Theory of Resonant X-Ray Scattering with Applications to high-Tc Cuprates

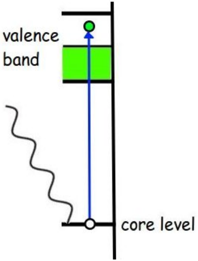
David Benjamin (Harvard), Eugene Demler (Harvard), Peter Abbamonte (Illinois), Israel Klich (UVA), Dmitry Abanin (Perimeter)

November 7, 2013

Plan

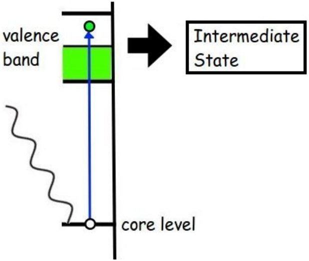
- Introduction
- REXS data
- Model
- Results
- Formalism
- RIXS results and data

Resonant x-ray scattering



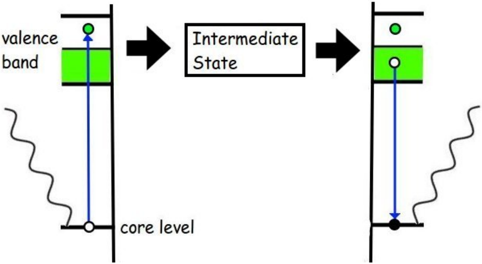
- Photon knocks core electron to valence band at $\mathbf{R}_m$.

Resonant x-ray scattering



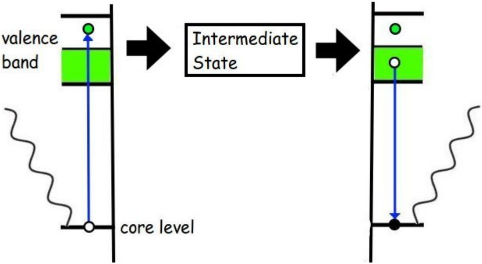
- Photon knocks core electron to valence band at $\mathbf{R}_m$.
- Things happen (optional)

Resonant x-ray scattering



- Photon knocks core electron to valence band at $\mathbf{R}_m$.
- Things happen (optional)
- Electron fills core hole at $\mathbf{R}_m$.

Resonant x-ray scattering

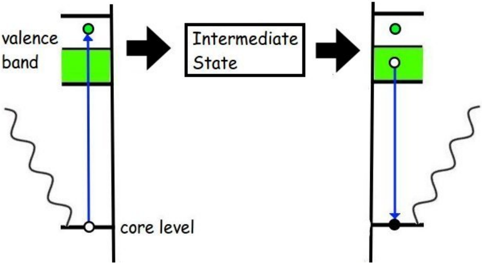


- Photon knocks core electron to valence band at $\mathbf{R}_m$.
- Things happen (optional)
- Electron fills core hole at $\mathbf{R}_m$.

Intensity $\propto$

$$\sum_f |A_{i\to f}|^2 \delta(E_f - E_i - \Delta\omega)$$

Resonant x-ray scattering



- Photon knocks core electron to valence band at $\mathbf{R}_m$.
- Things happen (optional)
- Electron fills core hole at $\mathbf{R}_m$.

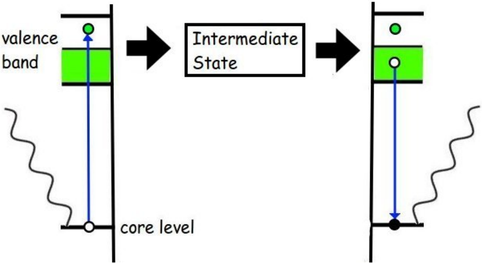
Intensity $\propto$

$$\sum_f |A_{i\to f}|^2 \delta(E_f - E_i - \Delta\omega)$$

$$A_{i\to f} = \sum_m e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{R}_m} \langle f | d_m \underbrace{(\omega + H_m - E_i + i\Gamma)^{-1}}_{\text{resonance}} d_m^\dagger | i \rangle,$$

where incident photon is $\mathbf{k}_i, \omega$, $1/\Gamma$ is core hole lifetime and $H_m = H_0 +$ core hole potential at $\mathbf{R}_m$, and outgoing photon is $\mathbf{k}_f, \omega - \Delta\omega$.

Resonant x-ray scattering



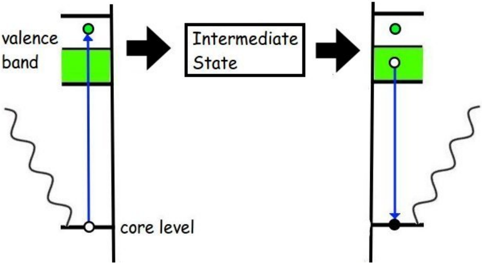
- Photon knocks core electron to valence band at $\mathbf{R}_m$.
- Things happen (optional)
- Electron fills core hole at $\mathbf{R}_m$.

Intensity $\propto$
$$\sum_f |A_{i\to f}|^2 \delta(E_f - E_i - \Delta\omega)$$

$$A_{i\to f} = \sum_m e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot\mathbf{R}_m} \langle f| d_m \underbrace{(\omega + H_m - E_i + i\Gamma)^{-1}}_{\text{resonance}} d_m^\dagger |i\rangle,$$

where incident photon is $\mathbf{k}_i, \omega$, $1/\Gamma$ is core hole lifetime and $H_m = H_0+$ core hole potential at $\mathbf{R}_m$, and outgoing photon is $\mathbf{k}_f, \omega - \Delta\omega$.

