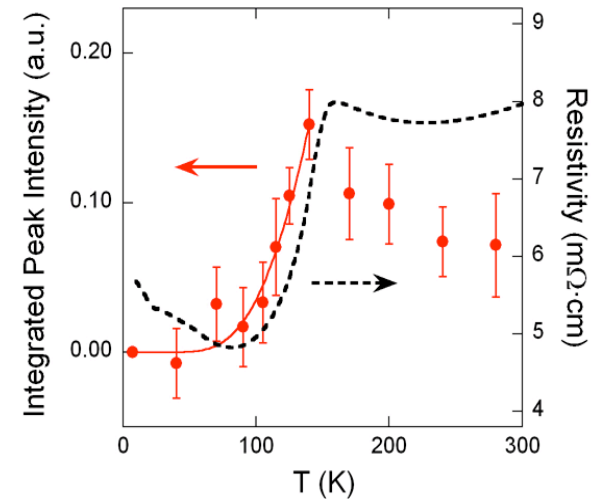
(one of the most important role of neutrons)



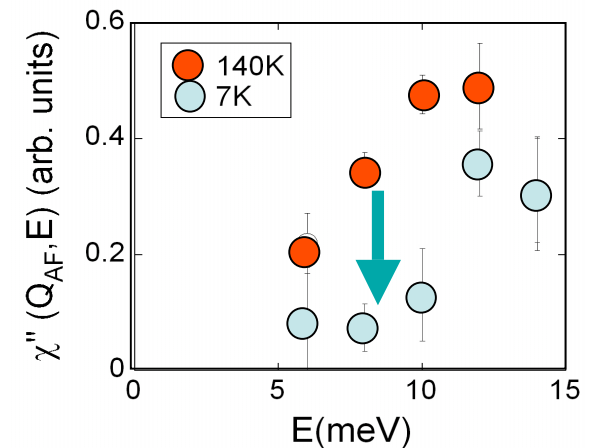
$S(|Q|, E)$ ($E_i = 30$ meV)

