Charge Dynamics in (ω, Q)-Space Studied by Inelastic X-ray Scattering

Jun'ichiro Mizuki

Quantum Beam Science Directorate

Japan Atomic Energy Agency (JAEA)

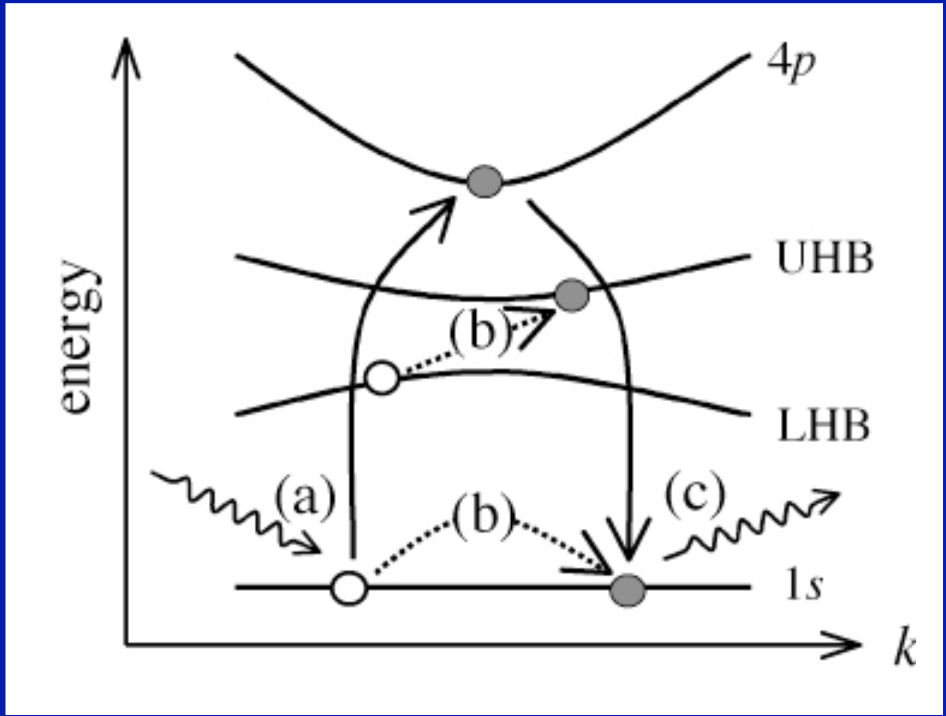
Inelastic X-ray scattering

[illegible]

[illegible]

- The first term: non-resonant inelastic scattering
  - All electrons (Ze) are contributed ⇒ phonon excitation
- The second term: resonant inelastic scattering (RIXS)
  - Electrons on the specific atom are contributed.
  - Resonance enhancement
  - Element specific ⇒ electronic excitation

RIXS of 3d transition elements



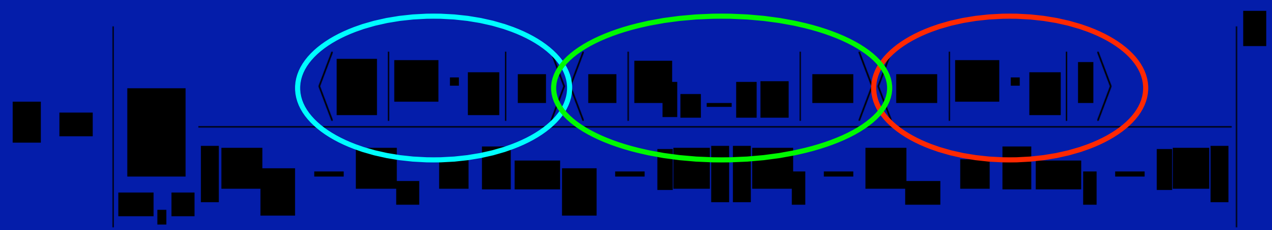
K-edge (1s→4p、several keV)

(a) absorption

(b) interaction between

1s core-hole and 3d electron

(c) X-ray emission



Inelastic Scattering

$$I(Q,E) \sim \left[V(Q)\right]^2 \left[1 - e^{-\beta E}\right]^{-1} \bullet \operatorname{Im}\chi(Q,E)$$

Interaction of probe

Generalized susceptibility

For neutrons → Spin susceptibility, Nuclear susceptibility

For X-rays, For electrons → Charge susceptibility

$$\chi(Q,E) = -(Q^2/4\pi^2 N)\ 1/\varepsilon(Q,E)$$

Dynamical dielectric function

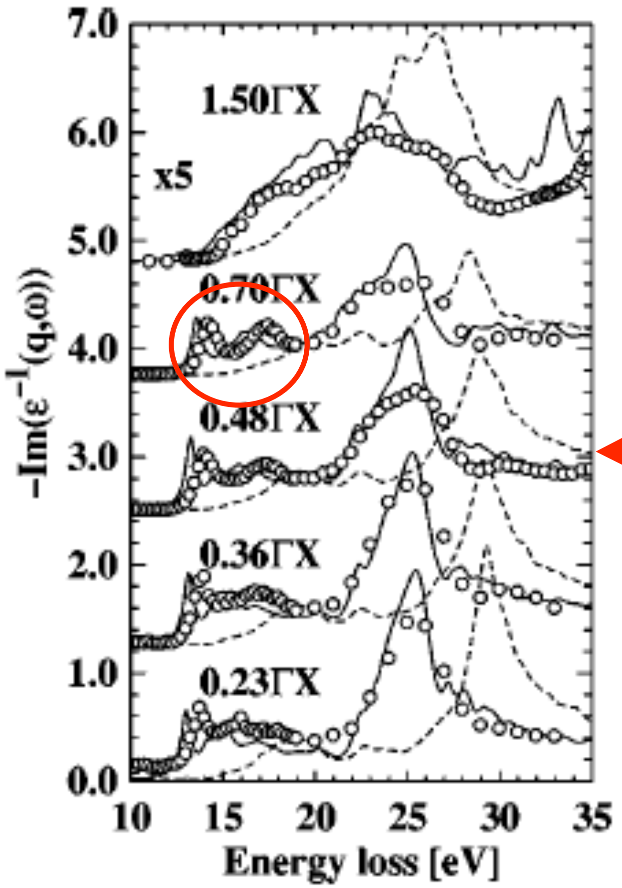
Effects of electron-hole interaction on the dynamic structure factor: Application to nonresonant inelastic x-ray scattering

J. A. Soininen
Department of Physics, POB 9, FIN-00014, University of Helsinki,

Eric L. Shirley
Optical Technology Division, Physics Laboratory, National Institute of Standards and Technol

(Received 24 January 2000)