Resonant x-ray scattering



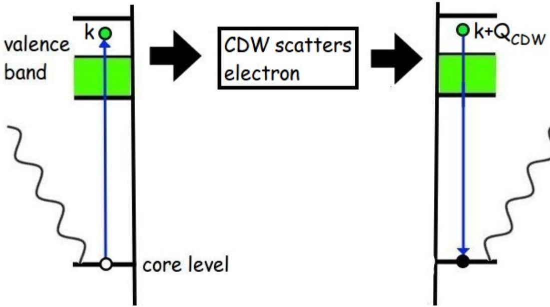
- Photon knocks core electron to valence band at $\mathbf{R}_m$.
- Things happen (optional)
- Electron fills core hole at $\mathbf{R}_m$.

Intensity $\propto \sum_f |A_{i\to f}|^2 \delta(E_f - E_i - \Delta\omega)$

$$A_{i\to f} = \sum_m e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot\mathbf{R}_m} \langle f | d_m \underbrace{(\omega + H_m - E_i + i\Gamma)^{-1}}_{\text{resonance}} d_m^\dagger | i \rangle,$$

where incident photon is $\mathbf{k}_i, \omega$, $1/\Gamma$ is core hole lifetime and $H_m = H_0 +$ core hole potential at $\mathbf{R}_m$, and outgoing photon is $\mathbf{k}_f, \omega - \Delta\omega$.

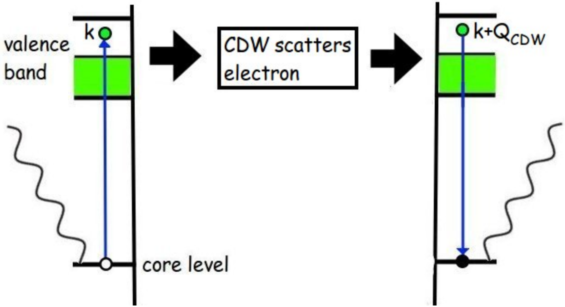
REXS: "valence-selective diffraction"



$$A_{i\to i} = \sum_m e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot\mathbf{R}_m} \langle i | d_m \underbrace{(\omega + H_m - E_i + i\Gamma)^{-1}}_{\text{resonance}} d_m^\dagger | i \rangle$$

- Photon knocks core electron to valence band.
- CDW elastically scatters electron, imparts momentum $\mathbf{Q}_{\mathrm{CDW}}$.
- Electron re-fills core hole, emitting photon.
- Enormously sensitive to valence electrons only.

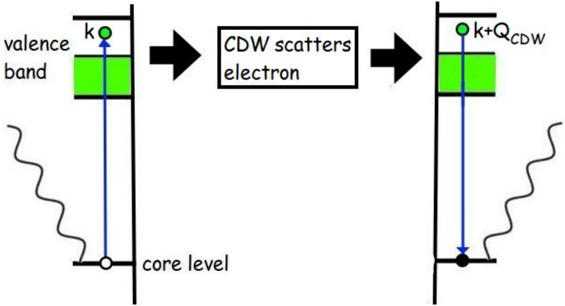
REXS: "valence-selective diffraction"



$$A_{i\to i} = \sum_m e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{R}_m} \langle i | d_m \underbrace{(\omega + H_m - E_i + i\Gamma)^{-1}}_{\text{resonance}} d_m^\dagger | i \rangle$$

- Photon knocks core electron to valence band.
- CDW elastically scatters electron, imparts momentum $\mathbf{Q}_{\text{CDW}}$.
- Electron re-fills core hole, emitting photon.
- Enormously sensitive to valence electrons only.

REXS: “valence-selective diffraction”

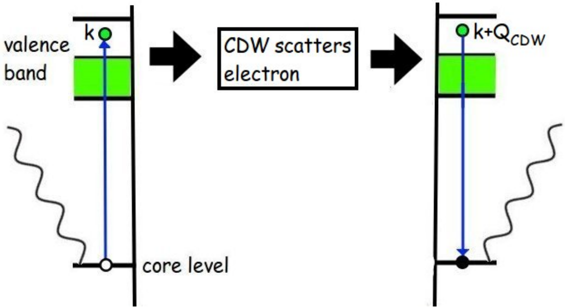


$$A_{i\to i} = \sum_m e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot\mathbf{R}_m} \langle i| d_m \underbrace{(\omega + H_m - E_i + i\Gamma)^{-1}}_{\text{resonance}} d_m^\dagger |i\rangle$$

Questions

- What does ω-dependence mean?
- What microscopic model describes cuprate REXS?

REXS: "valence-selective diffraction"



$$A_{i\to i} = \sum_m e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{R}_m} \langle i | d_m \underbrace{(\omega + H_m - E_i + i\Gamma)^{-1}}_{\text{resonance}} d_m^\dagger | i \rangle$$

Questions

- What does ω-dependence mean?
- What microscopic model describes cuprate REXS?

Two-peak spectrum in cuprate REXS

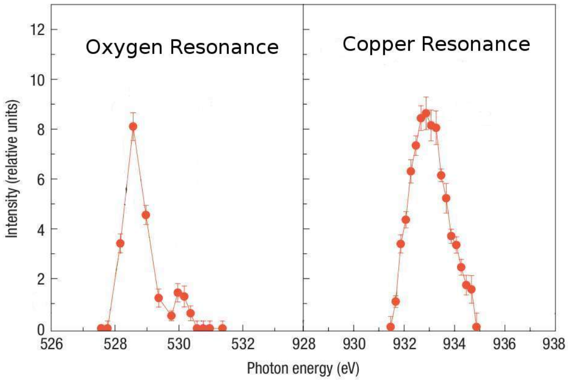


Figure: REXS of LBCO (x=1/8) at $\Delta\mathbf{q} = \mathbf{Q}_{\mathrm{CDW}} = (2\pi/4, 0, 0)$.