T- dependence

$S(Q=1.0 \sim 1.3 \text{ \AA}^{-1}, E=7.5 \sim 9 \text{ meV})$

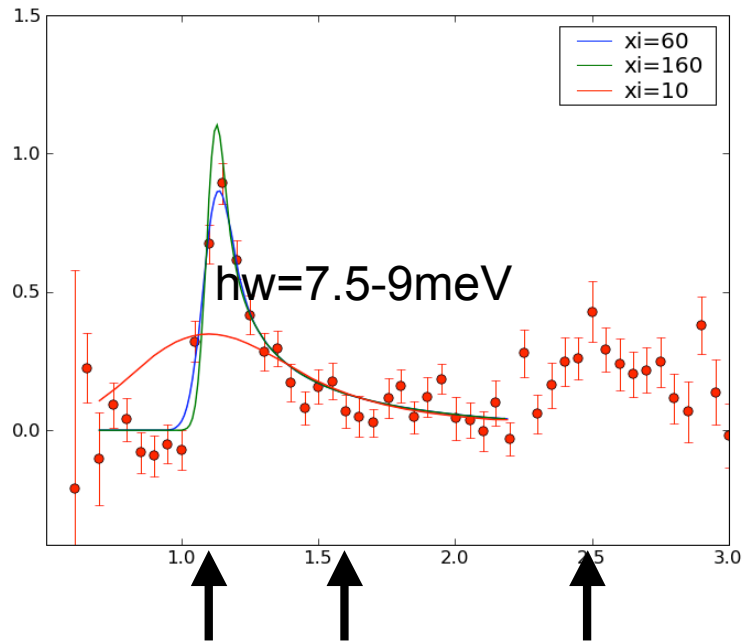


Spin gap formation



excitation from 2D-SDW

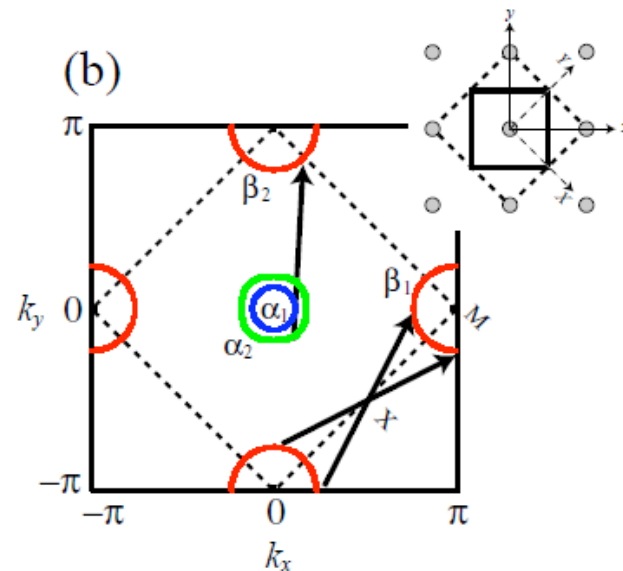
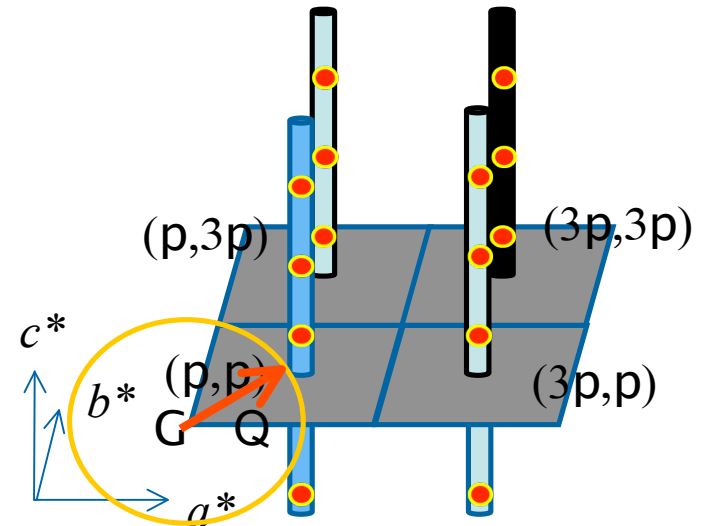
2D-SDW: Warren function



3D - AF long range order zone centers

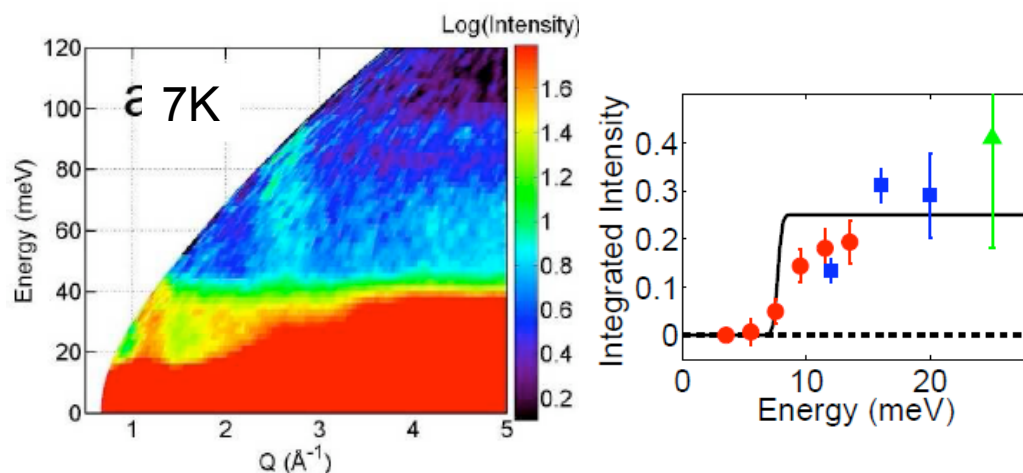
Static 3D-AF order and 2D-SDW in the inelastic region.

Existence of 2D-SDW



Nesting and unconventional S-wave SC
 Formation of SDW by a nesting
 Kuroki, Aoki, PRL 2008

BaFe₂As₂(T_c=0K), Spin wave excitation ?