P. R. B. 61 ('00) 16423

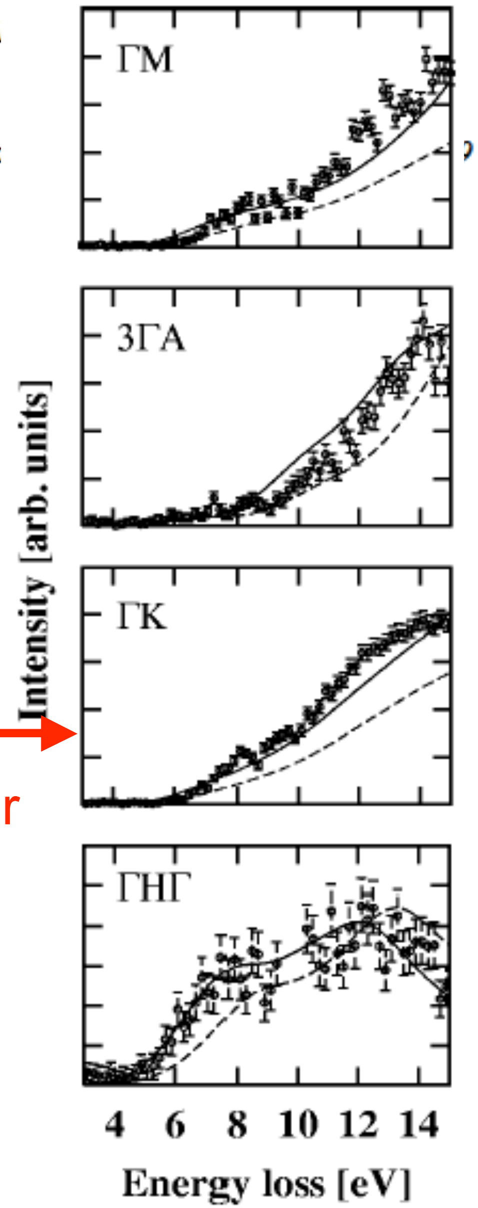


——— : including ele. –ho. inter.

······· : not including ele.-ho. Inter.

LiF
insulator

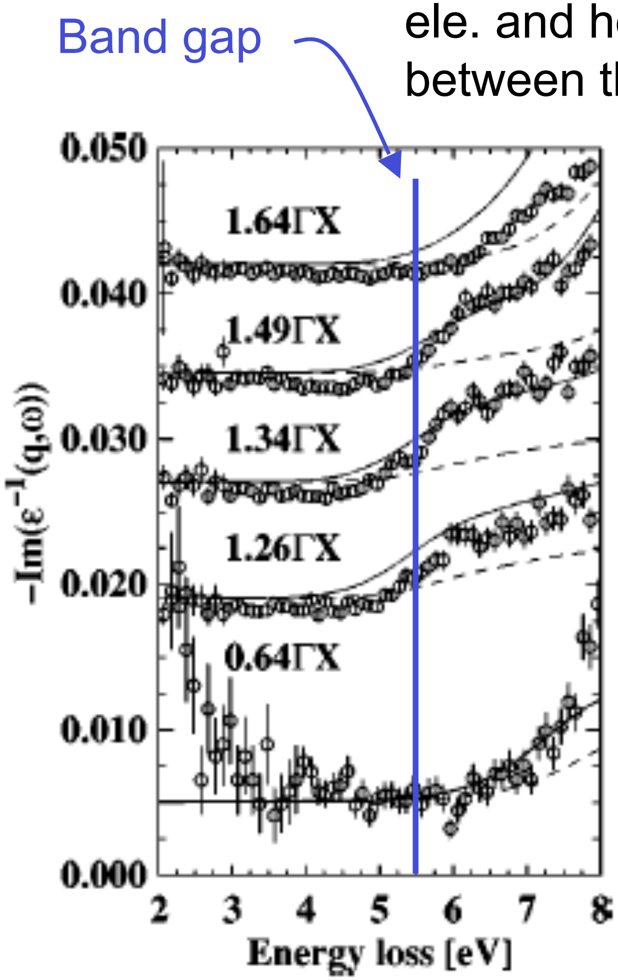
GaN
semiconductor

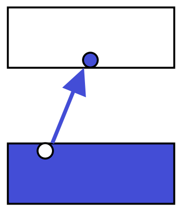


Non resonant IXS on Diamond

Propertied of an indirect band gap

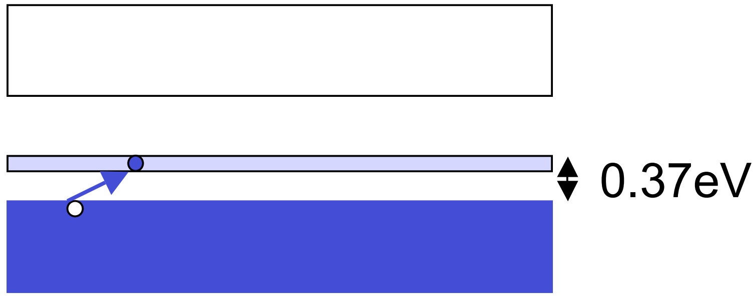
ele. and hol. interaction
between the band gap