Two-peak spectrum in cuprate REXS

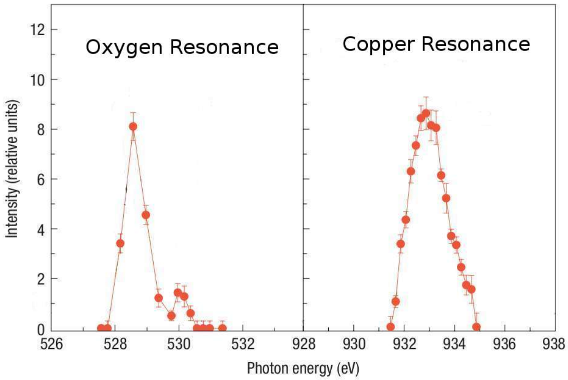
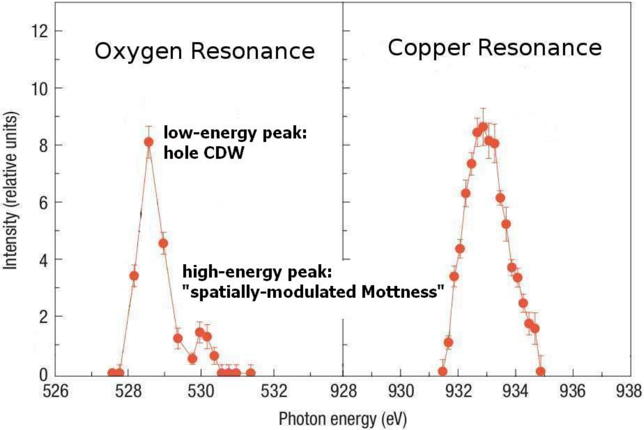


Figure: REXS of LBCO (x=1/8) at $\Delta\mathbf{q} = \mathbf{Q}_{\mathrm{CDW}} = (2\pi/4, 0, 0)$.

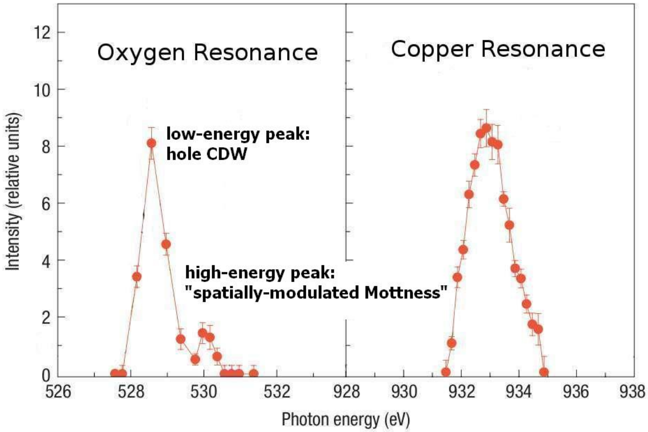
Questions

- What does ω-dependence mean? Why two peaks?
- What microscopic model describes cuprate REXS? Are quasiparticles enough?

Mott interpretation of two peaks in cuprate REXS



Mott interpretation of two peaks in cuprate REXS



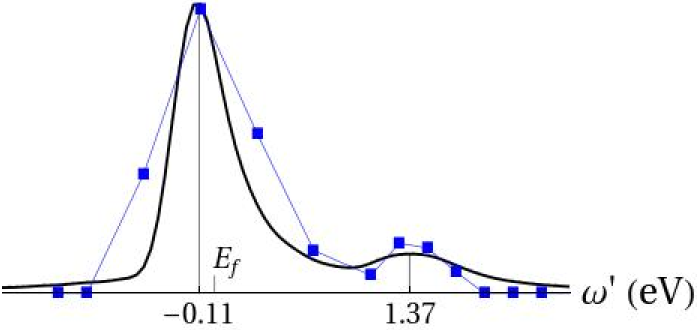
Problems with Mott interpretation

- Peak separation of 1.5 eV is too small for Hubbard gap.
- If second peak is Mott, it should be strong at Cu edge and weak at O edge.

A simple model agrees with experimental data

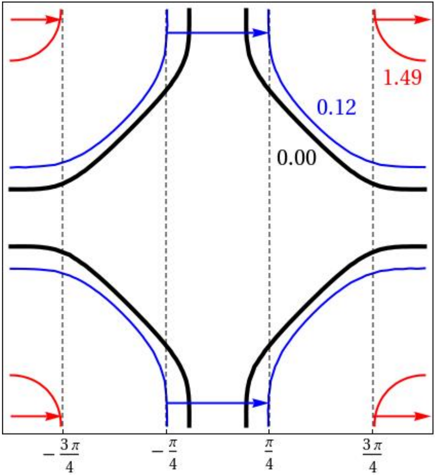
Results of a simple quasiparticle model:

$$H_m = \underbrace{\sum_{\mathbf{k}} \xi_{\mathbf{k}} d^\dagger_{\mathbf{k}} d_{\mathbf{k}}}_{\text{band structure}} + \underbrace{V \sum_{\mathbf{k}} \left(d^\dagger_{\mathbf{k}+\mathbf{Q}} d_{\mathbf{k}} + d^\dagger_{\mathbf{k}} d_{\mathbf{k}+\mathbf{Q}} \right)}_{\text{mean-field CDW}} + \underbrace{V_c d^\dagger_m d_m}_{\text{core hole potential}}$$



