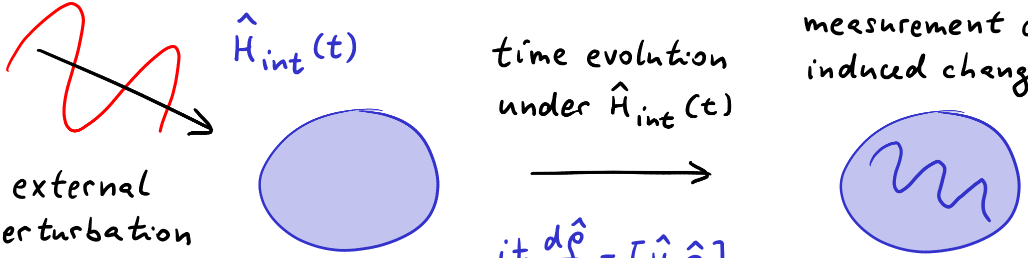
Many-body Green's Functions and experimental probes

① Linear response – Kubo Formula



$\hat H_{int}(t)$

external perturbation

system in equilibrium

time evolution under $\hat H_{int}(t)$

$$i\hbar\frac{d\hat\rho}{dt} = [\hat H, \hat\rho]$$

measurement of induced changes

$$\langle A\rangle = \mathrm{Tr}(\hat\rho\hat A)$$

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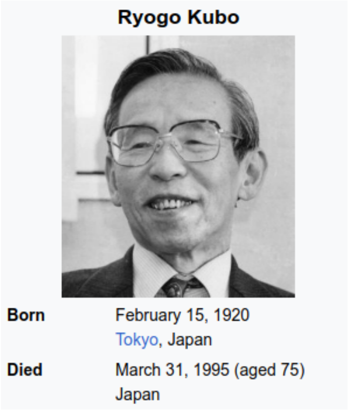


Ryogo Kubo

Born	February 15, 1920 Tokyo, Japan
Died	March 31, 1995 (aged 75) Japan

- evolution of the density operator – total Hamiltonian $\hat H + \hat H_{int}(t)$

$\hat\rho(t) = \hat\rho_0 + \Delta\hat\rho(t)$ $\hat\rho_0$: equilibrium $\frac{1}{Z}e^{-\beta\hat H}$, $\Delta\hat\rho$: induced changes

$$i\hbar\frac{d}{dt}\hat\rho = [\hat H + \hat H_{int}, \hat\rho] = \underbrace{[\hat H, \hat\rho_0]}_{0} + [\hat H, \Delta\hat\rho] + [\hat H_{int}, \hat\rho_0] + \underbrace{[\hat H_{int}, \Delta\hat\rho]}_{\text{beyond linear response}}$$

von Neumann equation

$$\rightarrow \quad i\hbar \frac{d}{dt}\Delta\hat{\rho}(t) = [\hat{H}, \Delta\hat{\rho}(t)] + [\hat{H}_{int}(t), \hat{\rho}_0]$$

Heisenberg picture for $\Delta\hat{\rho}$ and $\hat{H}_{int}$ - absorbs time-evolution due to $\hat{H}$

$$\Delta\hat{\rho}(t) = e^{\frac{i}{\hbar}\hat{H}t}\,\Delta\hat{\rho}(t)\,e^{-\frac{i}{\hbar}\hat{H}t} \qquad \hat{H}_{int}(t) = e^{\frac{i}{\hbar}\hat{H}t}\,\hat{H}_{int}(t)\,e^{-\frac{i}{\hbar}\hat{H}t}$$

Schrödinger picture

$$i\hbar\frac{d}{dt}\Delta\hat{\rho}(t) = i\hbar\left(\frac{d\,e^{\frac{i}{\hbar}\hat{H}t}}{dt}\Delta\hat{\rho}(t)\,e^{-\frac{i}{\hbar}\hat{H}t} + e^{\frac{i}{\hbar}\hat{H}t}\Delta\hat{\rho}(t)\,\frac{d\,e^{-\frac{i}{\hbar}\hat{H}t}}{dt}\right) + e^{\frac{i}{\hbar}\hat{H}t}\, i\hbar\,\frac{d\Delta\hat{\rho}}{dt}\, e^{-\frac{i}{\hbar}\hat{H}t}$$

$$= i\hbar\left(\frac{i}{\hbar}\hat{H}\,\Delta\hat{\rho}(t) - \frac{i}{\hbar}\Delta\hat{\rho}(t)\,\hat{H}\right) + e^{\frac{i}{\hbar}\hat{H}t}\left([\hat{H}, \Delta\hat{\rho}(t)] + [\hat{H}_{int}(t), \hat{\rho}_0]\right)e^{-\frac{i}{\hbar}\hat{H}t} = [\hat{H}_{int}(t), \hat{\rho}_0]$$

Final von Neumann equation $\quad i\hbar\frac{d}{dt}\Delta\hat{\rho}(t) = [\hat{H}_{int}(t), \hat{\rho}_0] \quad$ (all in Heisenberg pic.)

solution $\quad \Delta\hat{\rho}(t) = \frac{1}{i\hbar}\int_{-\infty}^{t}[\hat{H}_{int}(t'), \hat{\rho}_0]\,dt'$