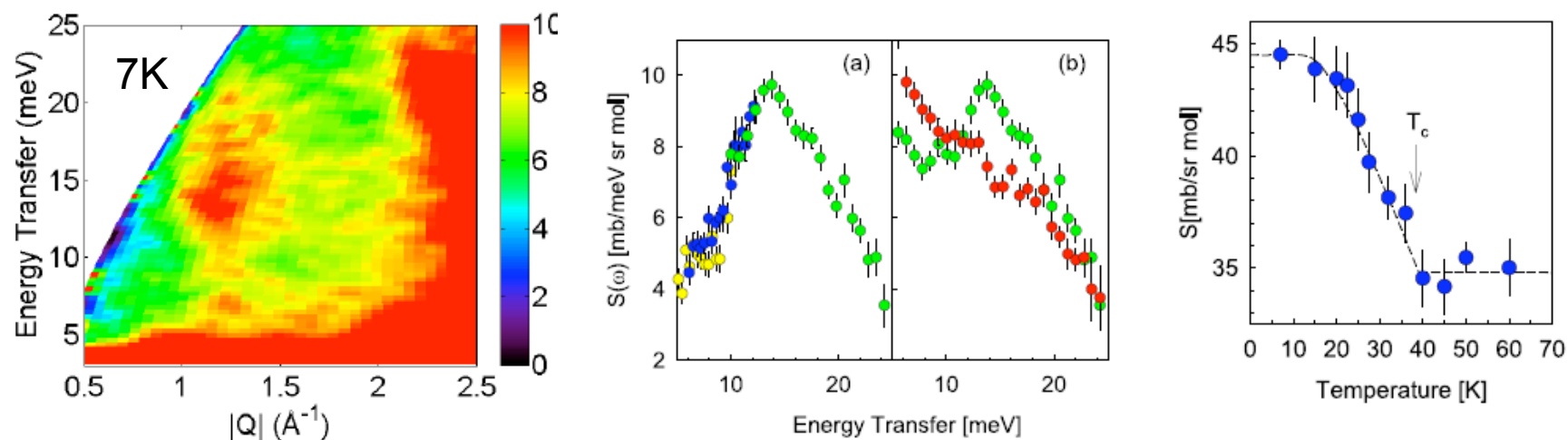


Similar experiments were rushed almost in the same time on the same instrument, MERLIN in ISIS.

Our Exp. date; 10 July
Christianson; 14 July
Ewings; after two above.