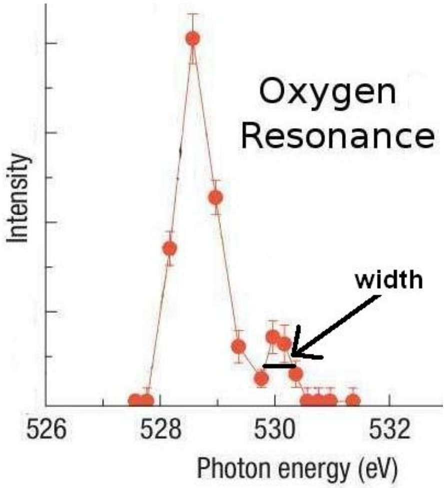
Band structure explains the two peaks

- Elastic scattering $|\mathbf{k}\rangle \rightarrow |\mathbf{k} + \mathbf{Q}_{CDW}\rangle$ needs $\xi_{\mathbf{k}} \approx \xi_{\mathbf{k}+\mathbf{Q}}$.
- Nesting of surface $\xi_{\mathbf{k}} = E$ yields peak at $\omega = E$.
- Contours tangent to degenerate lines $k_x = \pm(\pi - Q/2)$, $k_x = \pm Q/2$ are nested.

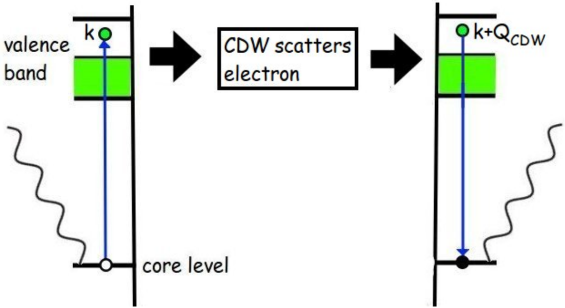


Long-lived quasiparticles

- Peaks are broadened by core hole and quasiparticle decay.
- 1/width gives lower bound for quasiparticle lifetime.
- Narrow high-energy peak implies long-lived quasiparticles!
- Complements magnetic oscillations and DMFT (PRL **110**, 086401)



REXS Formalism



$$A_{i\to i} = \sum_m e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot\mathbf{R}_m} \langle i|d_m(\omega + H_m - E_i + i\Gamma)^{-1} d_m^\dagger|i\rangle$$

$$= \int_0^\infty dt\, e^{(i\omega-\Gamma)t} \sum_m e^{i\mathbf{Q}_{CDW}\cdot\mathbf{R}_m} \underbrace{\langle i|d_m e^{-iH_m t} d_m^\dagger e^{-iH_0 t}|i\rangle}_{S_m(t)}$$

=Fourier transform of a history: excite, propagate, de-excite

REXS Formalism

$$S_m(t) = \langle i| d_m e^{-iH_m t} d_m^\dagger e^{-iH_0 t} |i\rangle$$

$$= \underbrace{\det\left((1-N) + U_m(t)N\right)^2}_{\text{Fermi sea}} \underbrace{\langle m| \left(\frac{N}{1-N} + U_m^{-1}(t)\right)^{-1} |m\rangle}_{\text{photoexcited electron}},$$

$$N \equiv (1 + \exp(\beta h_0))^{-1}, \quad U_m(t) \equiv e^{-ih_m t} e^{ih_0 t}$$

- Typo? No, $H_{m,0} = d_i^\dagger \left(h_{m,0}\right)_{ij} d_j$!
- N: *single-particle* Fermi sea occupation
- U_m *single-particle* time-evolution with core hole at $\mathbf{R}_m$
- $\det$: device for matrix elements of Slater determinant state
- $\det(\,)^2$: one Fermi sea for each spin
- $(1-N) + U_m(t)N$: time-evolve only occupied states.
- $|m\rangle$ Wannier orbital at $\mathbf{R}_m$.
- $\langle m|\,|m\rangle$: Propagator $\langle m|U_m(t)|m\rangle$ for $N = 0$, Pauli-blocking 0 for $N = 1$.

REXS Formalism

$$S_m(t) = \langle i| d_m e^{-iH_m t} d_m^\dagger e^{-iH_0 t} |i\rangle$$
$$= \underbrace{\det\left((1-N) + U_m(t)N\right)^2}_{\text{Fermi sea}} \underbrace{\langle m| \left(\frac{N}{1-N} + U_m^{-1}(t)\right)^{-1} |m\rangle}_{\text{photoexcited electron}},$$

$$N \equiv (1 + \exp(\beta h_0))^{-1}, \quad U_m(t) \equiv e^{-ih_m t} e^{ih_0 t}$$

- Typo? No, $H_{m,0} = d_i^\dagger \left(h_{m,0}\right)_{ij} d_j$!
- N: *single-particle* Fermi sea occupation
- U_m *single-particle* time-evolution with core hole at $\mathbf{R}_m$
- $\det$: device for matrix elements of Slater determinant state
- $\det(\,)^2$: one Fermi sea for each spin
- $(1-N) + U_m(t)N$: time-evolve only occupied states.
- $|m\rangle$ Wannier orbital at $\mathbf{R}_m$.
- $\langle m|\,|m\rangle$: Propagator $\langle m|U_m(t)|m\rangle$ for $N = 0$, Pauli-blocking 0 for $N = 1$.