- first order in $\hat{H}_{int}$
- higher orders arise from $[\hat{H}_{int}, \Delta\hat{\rho}]$

- evolution of the average $\langle A\rangle$

$$\langle A\rangle_t = \mathrm{Tr}\,\hat\rho\hat A \quad = \underbrace{\mathrm{Tr}\,\hat\rho_0\hat A}_{\text{equilibrium } \langle A\rangle_{eq}} \quad + \underbrace{\mathrm{Tr}\,\Delta\hat\rho(t)\hat A}_{\text{induced}}$$

$$\langle A\rangle_t - \langle A\rangle_{eq} = \mathrm{Tr}\left\{ e^{-\frac{i}{\hbar}\hat H t}\,\Delta\hat\rho(t)\,e^{\frac{i}{\hbar}\hat H t}\,\hat A \right\}$$

$\Delta\hat\rho(t)$ in Heisenberg

$$= \mathrm{Tr}\left\{\Delta\hat\rho(t)\,e^{\frac{i}{\hbar}\hat H t}\hat A e^{-\frac{i}{\hbar}\hat H t}\right\} = \mathrm{Tr}\left\{\Delta\rho(t)\,\hat A(t)\right\}$$

$$= \mathrm{Tr}\left\{\frac{1}{i\hbar}\int_{-\infty}^{t}\left[\hat H_{int}(t')\hat\rho_0 - \hat\rho_0\hat H_{int}(t')\right]dt'\;\hat A(t)\right\}$$

using cyclic property

$$= \frac{1}{i\hbar}\int_{-\infty}^{t}\mathrm{Tr}\left[\hat\rho_0\hat A(t)\hat H_{int}(t') - \hat\rho_0\hat H_{int}(t')\hat A(t)\right]dt'$$

Kubo Formula

$$\langle A\rangle_t - \langle A\rangle_{eq} = \frac{1}{i\hbar}\int_{-\infty}^{t}\mathrm{Tr}\,\hat\rho_0\left[\hat A(t),\hat H_{int}(t')\right]dt' = \frac{1}{i\hbar}\int_{-\infty}^{t}\left\langle\left[\underset{\uparrow}{\hat A(t)},\underset{\uparrow}{\hat H_{int}(t')}\right]\right\rangle_{eq}dt'$$

Heisenberg ops

- connection to many-body GF

external field

coupling to external field is of the form $\hat{H}_{int} = -\hat{B}\,\varphi$

internal variable of the system

$$\langle A\rangle_t = \langle A\rangle_{eq} - \frac{1}{i\hbar}\int_{-\infty}^{t} \langle[\hat{A}(t),\hat{B}(t')]\rangle_{eq}\,\varphi(t')\,dt'$$

$$= \langle A\rangle_{eq} + \int_{-\infty}^{\infty} \chi(t,t')\,\varphi(t')\,dt' \qquad \chi(t,t') = \frac{i}{\hbar}\langle[\hat{A}(t),\hat{B}(t')]\rangle_{eq}\,\vartheta(t-t')$$

susceptibility – negatively taken G_R

Ex1 magnetic susceptibility

electron magnetic moment $\hat{\bar{m}} = -g\mu_B\hat{\bar{S}}$

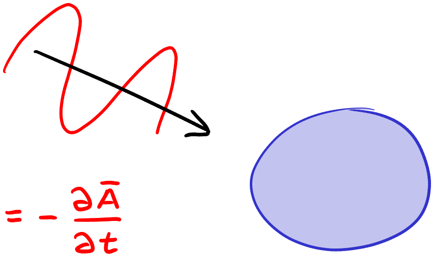
coupling to external mag. field $\hat{H}_{int} = -\sum \bar{m}\cdot\bar{B} = \sum_{q} g\mu_B\,\bar{S}_{-q}\cdot\bar{B}_q$

induced mag. moment $\langle m_q^\alpha\rangle_t = \int_{-\infty}^{\infty}\chi_{\alpha\beta}(q,t,t')\,B_q^\beta(t')\,dt'$

(α-component)

$$\hookrightarrow \quad \chi_{\alpha\beta} = (g\mu_B)^2\,\frac{i}{\hbar}\langle[\hat{S}_q^\alpha(t),\hat{S}_{-q}^\beta(t')]\rangle\,\vartheta(t-t')$$

Ex2 optical conductivity



$\bar{E} = -\frac{\partial \bar{A}}{\partial t}$

$\bar{A}(\bar{r}) = \sum_{q} e^{i\bar{q}\cdot\bar{r}}\bar{A}_q$

$$\xrightarrow[\text{time evolution}]{\hat{H}_{int} = -\hat{j}\cdot\bar{A}}$$

induced current density

$\langle\bar{j}\rangle = \sigma\bar{E}$

↑

optical conductivity

- coupling to EM field via vector potential entering the kinetic energy

$$\frac{\hbar}{i}\nabla \to \frac{\hbar}{i}\nabla - q\bar{A} \qquad \hat{H}_{int} = \hat{T}_A - \hat{T} \qquad \delta\hat{H}_{int} = -\hat{j}\cdot\delta\bar{A} \to \hat{j} = -\frac{\delta\hat{H}_{int}}{\delta\bar{A}}$$