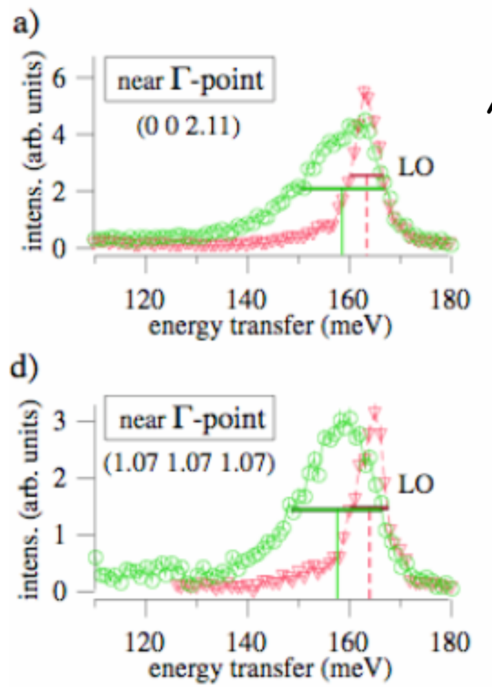


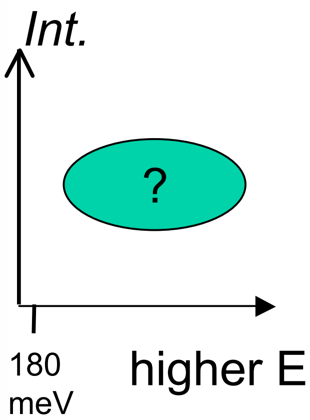


Caliebe et al., P.R.L. 84 ('00) 3907

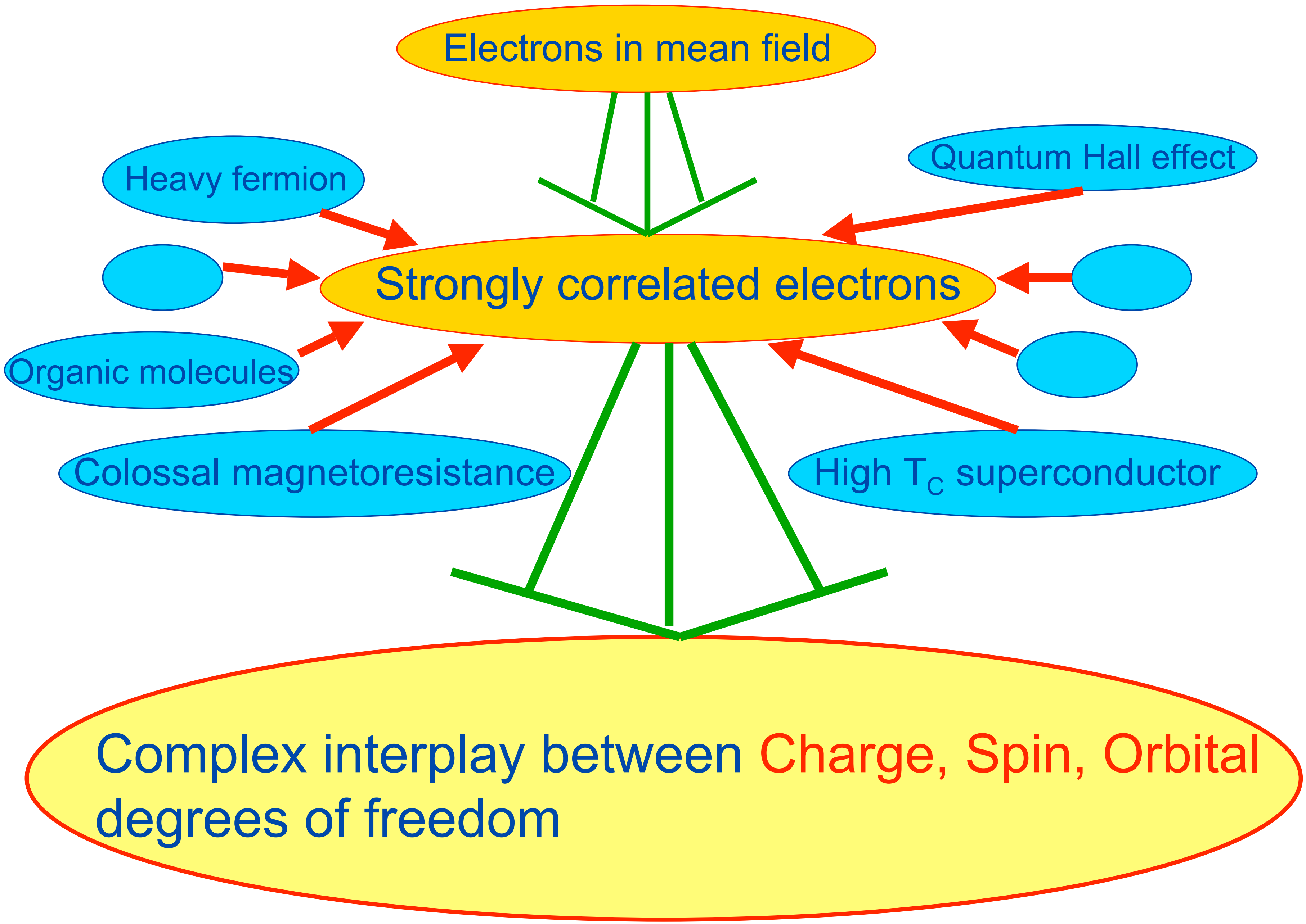
- ●Band engineering of Semiconductors,
- ●Supercondctor based on Semiconductors