REXS Formalism

$$S_m(t) = \langle i | d_m e^{-iH_m t} d_m^\dagger e^{-iH_0 t} | i \rangle$$

$$= \underbrace{\det\left((1-N) + U_m(t) N\right)^2}_{\text{Fermi sea}} \underbrace{\langle m | \left(\frac{N}{1-N} + U_m^{-1}(t) \right)^{-1} | m \rangle}_{\text{photoexcited electron}},$$

$$N \equiv (1 + \exp(\beta h_0))^{-1}, \quad U_m(t) \equiv e^{-ih_m t} e^{ih_0 t}$$

- Typo? No, $H_{m,0} = d_i^\dagger \left(h_{m,0}\right)_{ij} d_j$!
- N: *single-particle* Fermi sea occupation
- U_m *single-particle* time-evolution with core hole at $\mathbf{R}_m$
- $\det$: device for matrix elements of Slater determinant state
- $\det(\,)^2$: one Fermi sea for each spin
- $(1-N) + U_m(t)N$: time-evolve only occupied states.
- $|m\rangle$ Wannier orbital at $\mathbf{R}_m$.
- $\langle m| \, |m\rangle$: Propagator $\langle m | U_m(t) | m \rangle$ for $N = 0$, Pauli-blocking 0 for $N = 1$.

REXS Formalism

$$
\begin{aligned}
S_m(t) =& \langle i | d_m e^{-iH_m t} d_m^\dagger e^{-iH_0 t} | i \rangle \\
=& \underbrace{\det\left((1-N) + U_m(t) N\right)^2}_{\text{Fermi sea}} \underbrace{\langle m | \left(\frac{N}{1-N} + U_m^{-1}(t) \right)^{-1} | m \rangle}_{\text{photoexcited electron}},
\end{aligned}
$$

$$
N \equiv (1 + \exp(\beta h_0))^{-1}, \quad U_m(t) \equiv e^{-ih_m t} e^{ih_0 t}
$$

- Typo? No, $H_{m,0} = d_i^\dagger \left(h_{m,0}\right)_{ij} d_j$!
- N: *single-particle* Fermi sea occupation
- U_m *single-particle* time-evolution with core hole at $\mathbf{R}_m$
- $\det$: device for matrix elements of Slater determinant state
- $\det(\,)^2$: one Fermi sea for each spin
- $(1-N) + U_m(t)N$: time-evolve only occupied states.
- $|m\rangle$ Wannier orbital at $\mathbf{R}_m$.
- $\langle m| \, |m\rangle$: Propagator $\langle m | U_m(t) | m \rangle$ for $N = 0$, Pauli-blocking 0 for $N = 1$.

REXS Formalism

$$S_m(t) = \langle i | d_m e^{-iH_m t} d_m^\dagger e^{-iH_0 t} | i \rangle$$

$$= \underbrace{\det\left((1-N) + U_m(t) N\right)^2}_{\text{Fermi sea}} \underbrace{\langle m | \left(\frac{N}{1-N} + U_m^{-1}(t) \right)^{-1} | m \rangle}_{\text{photoexcited electron}},$$

$$N \equiv (1 + \exp(\beta h_0))^{-1}, \quad U_m(t) \equiv e^{-ih_m t} e^{ih_0 t}$$

- Typo? No, $H_{m,0} = d_i^\dagger \left(h_{m,0}\right)_{ij} d_j$!
- N: *single-particle* Fermi sea occupation
- U_m *single-particle* time-evolution with core hole at $\mathbf{R}_m$
- $\det$: device for matrix elements of Slater determinant state
- $\det(\,)^2$: one Fermi sea for each spin
- $(1-N) + U_m(t)N$: time-evolve only occupied states.
- $|m\rangle$ Wannier orbital at $\mathbf{R}_m$.
- $\langle m| \, |m\rangle$: Propagator $\langle m | U_m(t) | m \rangle$ for $N = 0$, Pauli-blocking 0 for $N = 1$.

Motivating the determinant formula

Consider $\langle e^X \rangle = \mathrm{tr}\left[e^X e^{-\beta H}\right] / \mathrm{tr}\left[e^{-\beta H}\right]$ for quadratic X, H.

- In basis where $X = \sum_\alpha \omega_\alpha \hat{n}_\alpha$

  $$\mathrm{tr}\left[e^X\right] = \prod_\alpha \sum_{n_\alpha=0,1} e^{n_\alpha \omega_\alpha} = \prod_\alpha (1 + e^{\omega_\alpha}) = \det\left(1 + e^X\right)$$

Motivating the determinant formula

Consider $\langle e^X \rangle = \mathrm{tr}\left[e^X e^{-\beta H}\right] / \mathrm{tr}\left[e^{-\beta H}\right]$ for quadratic X, H.

- In basis where $X = \sum_\alpha \omega_\alpha \hat{n}_\alpha$
  $$\mathrm{tr}\left[e^X\right] = \prod_\alpha \sum_{n_\alpha=0,1} e^{n_\alpha \omega_\alpha} = \prod_\alpha (1 + e^{\omega_\alpha}) = \det\left(1 + e^X\right)$$
- BCH: $e^X e^Y = e^Z$, Z quadratic, $\mathrm{tr}\left[e^X e^Y\right] = \det\left(1 + e^X e^Y\right)$.

Motivating the determinant formula

Consider $\langle e^X \rangle = \mathrm{tr}\left[e^X e^{-\beta H}\right] / \mathrm{tr}\left[e^{-\beta H}\right]$ for quadratic X, H.