$$\hat{T}_A = \int d^3\bar{r} \sum_G \hat{\psi}_G^+(\bar{r}) \frac{1}{2m}\left[\frac{\hbar}{i}\nabla + e\bar{A}(\bar{r})\right]^2 \hat{\psi}_G(\bar{r})$$

$$\hat{T}_A - \hat{T} = -\frac{1}{2}\int d^3\bar{r}\, \underbrace{\left(-\frac{e}{m}\bar{A}\hat{n}\right)}_{\hat{j}_d \text{ - diamagnetic}}\cdot\bar{A} - \int d^3\bar{r}\, \underbrace{\left(-\frac{e\hbar}{2mi}\right)\sum_G\left(\hat{\psi}_G^+\nabla\hat{\psi}_G - \hat{\psi}_G\nabla\hat{\psi}_G^+\right)}_{\hat{j}_p \text{ - paramagnetic current density}}\cdot\bar{A}$$

- electrons in a single band with the dispersion ε_k, vector potential $\bar{A}(\bar{r}) = \sum_q e^{i\bar{q}\cdot\bar{r}}\bar{A}_q$

$$\hat{j}_d^{\alpha}(q) = \sum_\beta \hat{\tau}_{\alpha\beta}\bar{A}_{\beta q} \qquad \hat{\tau}_{\alpha\beta} = \sum_{k\sigma}\frac{e^2}{\hbar^2}\frac{\partial \varepsilon_k^2}{\partial k_\alpha \partial k_\beta}\hat{c}^+_{k\sigma}\hat{c}_{k\sigma} \qquad \hat{j}_p^{\alpha}(q) = -e\sum_{k\sigma}\frac{1}{\hbar}\frac{\partial \varepsilon_k}{\partial k_\alpha}\hat{c}^+_{k\sigma}\hat{c}_{k+q\sigma}$$

For free particles with $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$: $\rightarrow \frac{e^2}{m}\delta_{\alpha\beta}\hat{c}^+_{k\sigma}\hat{c}_{k\sigma}$ $\qquad \frac{\hbar k_\alpha}{m} \leftarrow$

- application of kubo formula

$$\langle j\rangle_t = \langle j\rangle_{eq} - \frac{1}{i\hbar}\int_{-\infty}^{t}\langle[\hat{j}(t), \hat{H}_{int}(t')]\rangle_{eq}\,dt' \qquad \hat{H}_{int} = -\sum_\beta \hat{j}_p^{\beta}(q)A_{\beta q}$$

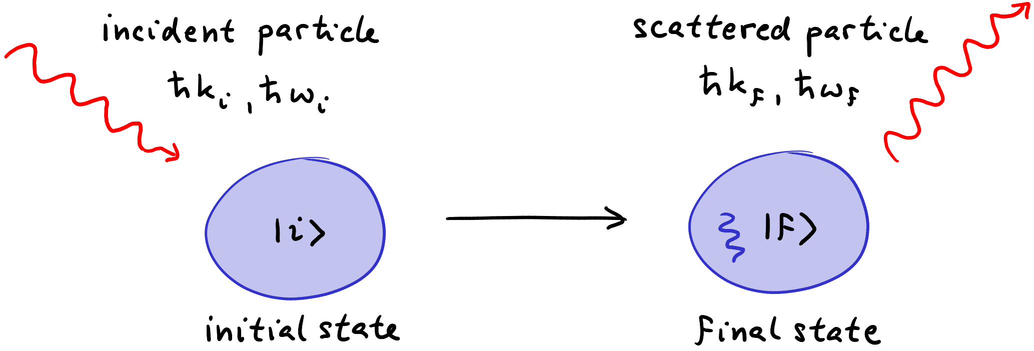
$$\langle j^\alpha\rangle = \underbrace{\sum_\beta \langle\hat{\tau}_{\alpha\beta}\rangle_{eq}A_\beta(t)}_{\text{diamagnetic}} + \underbrace{\int_{-\infty}^{\infty}dt\,\Pi_{\alpha\beta}(t-t')A_\beta(t')}_{\text{paramagnetic}} \qquad \xleftarrow{} \underbrace{\frac{i}{\hbar}\langle[\hat{j}_p^{\alpha}(t), \hat{j}_p^{\beta}(t')]\rangle\,\vartheta(t-t')}_{\text{current-current corr. fun.}}$$

optical conductivity

$$\sigma_{\alpha\alpha}(\omega) = \frac{\langle j_\alpha\rangle}{E_\alpha} = \frac{\langle\hat{\tau}_{\alpha\alpha}\rangle + \Pi_{\alpha\alpha}(\omega)}{i(\omega+i0^+)} \rightarrow \mathrm{Re}\,\sigma = -\pi\underbrace{\left[\langle\hat{\tau}\rangle + \mathrm{Re}\,\Pi(\omega=0)\right]}_{\text{compensated unless SC}}\delta(\omega) + \frac{\mathrm{Im}\,\Pi(\omega)}{\omega}$$

$$\bar{E} = i(\omega+i0^+)\bar{A}$$

② Scattering experiment – general description



system absorbs energy

$$E = \hbar\omega_i - \hbar\omega_f$$

and momentum

$$\hbar q = \hbar k_i - \hbar k_f$$

- quantitative description – differential cross-section

$$\frac{d^2\sigma}{d\Omega\, dE} = \frac{\#\text{ particles scattered into } d\Omega \,\&\, dE \text{ per time unit per target}}{\text{incoming flux} = \#\text{ particles per time unit per unit area}}$$