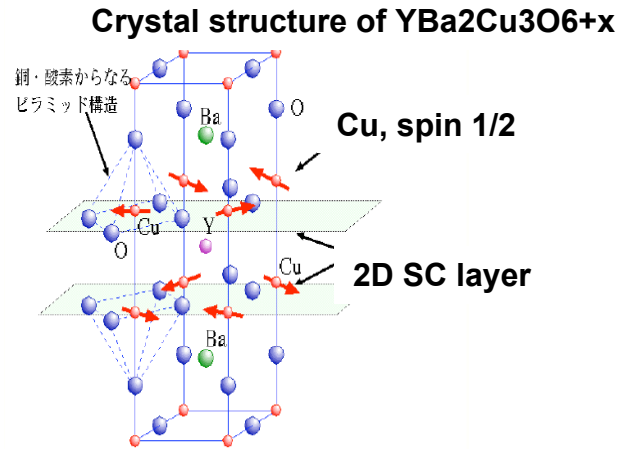
Ewings et al., cond-mat Aug. 2008

Ba_{0.6}K_{0.4}Fe₂As₂ (T_c=38K), Resonance peak in the SC states



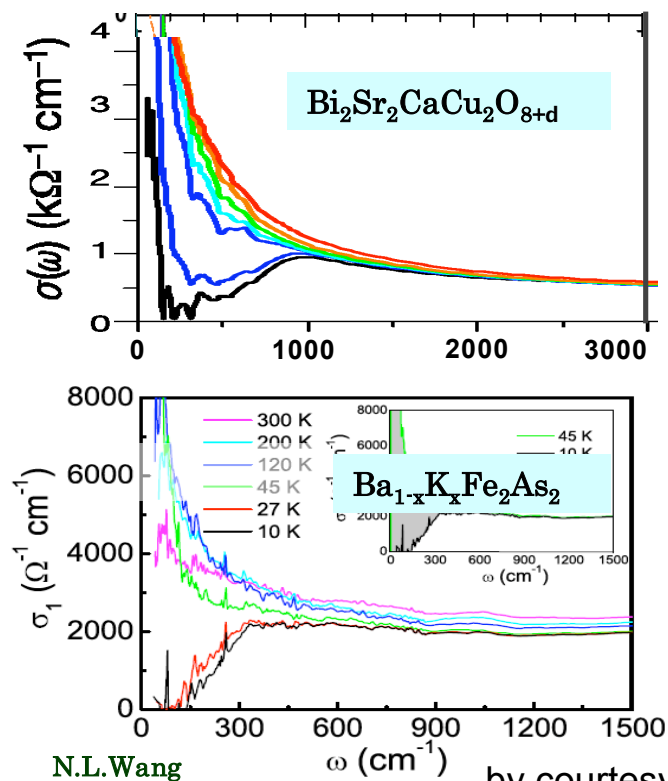
Christianson et al. cond-mat July 2008

Oxide High T_c superconductor

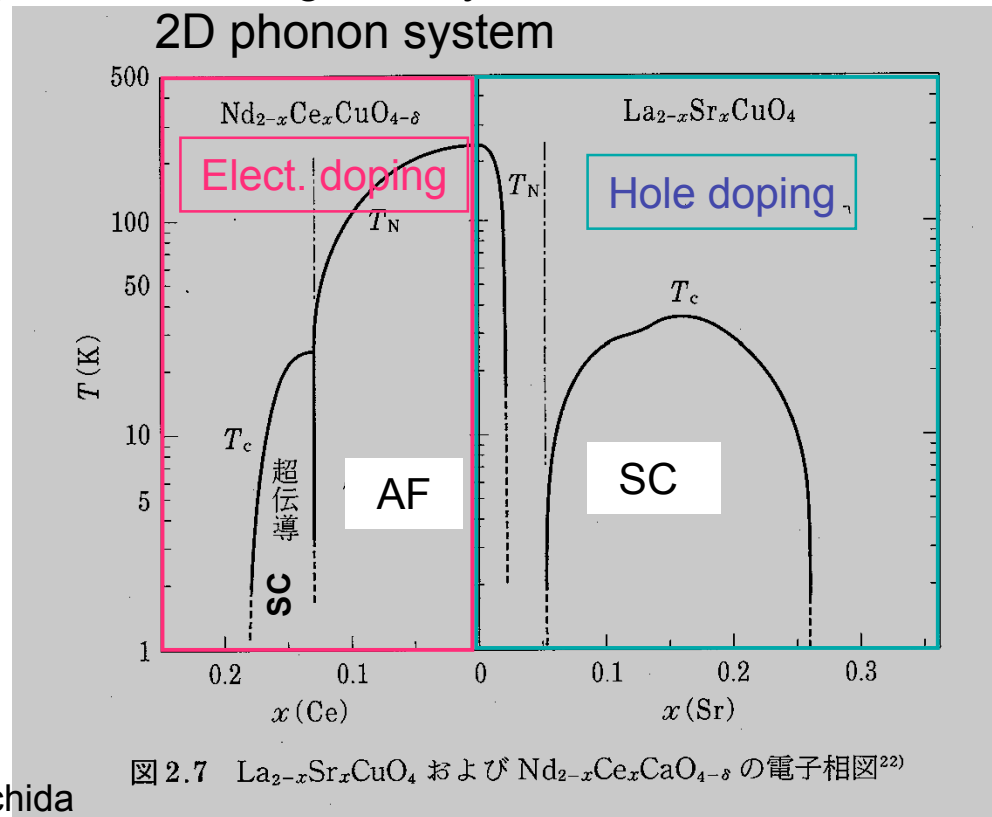


- Strong U ($\sim 8\text{eV}$);
- strongly correlated electron system (half filling system)
 - \Rightarrow Mott insulator
- 2D electron system ($3d(X^2-Y^2)$, spin=1/2, charge transfer to the oxygen 2ps)
- 2D magnetic system
- 2D phonon system