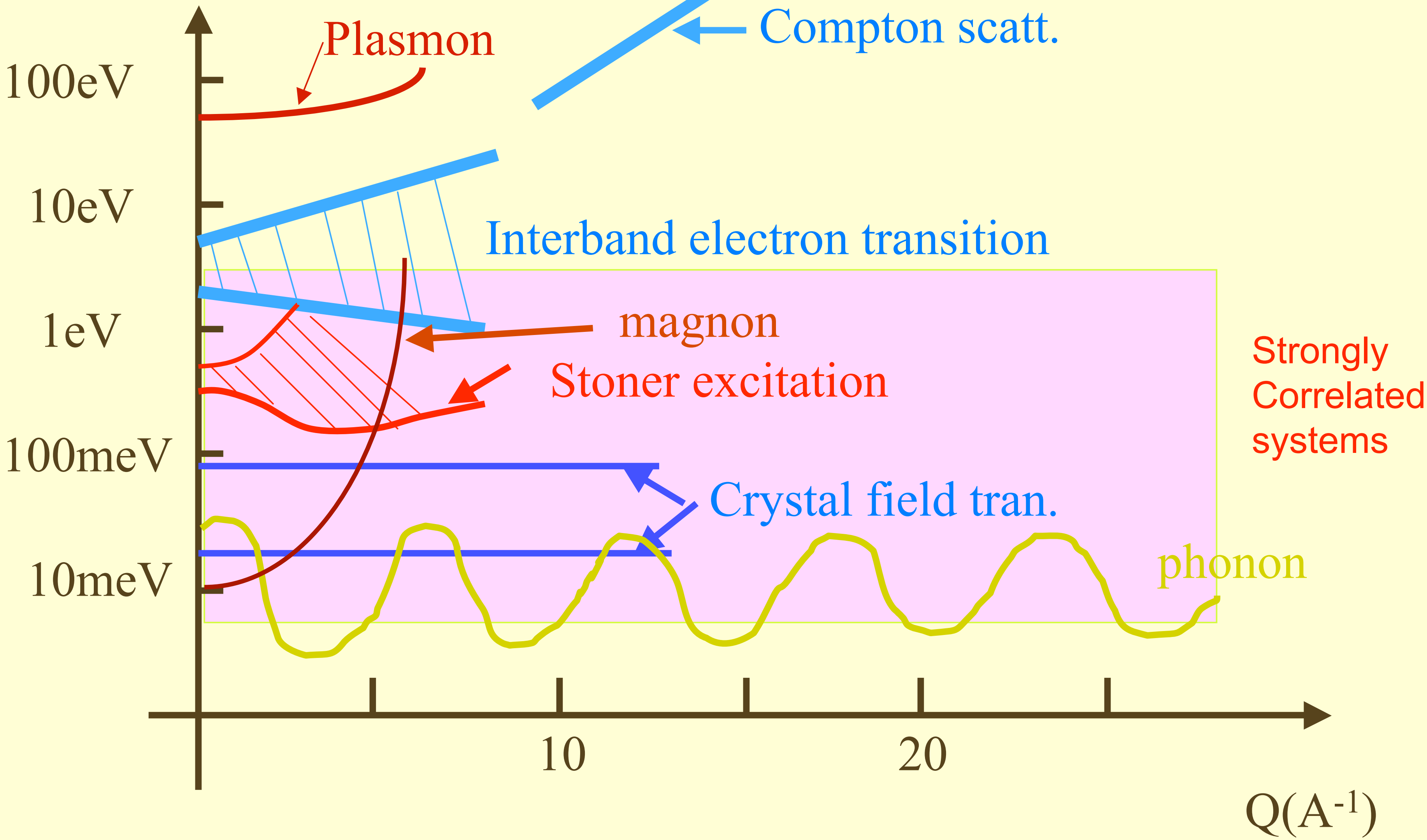


M. Hoesch, J. M. et al., P. R. B. 75 ('07) 140508(R)

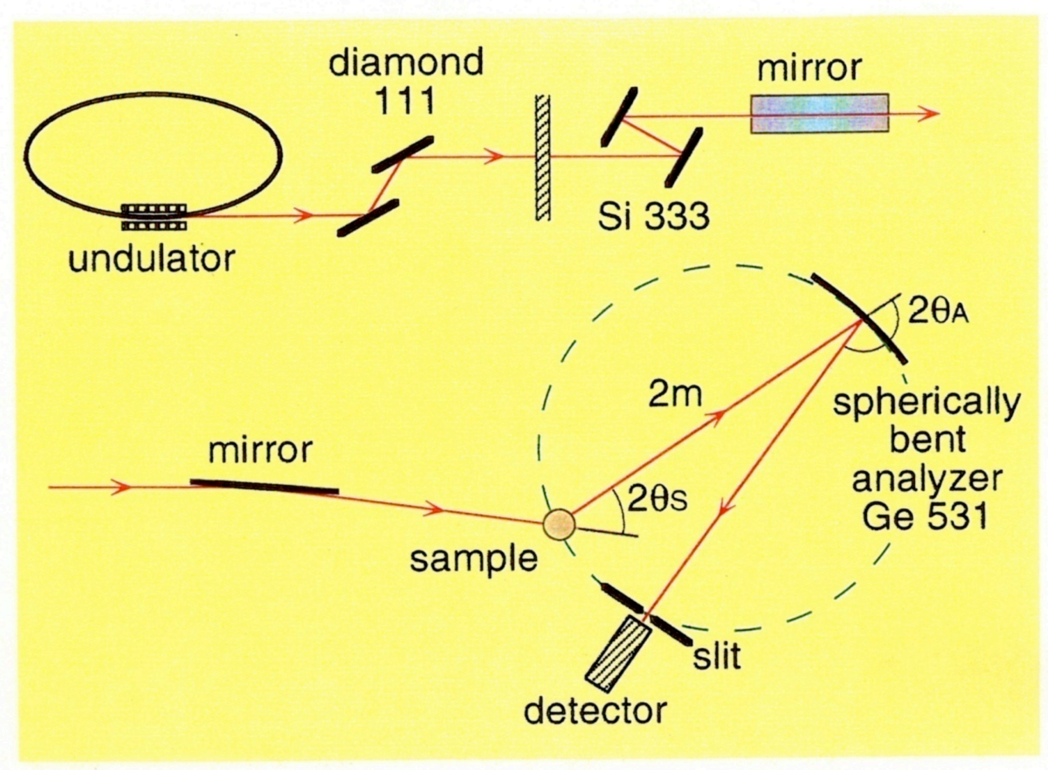

Electrons in mean field
Heavy fermion
Quantum Hall effect
Strongly correlated electrons
Organic molecules
Colossal magnetoresistance
High T_C superconductor
Complex interplay between Charge, Spin, Orbital degrees of freedom

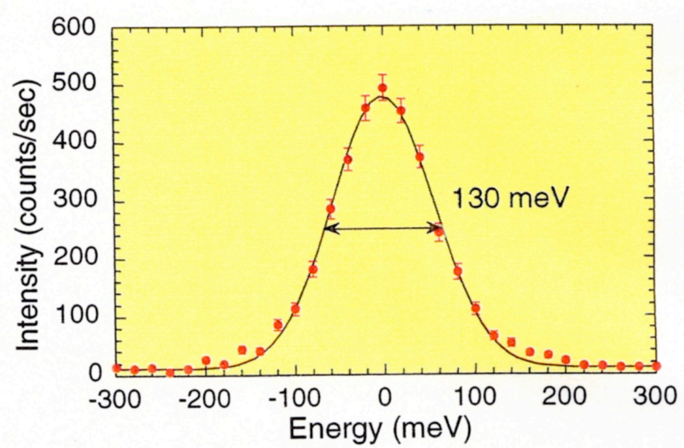
Elementary Excitations in Solids

Text book



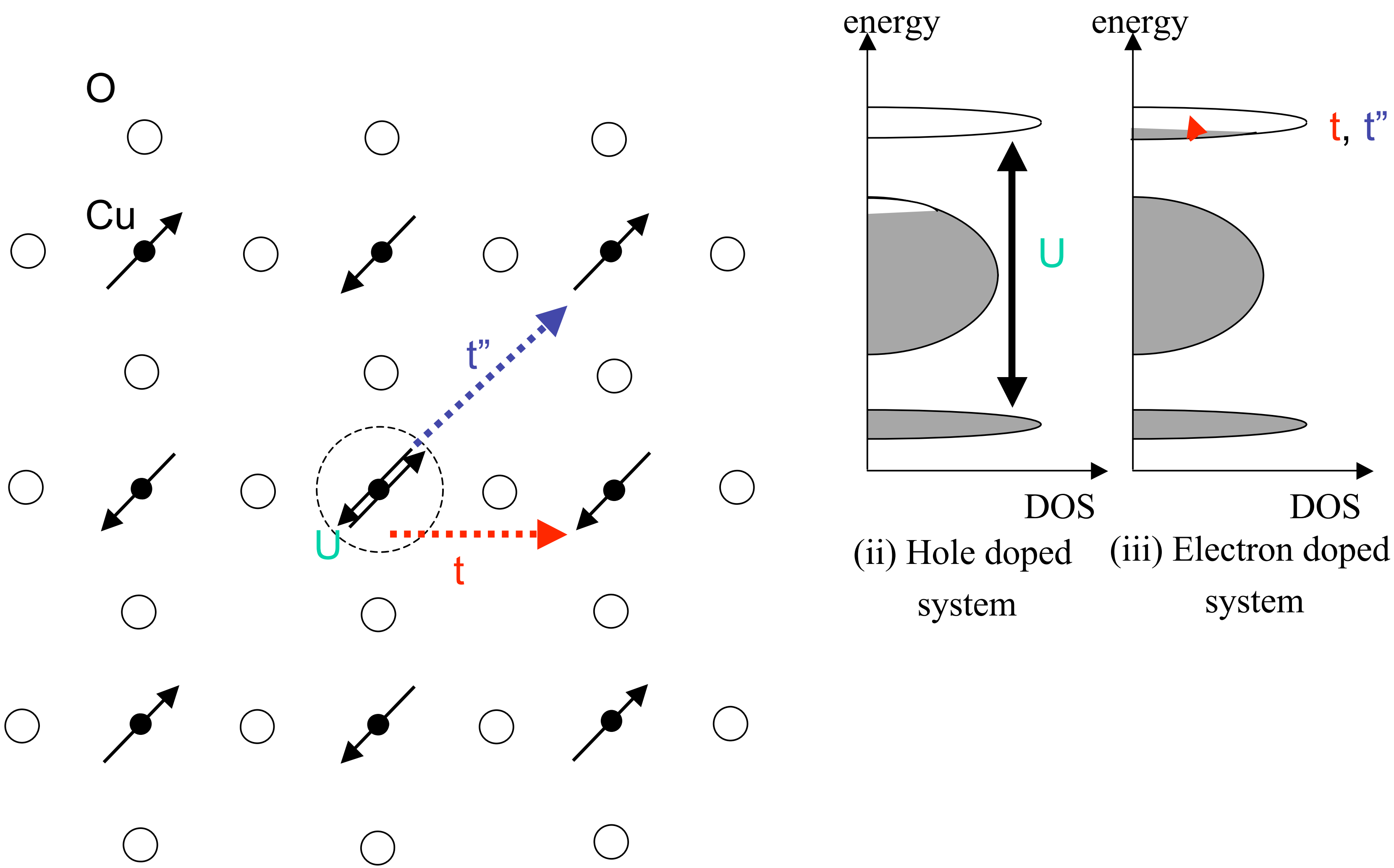
Set-up of Inelastic Scattering Spectrometer at BL-11XU