- Fermi's Golden rule

$$\frac{d^2\sigma}{d\Omega\, dE} \sim \sum_{i\,f} \Big| \overbrace{\langle k_f| \otimes \langle f|}^{\text{final}} \; \hat{M} \; \overbrace{|i\rangle \otimes |k_i\rangle}^{\text{initial}} \Big|^2 \; \delta(E_f + \hbar\omega_f - E_i - \hbar\omega_i)$$

relevant states

↑ scattering operator

energy conservation

in thermal equilibrium

$$\frac{d^2\sigma}{d\Omega\, dE} \sim \frac{1}{Z}\sum_{if} e^{-\beta E_i}\, |\langle f|\overset{\substack{\text{momentum transfer}\\ \downarrow}}{\hat{M}_{-q}}|i\rangle|^2\, \delta[E_f - E_i - \overbrace{(\hbar\omega_i - \hbar\omega_f)}^{\text{energy transfer } E}] = \underset{\text{structure factor}}{S(q,E)}$$

scattering operator acting on the system

- typically $\hat{H}_{int}$, but may be more complex
- $|k_i\rangle, |k_f\rangle$ as external parameters, usually $\hat{M}$ depends on momentum transfer q

- connection to GF

bosonic GF in energy domain $$G_R(E) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, e^{\frac{i}{\hbar}(E+i0^+)t}\, \langle[\hat{A}(t), \hat{A}^+]\rangle\, \vartheta(t)$$

Spectral function

$$A(E) = \frac{1}{Z}\sum_{mn} e^{-\beta E_m}\left\{|\langle n|\hat{A}^+|m\rangle|^2\,\delta[E-(E_n-E_m)] - |\langle n|\hat{A}|m\rangle|^2\,\delta[E+(E_n-E_m)]\right\}$$

↖ relabel $m \leftrightarrow n$ & $e^{-\beta E_m} = e^{-\beta E_n}\, e^{-\beta(E_m-E_n)}$

$$= \frac{1}{Z}\sum_{mn} e^{-\beta E_m}\, |\langle n|\hat{A}^+|m\rangle|^2\,\delta[E-(E_n-E_m)]\,(1-e^{-\beta E})$$

susceptibility $$\chi(q,E) = \frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, e^{\frac{i}{\hbar}(E+i0^+)t}\langle [\underset{\hat A}{\hat M_q(t)}, \underset{\hat A^+}{\hat M_{-q}}]\rangle\, \vartheta(t)$$

$$S(q,E) = (1-e^{-\beta E})^{-1} A = (1-e^{-\beta E})^{-1}\left(-\frac{1}{\pi}\mathrm{Im}\, G_R\right) = \underbrace{(1-e^{-\beta E})^{-1}}_{N_B(E)+1}\frac{1}{\pi}\mathrm{Im}\,\chi$$

$$= \frac{1}{\pi}[N_B(E)+1]\,\mathrm{Im}\,\chi(q,E)$$

- sum rule $\int dE\,[N_B(E)+1]\,A(E) = \langle \hat A \hat A^+\rangle$

$$\int_{-\infty}^{\infty} S(q,E)\,dE = \frac{1}{\pi}\int_{-\infty}^{\infty} dE\,[N_B(E)+1]\,A(E) = \frac{1}{\pi}\langle \hat M_q \hat M_{-q}\rangle$$

→ structure factor = energy-resolved correlations

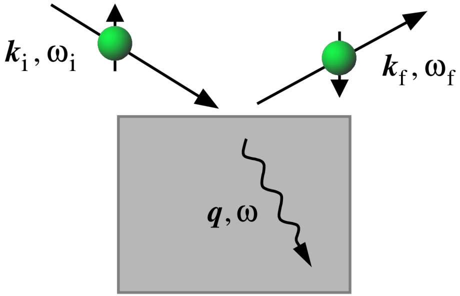
- emission × absorption intensities

anti-Stokes: excitation destroyed $E<0$

Stokes: excitation created $E>0$

$$\frac{S(-q,-E)}{S(q,E)} = \frac{(1-e^{+\beta E})^{-1}}{(1-e^{-\beta E})^{-1}}\,\overbrace{\frac{\chi(-q,-E)}{\chi(q,E)}}^{-1} = e^{-\beta E}$$

③ Neutron scattering



- neutron – no charge, magnetic moment

$$\hat{\bar{m}}_n = -g\mu_N \frac{1}{\hbar}\hat{\bar{I}} \quad \leftarrow \text{spin-}\tfrac{1}{2}$$

g-factor $g = 3.826\ldots$

nuclear magneton $\mu_N = \frac{e\hbar}{2m_p}$

- interactions of neutrons with the sample

1) nuclei – heavy, small mag. moment

contact interaction

potential $\sim \sum_{R} \delta(\bar{r} - \underset{\substack{\uparrow \\ \text{lattice}}}{\bar{R}} - \underset{\substack{\uparrow \\ \text{phonons}}}{\bar{u}_R})$