- In basis where $X = \sum_\alpha \omega_\alpha \hat{n}_\alpha$

  $$\mathrm{tr}\left[e^X\right] = \prod_\alpha \sum_{n_\alpha=0,1} e^{n_\alpha \omega_\alpha} = \prod_\alpha (1 + e^{\omega_\alpha}) = \det\left(1 + e^X\right)$$

- BCH: $e^X e^Y = e^Z$, Z quadratic, $\mathrm{tr}\left[e^X e^Y\right] = \det\left(1 + e^X e^Y\right)$.
- Insertions: $\mathrm{tr}\left[d_m^\dagger d_n e^Z\right] = \sum_{\alpha,\beta} \langle \alpha | n \rangle \langle m | \beta \rangle \mathrm{tr}\left[d_\alpha^\dagger d_\beta e^Z\right] =$

  $$\sum_\alpha \langle m|\alpha\rangle\langle\alpha|n\rangle \mathrm{tr}\left[\hat{n}_\alpha e^Z\right] = \sum_\alpha \langle m|\alpha\rangle\langle\alpha|n\rangle \prod_{\gamma\neq\alpha} (1 + e^{\omega_\gamma}) \sum_{n_\alpha=0,1} n_\alpha e^{n_\alpha \omega_\alpha} = \sum_\alpha \langle m|\alpha\rangle\langle\alpha|n\rangle \frac{\det(1+e^Z)}{1+e^{\omega_\alpha}} e^{\omega_\alpha} =$$

  $$\sum_\alpha \langle m| \frac{e^Z}{1+e^Z} |\alpha\rangle\langle\alpha|n\rangle \det(1+e^Z) =$$

  $$\langle m| \frac{e^Z}{1+e^Z} |n\rangle \det(1+e^Z)$$

Summary of REXS

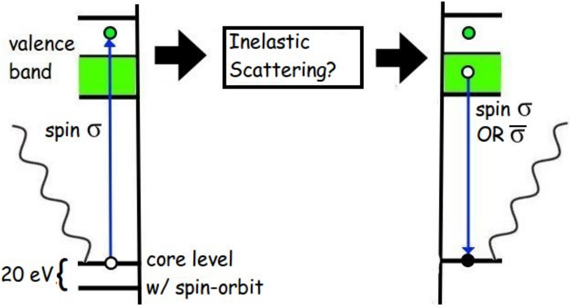
Questions

- What does ω-dependence mean? Why two peaks?
- What microscopic model describes cuprate REXS? Are quasiparticles enough?

Answers

- Band structure explains everything, core hole improve quantitative agreement, and high-energy quasiparticles are surprisingly well-defined!
- DMFT long-lived quasiparticles: PRL **110**, 086401

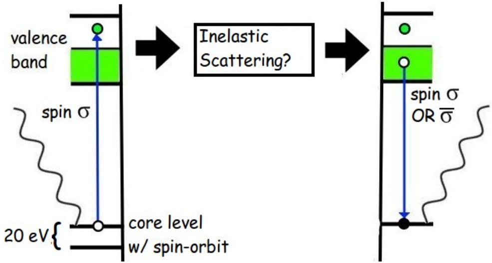
RIXS Formalism



$$A_{i\to f} = \sum_{m,\sigma} e^{i(\mathbf{k}_f - \mathbf{k}_i)\cdot \mathbf{R}_m} \langle f | d_{m,\sigma \text{ OR } \bar{\sigma}} (\omega + H_m - E_i + i\Gamma)^{-1} d^{\dagger}_{m,\sigma} | i \rangle$$

- Due to spin-orbit of core level, spin-flip is possible
- Polarized incoming beam can select either spin-flip or non-spin-flip.

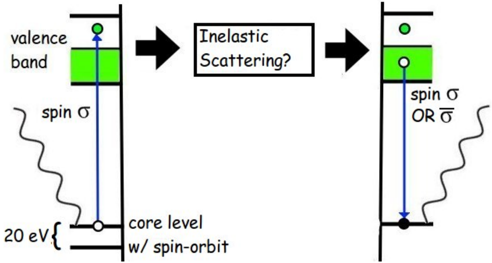
RIXS Formalism



As in REXS we have the Fourier transform of a history:

$$I \propto \int_{-\infty}^{\infty} ds \int_{0}^{\infty} dt \int_{0}^{\infty} d\tau \, e^{i\omega(t-\tau) - is\Delta\omega - \Gamma(t+\tau)} \sum_{mn} e^{i\mathbf{Q}\cdot(\mathbf{R}_m - \mathbf{R}_n)} \chi_{\rho\sigma} \chi_{\mu\nu} S^{mn}_{\rho\sigma\mu\nu},$$

RIXS Formalism



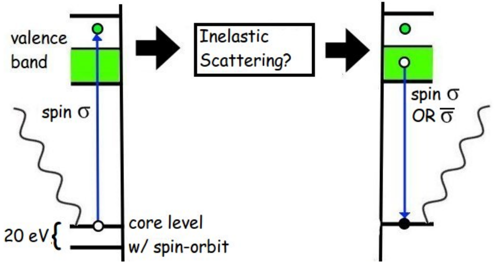
As in REXS we have the Fourier transform of a history:

$$I \propto \int_{-\infty}^{\infty} ds \int_{0}^{\infty} dt \int_{0}^{\infty} d\tau \, e^{i\omega(t-\tau) - is\Delta\omega - \Gamma(t+\tau)} \sum_{mn} e^{i\mathbf{Q}\cdot(\mathbf{R}_m - \mathbf{R}_n)} \chi_{\rho\sigma}\chi_{\mu\nu} S^{mn}_{\rho\sigma\mu\nu},$$

$$S^{mn}_{\rho\sigma\mu\nu} = \langle e^{iH\tau} d_{n\rho} e^{-iH_n\tau} d^{\dagger}_{n\sigma} e^{iHs} d_{m\mu} e^{iH_m t} d^{\dagger}_{m\nu} e^{-iH(t+s)} \rangle.$$