Observed energy Resolution at 6.5 keV

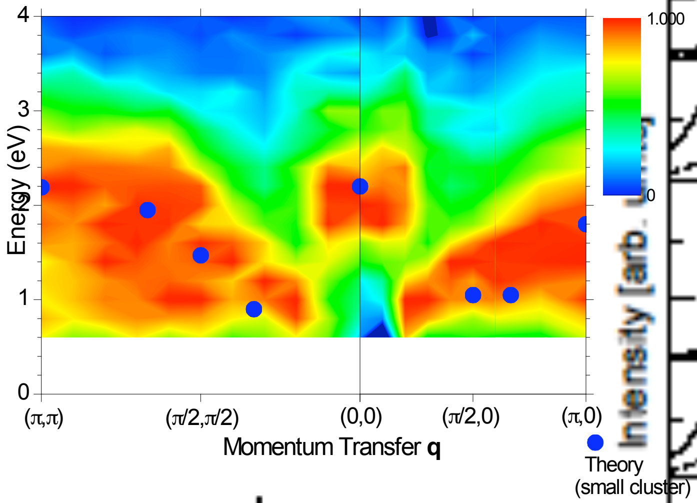
Schematic diagram of electronic states

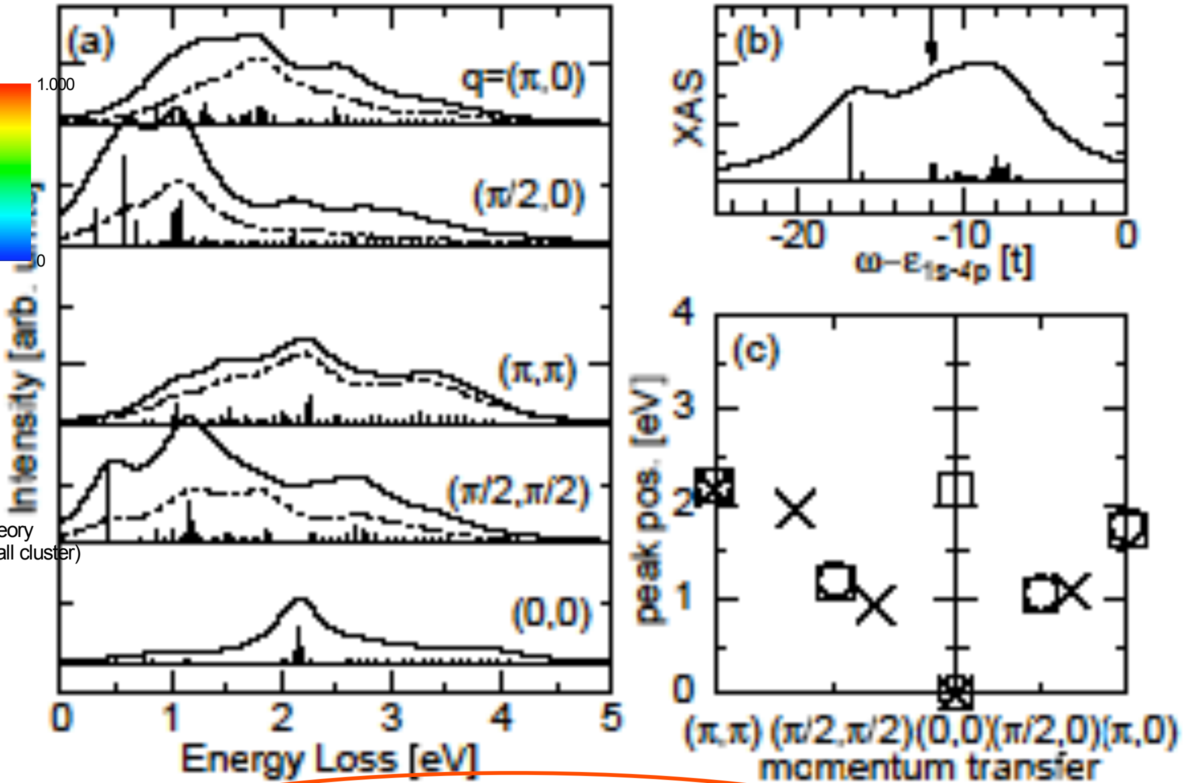


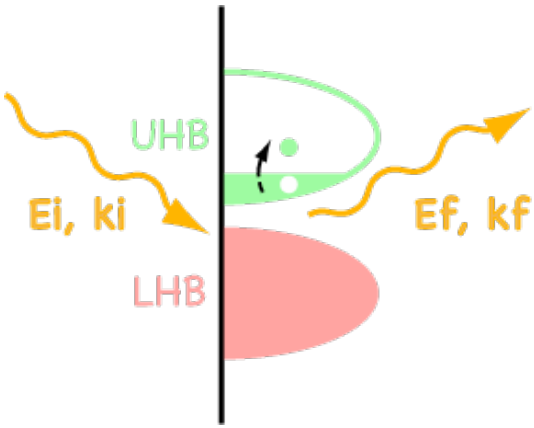
Electron doping

X=0.15

Calculated by K. Tsutsui







—— RIXS spectra

······· Dynamical density response function

The electron involved in dynamical density response function can be selected by RIXS !

K. Ishii, J. M. et al.,PRL. 94 ('05)207003

toward future

Required energy resolution

- Inter-band excitation: "U"~2eV

  Excitations across the Mott / charge-transfer gap

  ΔE~0.5eV

- Intra-band excitation: "*t*"~0.4eV

  Excitations within bands across the Fermi level

  ΔE~0.1eV

- Low-energy excitation: "*J*"~0.1eV

  Excitations related to the spin degree of freedom

  ΔE~0.05eV

Dynamical structure factor of IXS in the phonon energy region

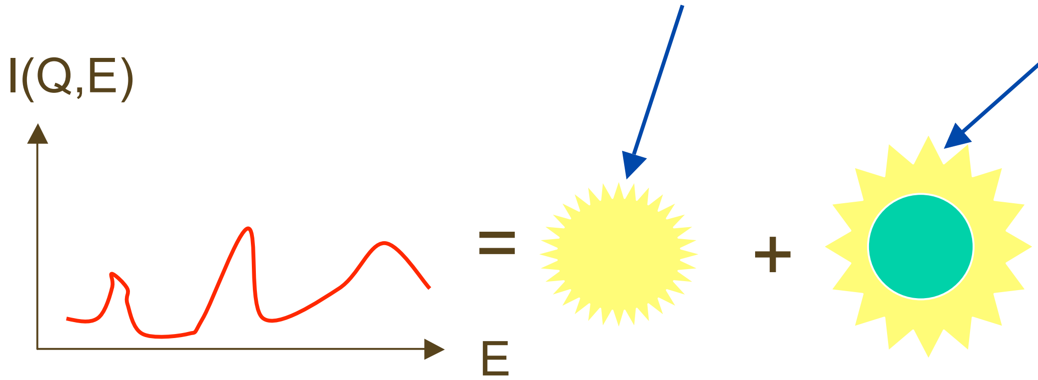
$$\varepsilon(Q,\omega)=\varepsilon_{el}(Q,\omega)+\varepsilon_{ion}(Q,\omega)-1$$

↓

$$\chi(Q,\omega)= -(Q^2/4\pi^2 N)\ 1/\varepsilon(Q,\omega)$$

↓

$$I(Q,\omega)= F(\varepsilon_{el})+G(\varepsilon_{el})\cdot H(\varepsilon_{ion})$$