2) electrons – light, large mag. moment

dipole-dipole interaction $-\hat{\bar{m}}_n \cdot \bar{B}_e$

dipolar field from electron ↗

$$\hat{\bar{m}}_e = -\mu_B \frac{1}{\hbar}(g\hat{\bar{S}} + \hat{\bar{L}}) \qquad g = 2.002\ldots$$

Bohr magneton $\mu_B = \frac{e\hbar}{2m_e}$

- non-magnetic scattering (nuclear)

$$\langle k_f| \otimes \langle f| \hat{H}_{int} |i\rangle \otimes |k_i\rangle = \int d^3\bar{r}\; e^{-i\bar{k}_f\cdot\bar{r}}\, e^{i\bar{k}_i\cdot\bar{r}} \langle f| \sum_R \delta(\bar{r}-\bar{R}-\hat{\bar{u}}_R)|i\rangle =$$

↖ ↗

neutron wave functions $|k\rangle \rightarrow e^{i\bar{k}\cdot\bar{r}}$

$$= \langle f|\sum_R e^{i\bar{q}\cdot\bar{R}}\, e^{i\bar{q}\cdot\hat{\bar{u}}_R}\,|i\rangle \approx \langle f|\sum_R e^{i\bar{q}\cdot\bar{R}}|i\rangle + i\bar{q}\cdot\langle f|\overbrace{\sum_R e^{i\bar{q}\cdot\bar{R}}\,\hat{\bar{u}}_R}^{\text{Fourier component } \hat{\bar{u}}_{-q}}|i\rangle$$

$\bar{q} = \bar{k}_i - \bar{k}_f$ ↖ expand as $\hat{1} + i\bar{q}\cdot\hat{\bar{u}}_R$

1) elastic neutron scattering – $\langle f|\sum_R e^{i\bar{q}\cdot\bar{R}}|i\rangle \rightarrow |f\rangle = |i\rangle$, $E = 0$

static structure factor $\sum_R e^{i\bar{q}\cdot\bar{R}} \sim \sum_G \delta_{\bar{q},\bar{G}}$ Bragg peaks → lattice geometry

2) inelastic neutron scattering (INS)

dynamic structure factor $i\bar{q}\cdot\langle f|\hat{u}_{-q}|i\rangle \sim \langle f|\overbrace{\hat{a}_{-q} + \hat{a}^{+}_{q}}^{\text{phonon operators}}|i\rangle$

→ phonon dynamics (via $\bar{q}$-scan of $E = \hbar\omega_q$)

- magnetic scattering of neutrons due to $-\hat{\bar{m}}_n \cdot \hat{\bar{B}}_e$

magnetic field of electron magnetic moment $\hat{\bar{m}}_e$ at origin: $\hat{\bar{B}}_e = \nabla \times \hat{\bar{A}} = \nabla \times \left[\frac{\mu_0}{4\pi} \left(\hat{\bar{m}}_e \times \frac{\bar{r}}{r^3} \right) \right]$

$$\langle k_f | \otimes \langle f | \hat{H}_{int} | i \rangle \otimes | k_i \rangle \sim \int d^3\bar{r}\, e^{-i\bar{k}_f \cdot \bar{r}} e^{i\bar{k}_i \cdot \bar{r}} \sum_j \langle f | \nabla \times \left(\hat{\bar{m}}_j \times \frac{\bar{r} - \hat{\bar{r}}_j}{|\bar{r} - \hat{\bar{r}}_j|^3} \right) | i \rangle =$$

sum over electrons

$$\langle f | \sum_j e^{i\bar{q}\cdot\hat{\bar{r}}_j} \frac{\bar{q} \times (\hat{\bar{m}}_j \times \bar{q})}{q^2} | i \rangle = \langle f | \bar{q}^0 \times (\hat{\bar{M}}_{-q} \times \bar{q}^0) | i \rangle = \langle f | \hat{\bar{M}}_{-q} - (\hat{\bar{M}}_{-q} \cdot \bar{q}^0)\, \bar{q}^0 | i \rangle$$

M component ⊥ $\bar{q}$

non-polarized case - scalar product $\langle \, \rangle^* \cdot \langle \, \rangle$

$$|\langle \dots \rangle|^2 = \langle i | \hat{\bar{M}}_{\perp q} | f \rangle \cdot \langle f | \hat{M}_{\perp, -q} | i \rangle = \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q^2} \right) \langle i | \hat{M}^\alpha_q | f \rangle \langle f | \hat{M}^\beta_{-q} | i \rangle$$

Final structure factor

$$S(q, E) \sim \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q^2} \right) [N_B(E) + 1]\, \mathrm{Im}\, \chi_{\alpha\beta}(q, E)$$

with $\chi_{\alpha\beta}(q, t) = \frac{i}{\hbar} \langle [\hat{M}^\alpha_q(t), \hat{M}^\beta_{-q}] \rangle\, \theta(t)$