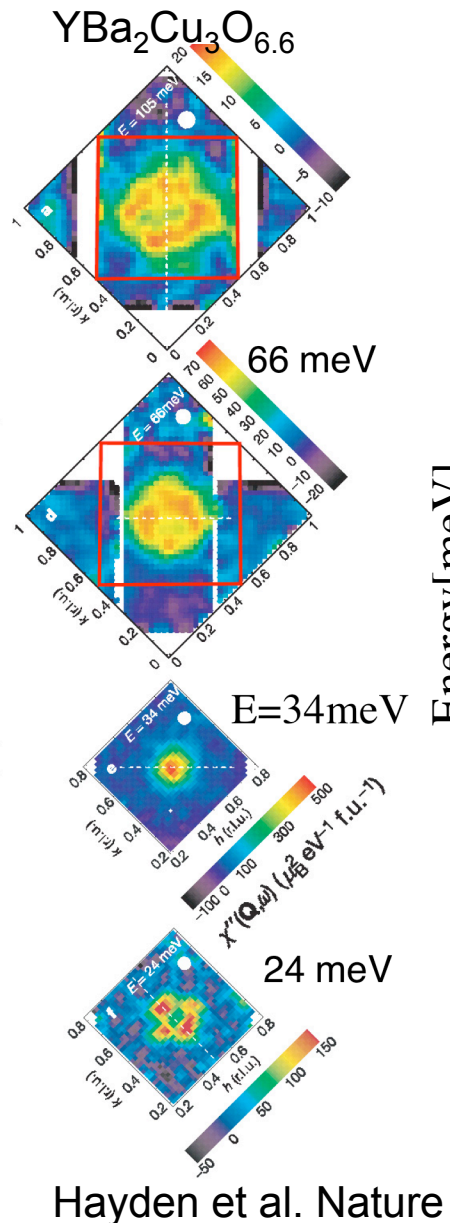
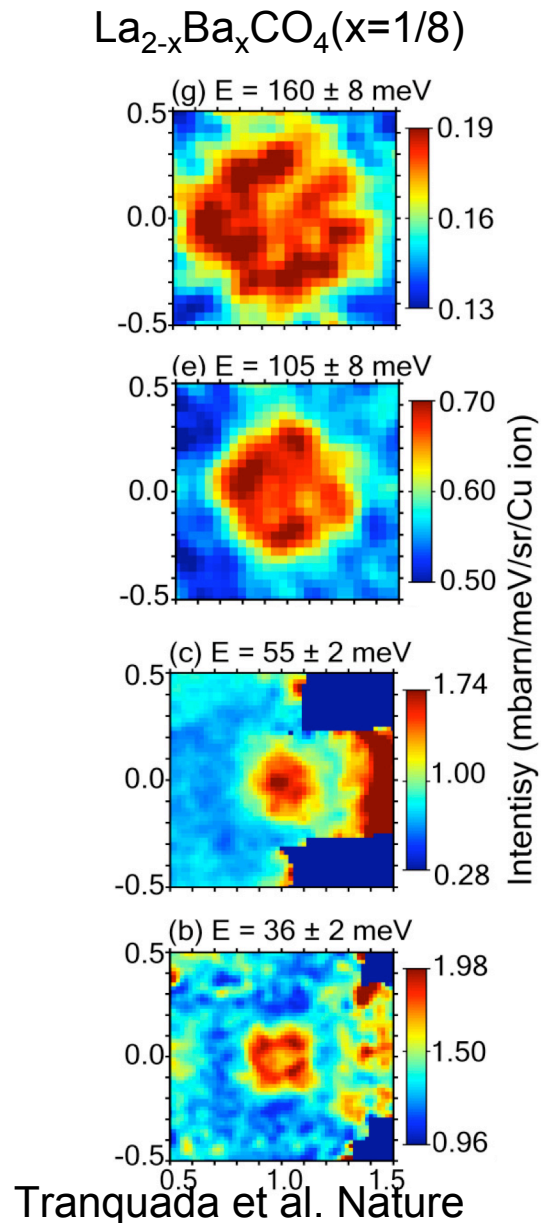
Resemblance in the optical conductivity