- $\chi_{\alpha\beta}$: polarization-dependent balance between spin-flip and non-flip
- Forward and backward time "Keldysh" histories

RIXS Formalism



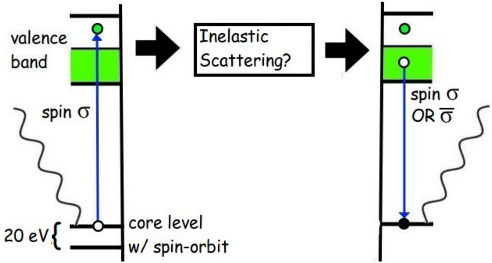
As in REXS we have the Fourier transform of a history:

$$I \propto \int_{-\infty}^{\infty} ds \int_{0}^{\infty} dt \int_{0}^{\infty} d\tau \, e^{i\omega(t-\tau)-is\Delta\omega-\Gamma(t+\tau)} \sum_{mn} e^{i\mathbf{Q}\cdot(\mathbf{R}_m-\mathbf{R}_n)} \chi_{\rho\sigma}\chi_{\mu\nu} S^{mn}_{\rho\sigma\mu\nu},$$

$$S^{mn}_{\rho\sigma\mu\nu} = \langle e^{iH\tau} d_{n\rho} e^{-iH_n\tau} d^{\dagger}_{n\sigma} e^{iHs} {\color{red} d_{m\mu} e^{iH_m t} d^{\dagger}_{m\nu}} e^{-iH(t+s)} \rangle.$$

- $\chi_{\alpha\beta}$: polarization-dependent balance between spin-flip and non-flip
- Forward and backward time "Keldysh" histories

RIXS Formalism



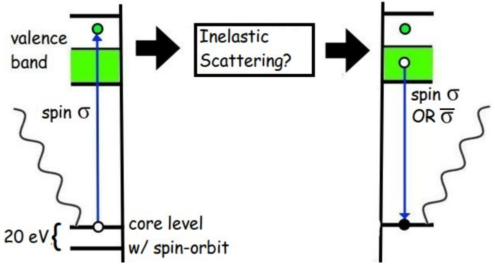
As in REXS we have the Fourier transform of a history:

$$I \propto \int_{-\infty}^{\infty} ds \int_0^{\infty} dt \int_0^{\infty} d\tau \, e^{i\omega(t-\tau)-is\Delta\omega-\Gamma(t+\tau)} \sum_{mn} e^{i\mathbf{Q}\cdot(\mathbf{R}_m-\mathbf{R}_n)} \chi_{\rho\sigma}\chi_{\mu\nu} S^{mn}_{\rho\sigma\mu\nu},$$

$$S^{mn}_{\rho\sigma\mu\nu} = \langle e^{iH\tau} d_{n\rho} e^{-iH_n\tau} d^{\dagger}_{n\sigma} e^{iHs} d_{m\mu} e^{iH_m t} d^{\dagger}_{m\nu} e^{-iH(t+s)} \rangle.$$

- $\chi_{\alpha\beta}$: polarization-dependent balance between spin-flip and non-flip
- Forward and backward time "Keldysh" histories

RIXS Formalism



As in REXS we have the Fourier transform of a history:

$$I \propto \int_{-\infty}^{\infty} ds \int_0^{\infty} dt \int_0^{\infty} d\tau \, e^{i\omega(t-\tau) - is\Delta\omega - \Gamma(t+\tau)} \sum_{mn} e^{i\mathbf{Q}\cdot(\mathbf{R}_m - \mathbf{R}_n)} \chi_{\rho\sigma} \chi_{\mu\nu} S^{mn}_{\rho\sigma\mu\nu},$$

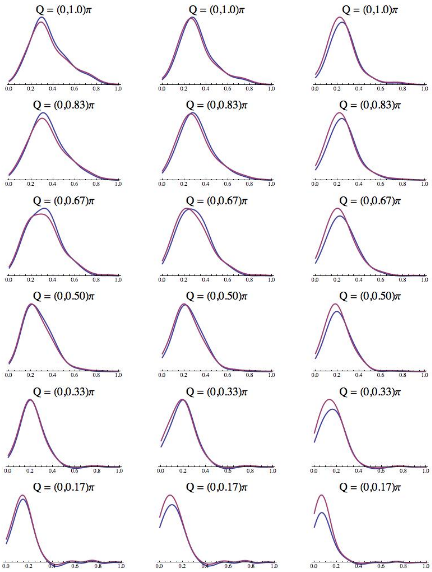
$$S^{mn}_{\rho\sigma\mu\nu} = \det(F) \Big[\langle n\rho | (1-N) F^{-1} e^{-ih_n \tau} | n\sigma \rangle$$

$$\times \langle m\mu | e^{-ih_0 s} e^{ih_n \tau} (1-N) F^{-1} U_{mn} | m\nu \rangle$$

$$+ \langle n\rho | (1-N) F^{-1} U_{mn} | m\nu \rangle \, \langle m\mu | e^{ih_m t} U_0 N F^{-1} e^{-ih_n \tau} | n\sigma \rangle \Big] .$$

where $U_{mn} = e^{-ih_n\tau} e^{ih_0 s} e^{ih_m t}$, and $U_0 = e^{i(\tau - t - s)h_0}$, and $F = 1 - N + U_{mn} U_0 N$.