elastic part $(E = 0)$

→ magnetic Bragg peaks

inelastic part

→ magnetic excitations

OAK RIDGE
National Laboratory

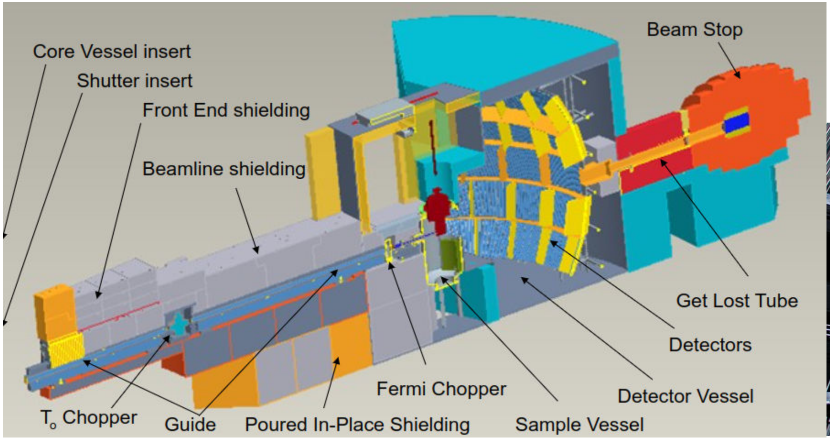
ORNL hosts two of the world's most powerful sources of neutrons for research:

High Flux Isotope Reactor (HFIR)

85MW reactor constructed 1965 to produce Pu, Cm, ...

Spallation Neutron Source (SNS)

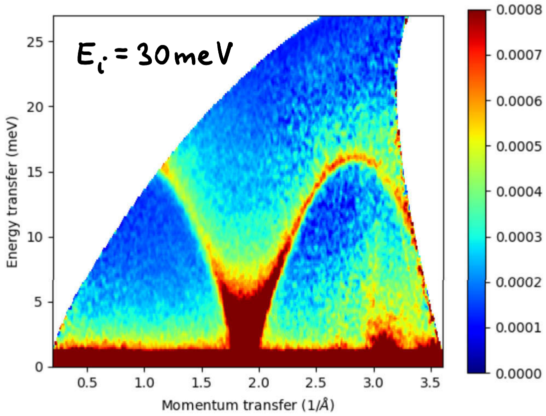
neutrons produced by microsecond proton pulses to a steel target filled with liquid mercury



SEQUOIA

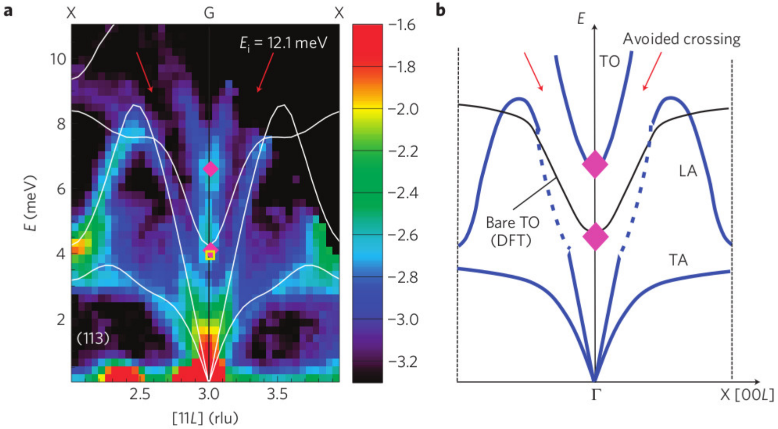
direct geometry time-of-flight chopper spectrometer

- INS on graphite

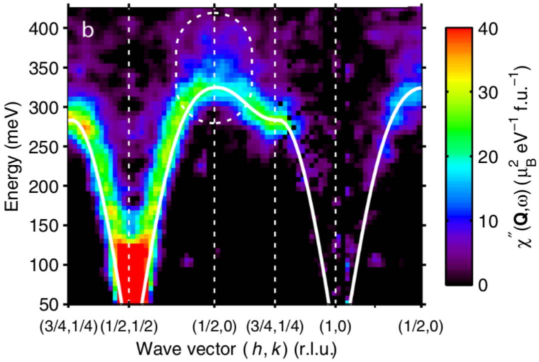


YQ Cheng, ORNL

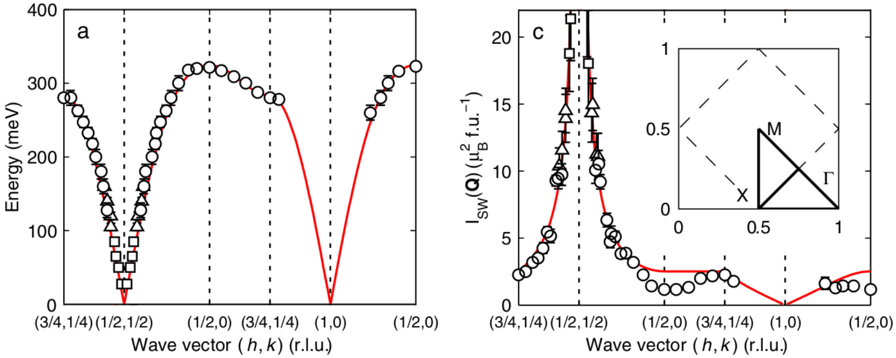
- INS on PbTe – anharmonic effects



Delaire et al., Nat. Mater. 10, 614 (2011)



La_2CuO_4



Headings et al., Phys. Rev. Lett. 105, 247001 (2010)