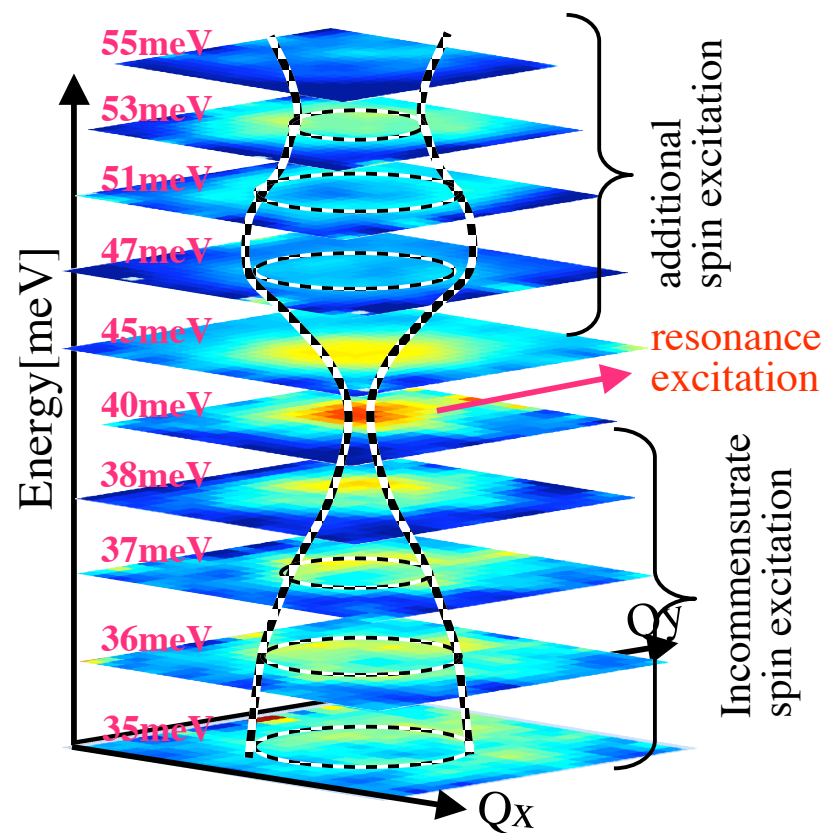
by courtesy of Uchida



Common feature in the magnetic excitation in the oxide high T_c superconductors



Hourglass shape in the magnetic excitation

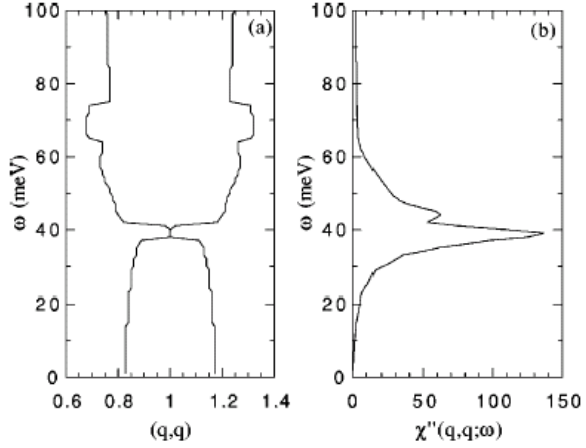
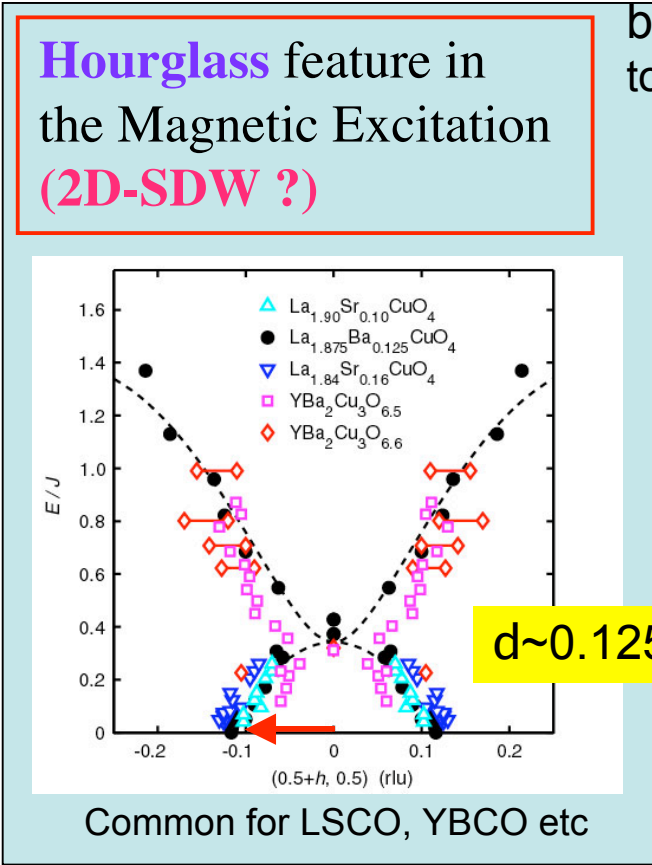
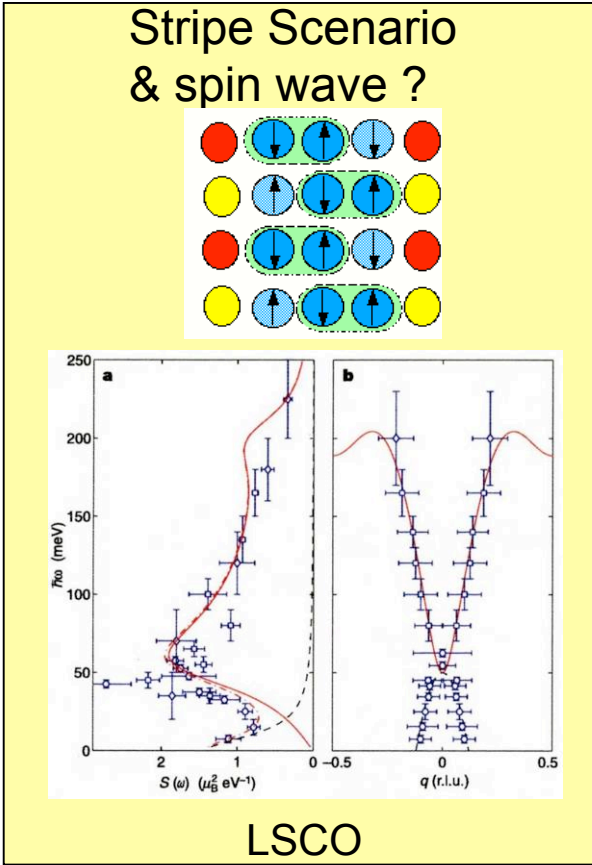