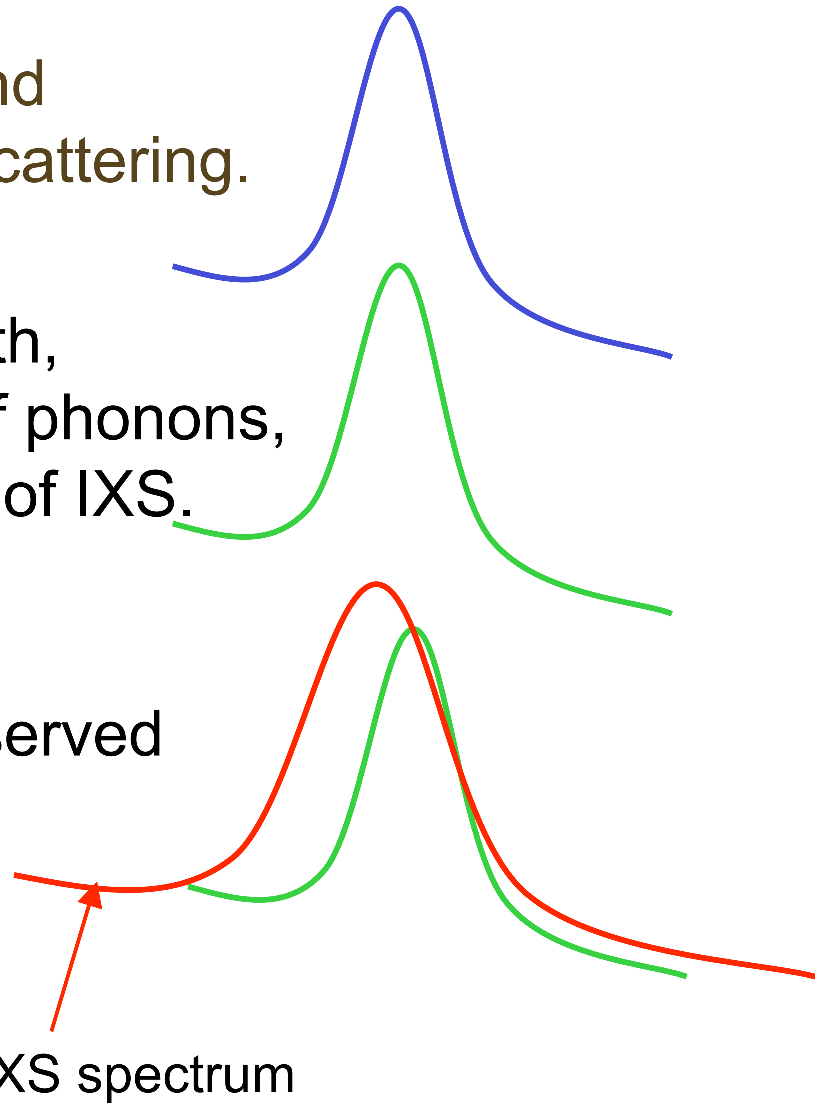
How to get the information on electric dynamical function

Collaboration between X-rays and Neutrons

1. Measure the phonon spectrum and dispersion by Neutron Inelastic Scattering.

2. Derive the information on the width, eigenvector and structure factor of phonons, and calculate the phonon intensity of IXS. (C-IXS)

3. Compare the C-IXS with the observed IXS spectrum.



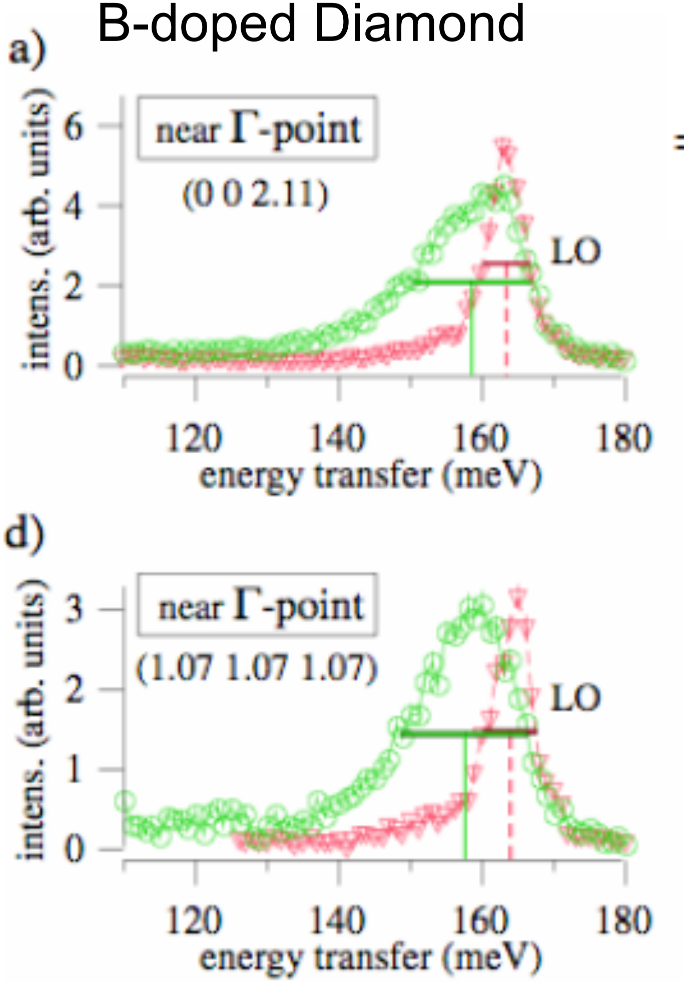
$$\epsilon(\mathbf{q},\omega)=\epsilon_{el}(\mathbf{q},\omega)+\epsilon_{ion}(\mathbf{q},\omega)-1.$$

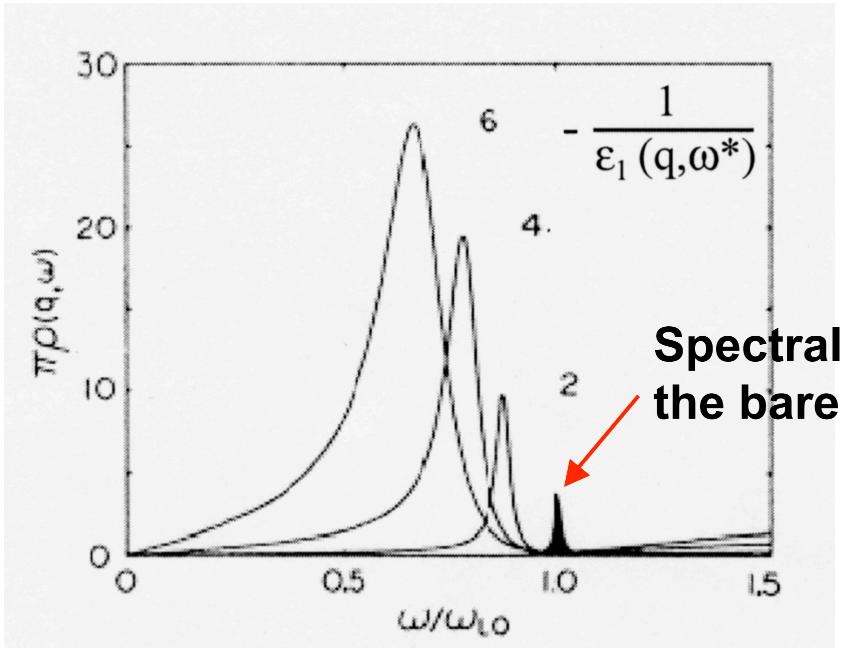
$$I(\mathrm{q},\boldsymbol{\omega}) = -\frac{1}{\pi}\mathrm{Im}\left[\frac{1}{\epsilon(\mathbf{q},\omega)}\right]$$