④ Light scattering

- quantized vector potential (Coulomb gauge $\nabla \cdot \bar{A} = 0$)

$$\hat{A}(\bar{r}) = \frac{1}{\sqrt{\Omega}} \sum_{q\lambda} e^{i\bar{q}\cdot\bar{r}} \; \bar{e}_{q\lambda} \sqrt{\frac{\hbar}{2\varepsilon_0 \omega_q}} \left(\hat{a}_{q\lambda} + \hat{a}^{+}_{-q\lambda} \right)$$

photon polarization ↗ photon frequency $\omega_q = cq$

- coupling of charged particles to EM field

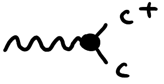
$$\langle k_f | \otimes \langle f | \; \hat{H}_{int} \; | i \rangle \otimes | k_i \rangle$$

$$\hat{H}_{int} = - \sum_{q} \hat{j}_p^{\alpha}(q) \, \hat{A}^{\alpha}_{-q} + \frac{1}{2} \sum_{q_1 q_2} \hat{\tau}_{\alpha\beta}(q_1+q_2) \, \hat{A}^{\alpha}_{-q_1} \hat{A}^{\beta}_{-q_2}$$

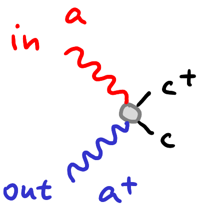
one-photon $(\hat{a}+\hat{a}^{+})$ two-photon $(\hat{a}+\hat{a}^{+})(\hat{a}+\hat{a}^{+})$

diagrammatically:

$\hat{j}_p \cdot A$



$\hat{\tau} \cdot A \cdot A$

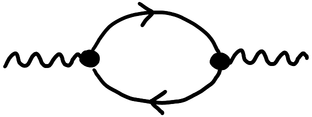


- scattering to second order in $\hat{H}_{int}$ (to capture resonant Raman & RIXS)

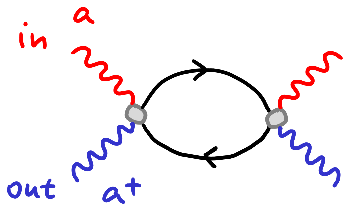
$$S(q,E) \sim |\langle \bar{k}_f \bar{e}_f| \otimes \langle f| \Big(\underbrace{\hat{H}_{int}}_{\text{First order}} + \underbrace{\hat{H}_{int} \frac{1}{\hat{H}-E_i} \hat{H}_{int}}_{\text{second order}} \Big) |i\rangle \otimes |\bar{k}_i \bar{e}_i\rangle|^2 \, \delta(E_f - E_i - E)$$

1) $\langle f|\hat{j}_p(q)|i\rangle$ single-photon absorption

→ optical conductivity



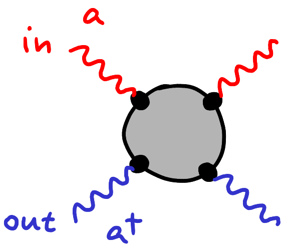
2) $\langle f|\hat{\tau}_{\alpha\beta}(q)|i\rangle$ non-resonant Raman channel

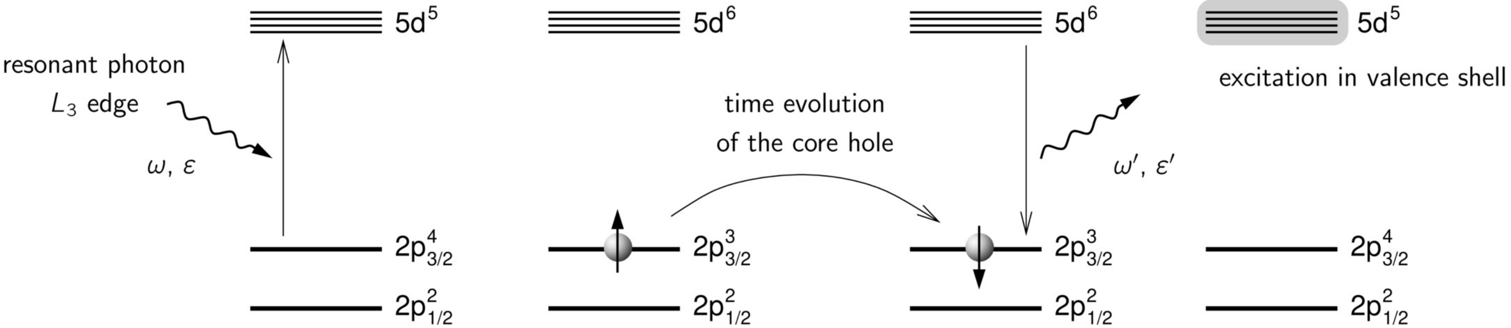


3) $$\langle f| \sum_q \hat{j}_p(q)\hat{A}_{-q} \frac{1}{\hat{H}-E_i} \sum_q \hat{j}_p(q)\hat{A}_{-q} |i\rangle$$