Yokoo et al. J. Neutron Research

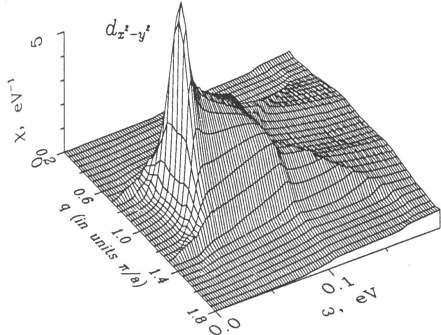
Anomalous Magnetic Excitation

Imc can be obtained from the Fermi Surface character

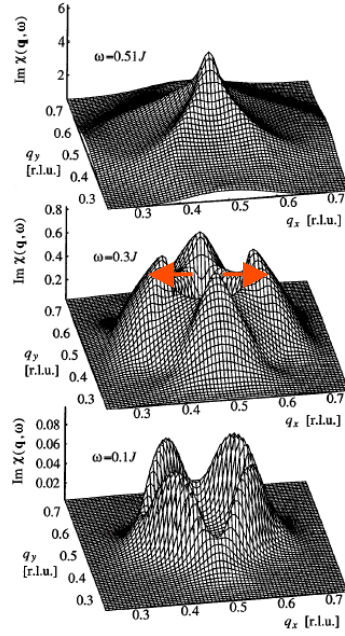
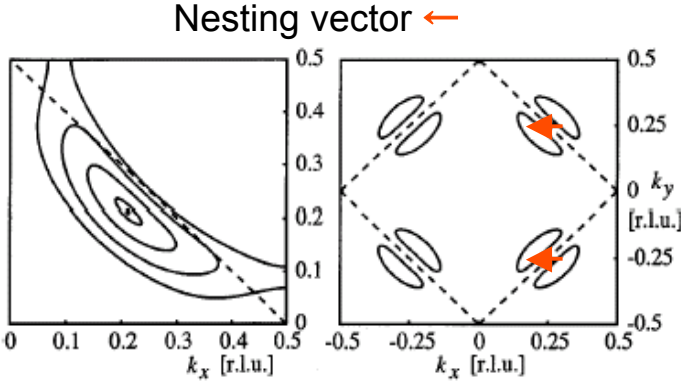
by RPA (electron state to)



Norman PRB 2000



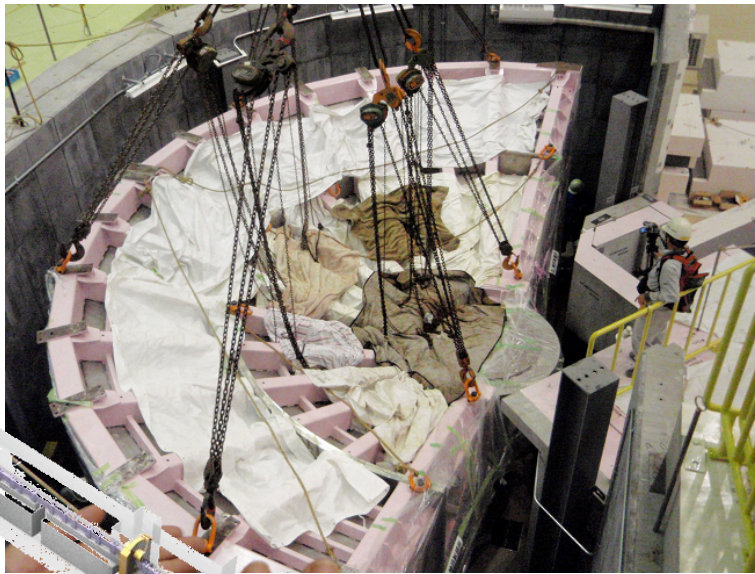
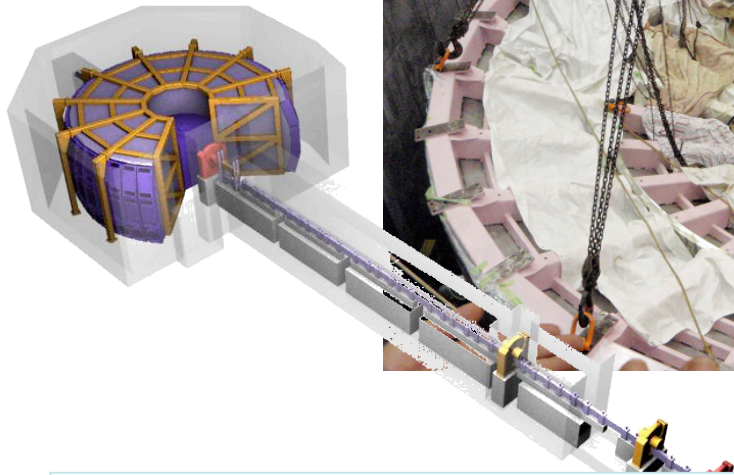
Yakovenko 1995