(electric + phonon) part

$$= -\frac{1}{\pi}\mathrm{Im}\left[\frac{1}{\epsilon_{el}(\mathbf{q},\omega)}\right] + \frac{\omega_{LO}^2(\mathbf{q})-\omega_{TO}^2}{\epsilon_{el}(\mathbf{q},\omega_{LO}^*)^2}\,\delta(\omega^2-\omega_{LO}^{*2}),$$

B-doped Diamond

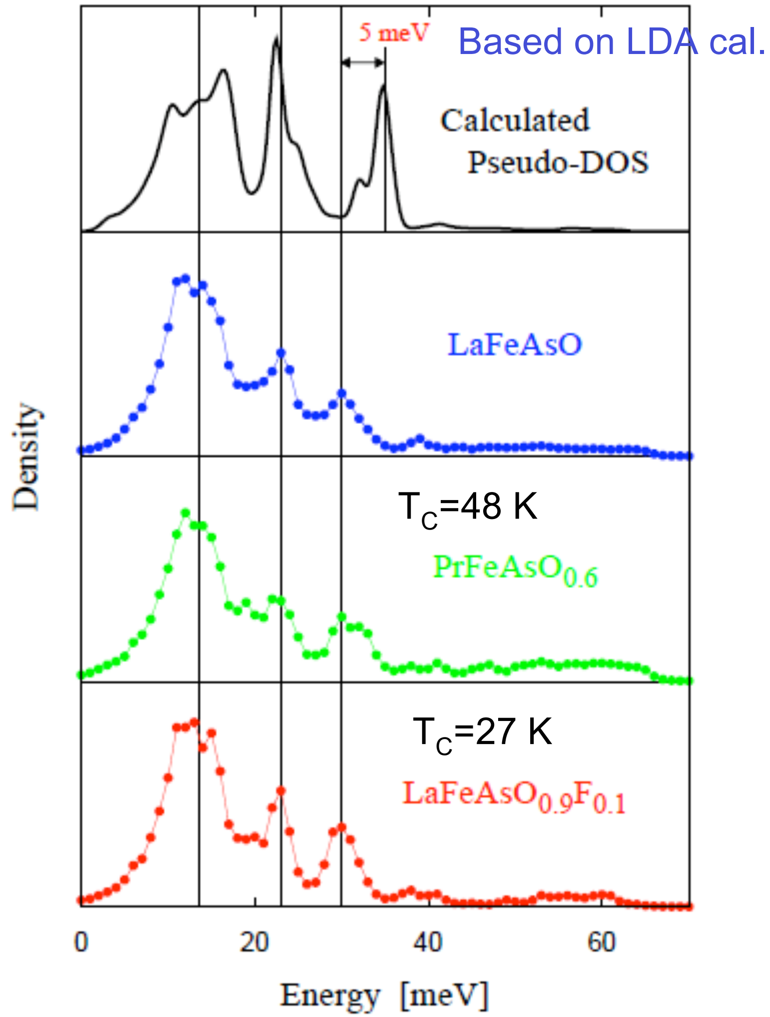


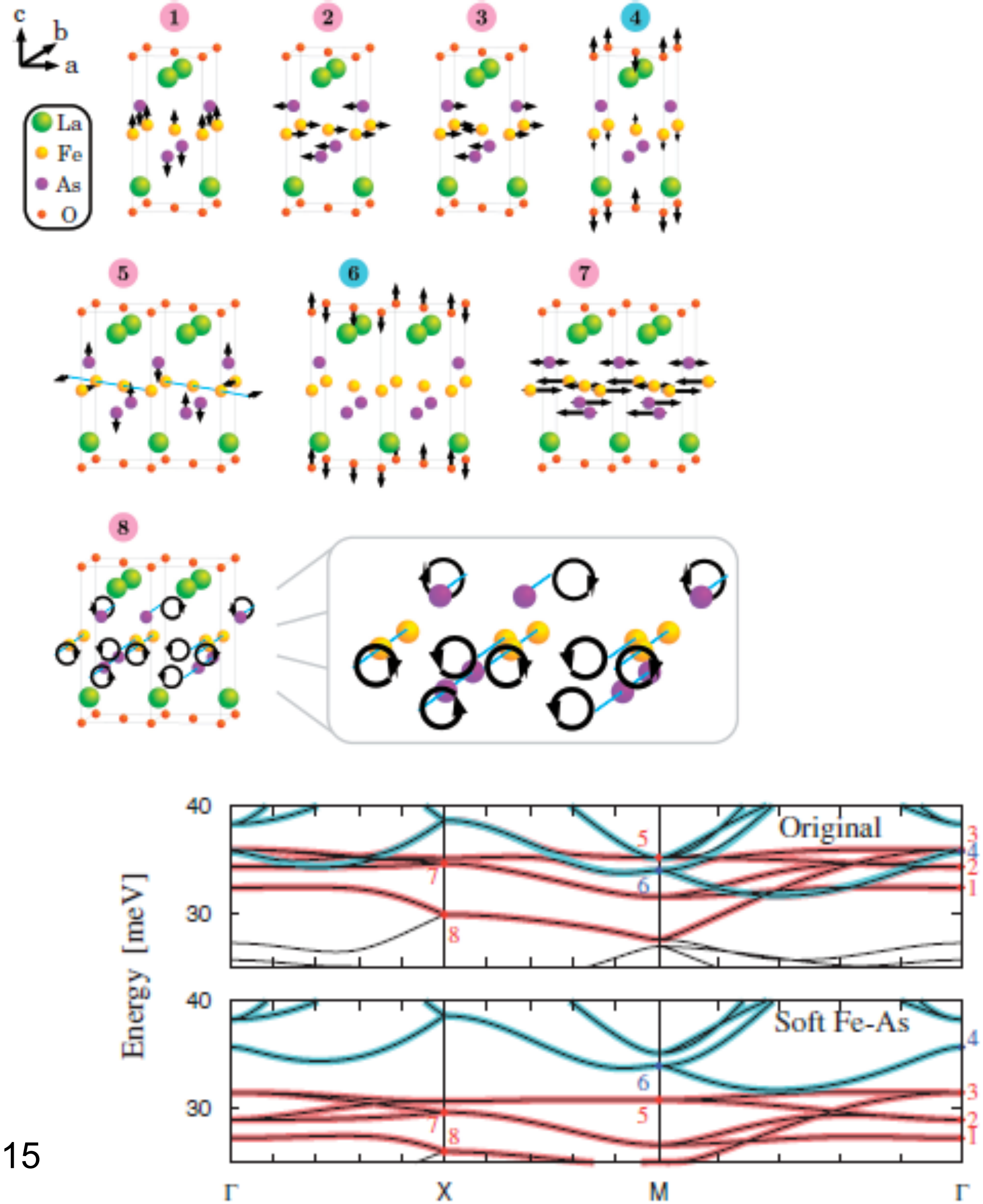


Spectral intensity of the bare LO-phonon

M. Tachiki et al., Phys. Rev. B38, ('88) 218.

Phonon DOS of Fe-based super.