↖ dipole transitions ↗

$$= \langle f|\hat{R}|i\rangle$$ resonant Raman channel





resonant photon

L_3 edge

ω, ε

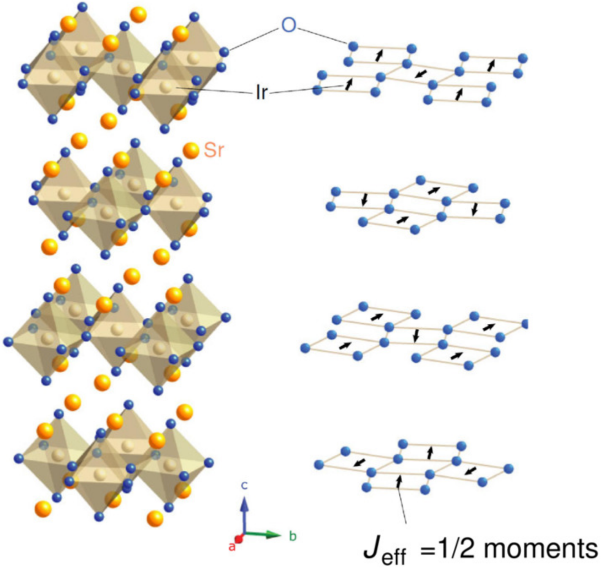
time evolution

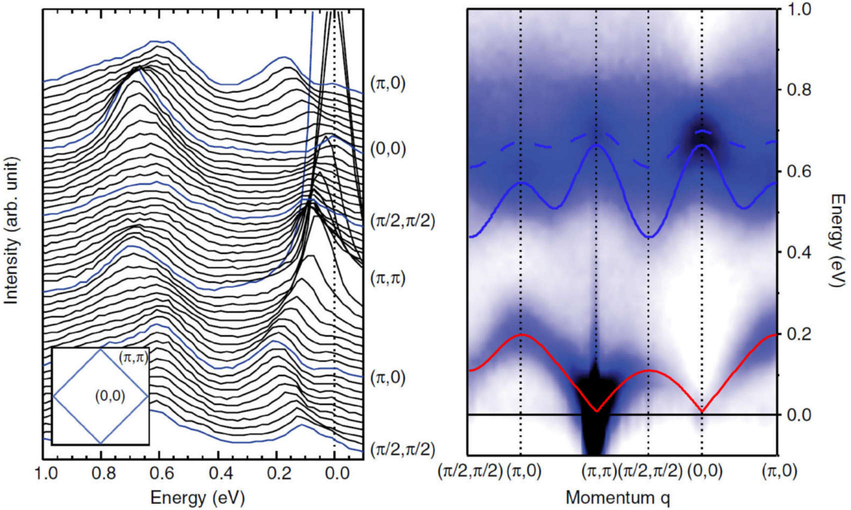
of the core hole

ω', ε'

excitation in valence shell

Sr_2IrO_4



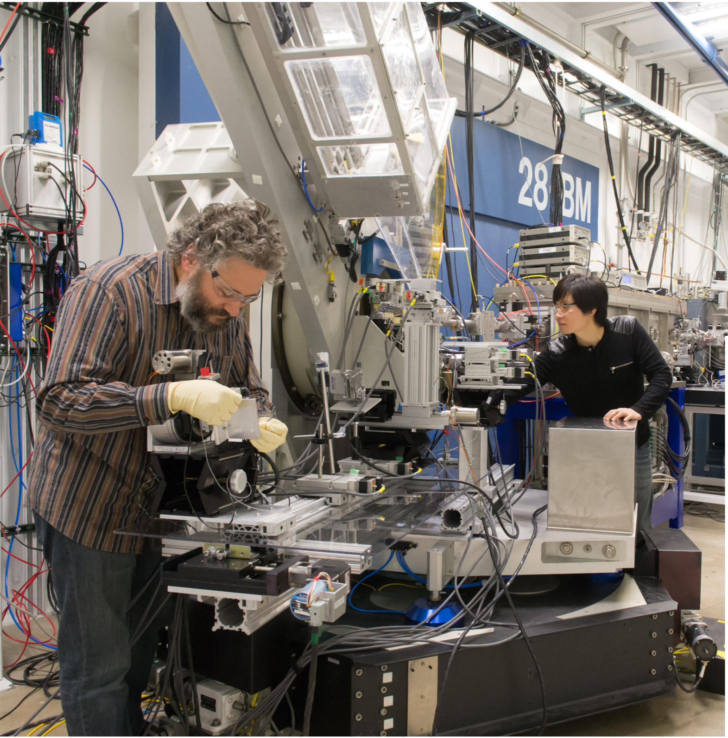


Kim et al., Phys. Rev. Lett. 108, 177003 (2012)

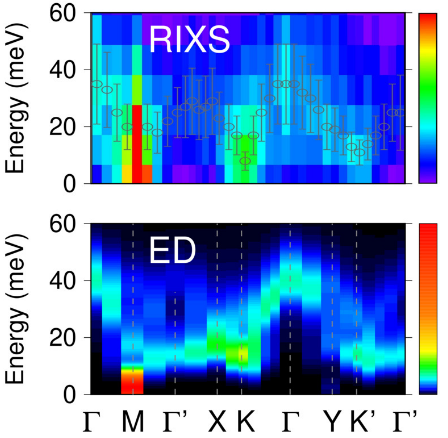
Argonne
NATIONAL
LABORATORY

RIXS at Advanced Photon Source

- designed for iridium L_3 edge (11.215keV)
- high resolution of 10meV



Kim et al., Phys. Rev. X 10, 021034 (2020)



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