Brinckmann and Lee, PRL 1999

Summary and guess

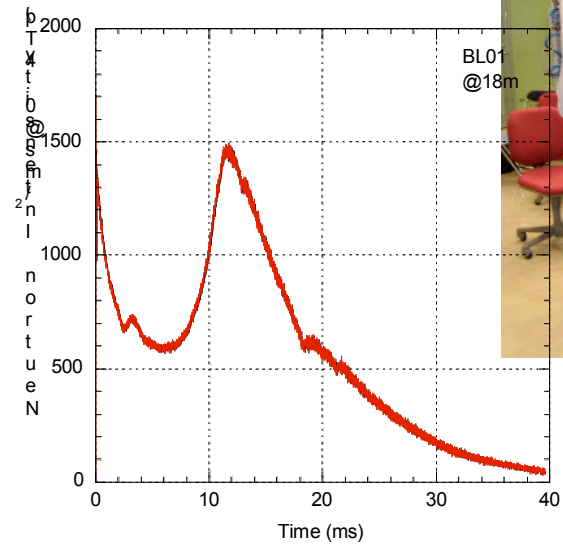
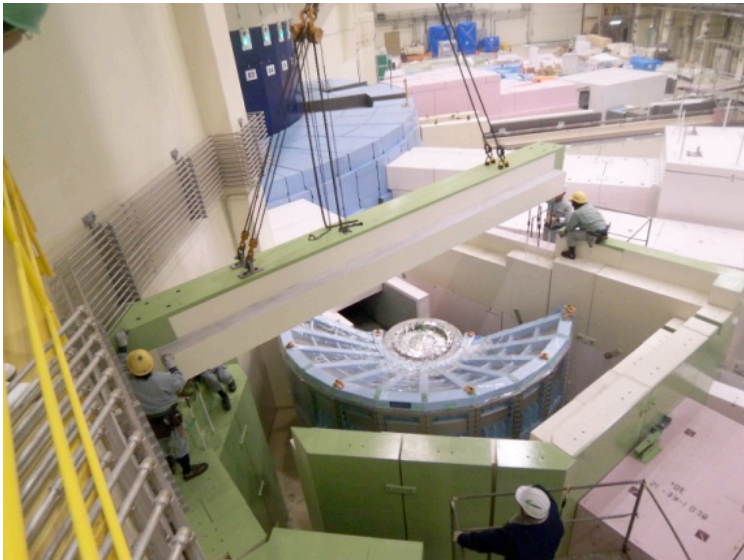
- 1) Strongly correlated electron system (SCES) gives various exotic physical properties.
- 2) Low dimensionality and the Fermi surface topology is important.
- 3) The discovery of the Fe-pnictide is very important for itself, but also stimulating reconsideration of physics of Oxide HTCSC.
- 4) It seems that **electron-electron correlation (nesting)** has an importance.
- 5) Studying dynamics of materials, by means of Neutron, X-ray, ARPES, Muon, is very important to understand the intrinsic mechanism of physical properties of SCES.
- 6) IMSS has those tools in hand, and hence the formation of the **Condensed Matter Research Center** is very timely to extend and enhance the activity of IMSS.
- 7) J-PARC can have an important role for it.



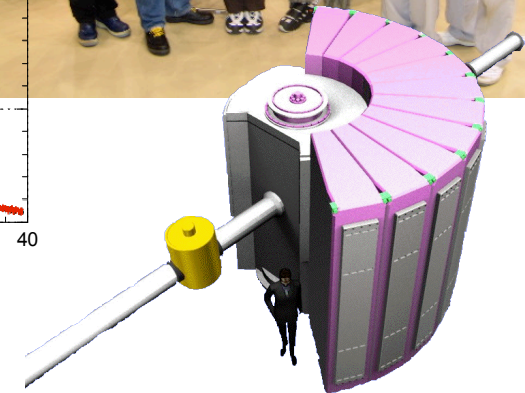
J-PARC neutron facility will provide excellent opportunities to study strongly correlated electron systems.

END

4SEASONS & AMATERAS will come on line soon.



The first neutrons on May 30.



END