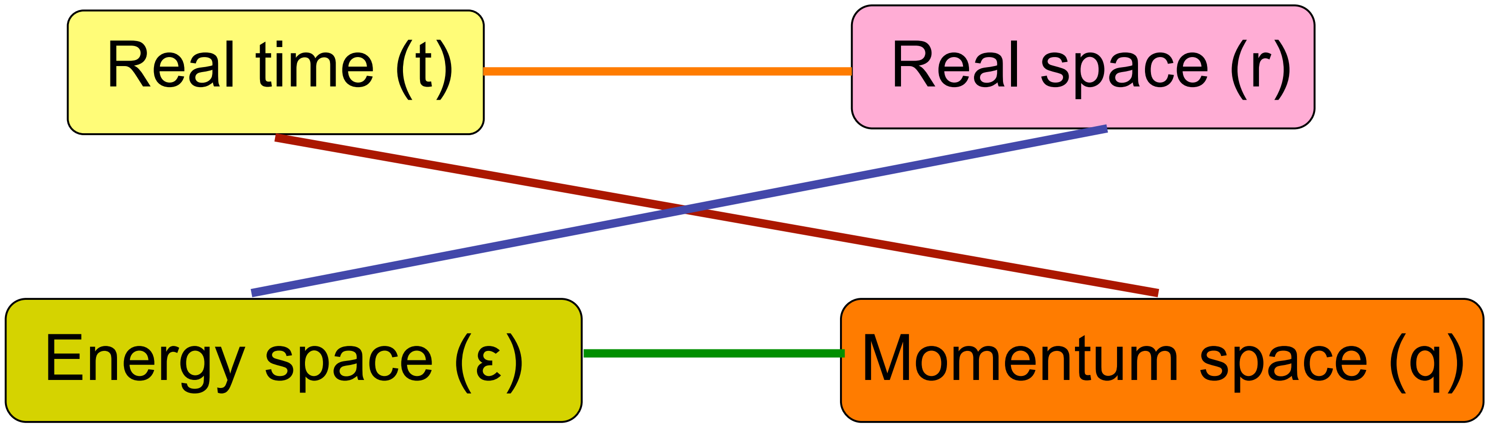




T. Fukuda, et al., J. Phys. Soc. Jpn. 77 ('08) 103715

Observation space

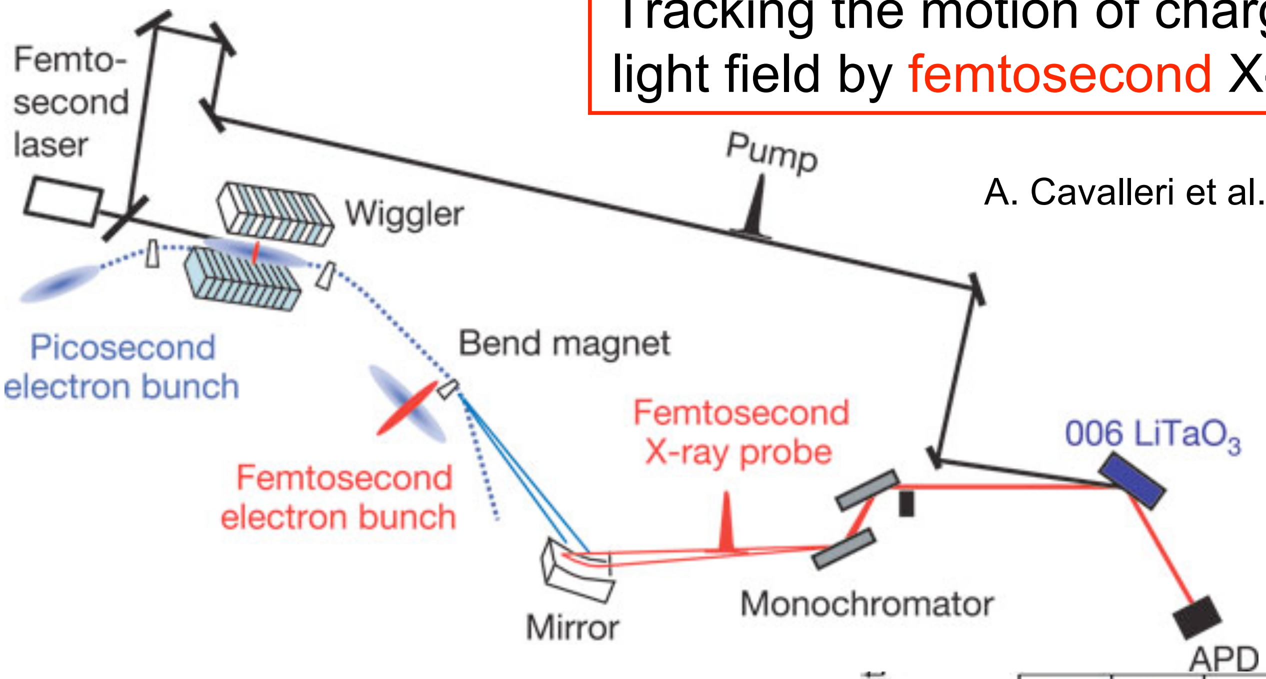
In what space should we measure physical properties?



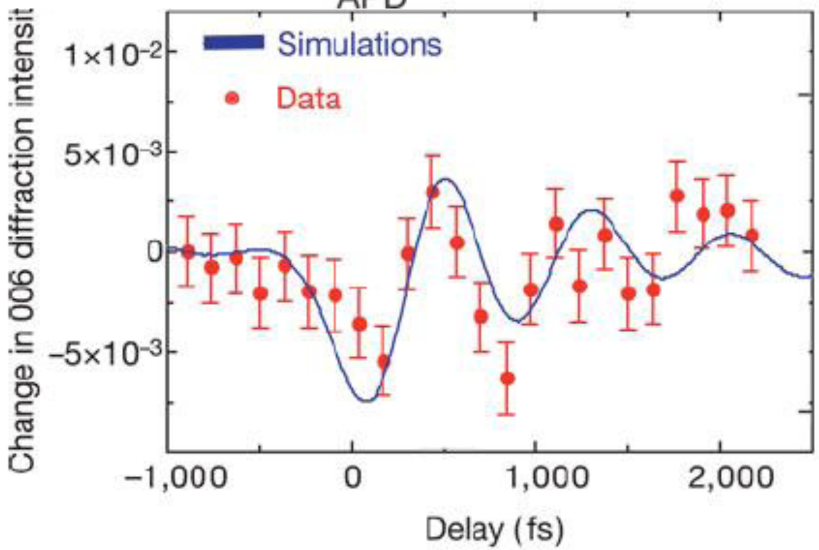
Dynamics in time domain

Tracking the motion of charges in a terahertz light field by femtosecond X-ray diffraction

A. Cavalleri et al., Nature 442 (‘06) 664



Time-dependent
Structure factor



Excitation of phonon polaritons in $LiTaO_3$

Collaborators for RIXS:

Experiment

K. Ikeuchi, I. Jarrige, M. Yoshida, T. Inami, J. Mizuki (SPring-8/JAEA)

H. Hiraka, K. Yamada, K. Kudo, Y. Koike, Y. Murakami (Tohoku Univ)

Y. Endoh (IIAS)

Theory

K. Tsutsui (SPring-8/JAEA)

T. Tohyama (Kyoto Univ.)

S. Maekawa (Tohoku Univ.)

Beamline

H. Ishii, Y. Q. Cai (Taiwan-BL, SPring-8)

Collaborators for Fe- based Superconductors:

JAEA

- T. Fukuda, S. Shamoto, M. Ishikado, J. Mizuki, M. Arai,

SPring-8/RIKEN, JASRI

- A. Q. R. Baron, S. Tsutsui, H. Uchiyama

JST

- H. Nakamura, M. Machida

AIST

- A. Iyo, H. Kito, H. Eisaki

TIT

- H. Hosono

Importance of the collaboration between Experiment and theory