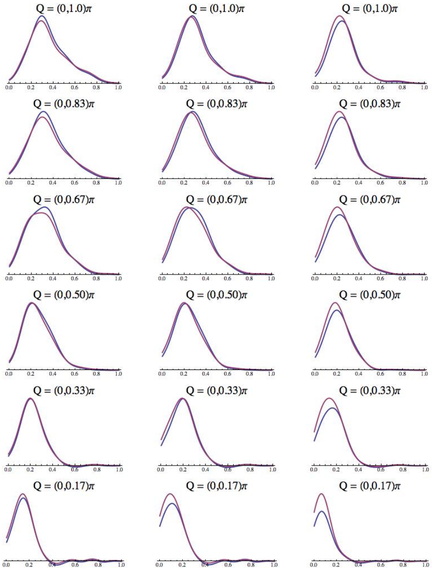
Surprise: band structure yields dispersing peaks!



- left to right: doping $x = 0.15, 0.25, 0.40$
- bottom to top: momentum transfer $\mathbf{Q} = 0.17(\pi, 0) \ldots (\pi, 0)$
- each plot: intensity vs. energy transfer $0 \leq \Delta\omega \leq 1$ eV in spin-flip channel.
- blue and purple: core hole potential $U_c = 0.0, -0.5$ eV.

Surprise: band structure yields dispersing peaks!

Same energy, widths, long high-energy tail, and doping-insensitivty.



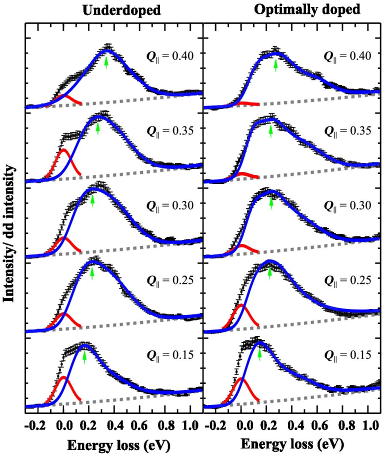


Figure: Bi-2212 data from Mark Dean et al, PRL **110**,147001 (2013)

Surprise: core hole separates spin-flip from non-flip!

Can quasiparticles do this?

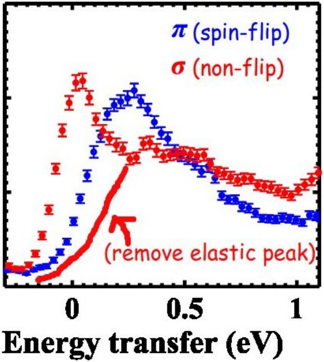


Figure: Bi-2212 spin-flip and non-flip channels from Mark Dean et al, PRL **110**,147001 (2013)

Surprise: core hole separates spin-flip from non-flip!

Can quasiparticles do this?

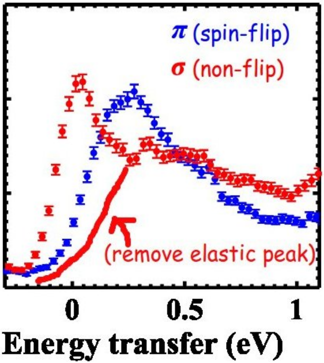


Figure: Bi-2212 spin-flip and non-flip channels from Mark Dean et al, PRL **110**,147001 (2013)

Yes.

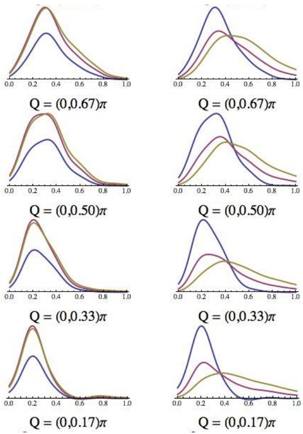


Figure: Left: spin-flip lineshapes, right: non-flip lineshapes for core hole strengths $U_c = 0.0, -0.25, -0.5$ eV.

Summary

RIXS

- Quasiparticles, core hole mimic magnon's lineshape!
- Relevant to "pairing glue."
- Spin flip insensitive to core hole. . . diagrammatics?

REXS

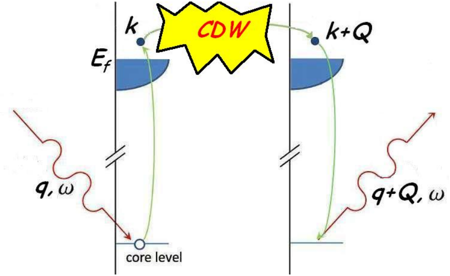
- Band structure
- Long-lived quasiparticles

Model

$$H = \sum_{\mathbf{k}} \xi_{\mathbf{k}} d^{\dagger}_{\mathbf{k}} d_{\mathbf{k}} + V \sum_{\mathbf{k}} \left(d^{\dagger}_{\mathbf{k}+\mathbf{Q}} d_{\mathbf{k}} + d^{\dagger}_{\mathbf{k}} d_{\mathbf{k}+\mathbf{Q}} \right) + V_c d^{\dagger}_j d_j \qquad (1)$$

$$\xi_{\mathbf{k}} = -t(\cos k_x + \cos k_y) + 4t_1 \cos k_x \cos k_y - 2t_2(\cos 2k_x + \cos 2k_y), \qquad (2)$$

$$\langle g| \sum_j p^{\dagger}_j d_j e^{-i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{R}_j} |n\rangle \qquad d^{\dagger}_{\mathbf{k}+\mathbf{Q}} d_{\mathbf{k}} \qquad \langle n| \sum_j d^{\dagger}_j e^{i\mathbf{k}\cdot\mathbf{R}_j} |g\rangle$$



Energy Domain to Time Domain

$$I(\omega, \mathbf{Q}) \propto \left| \sum_{j,n,\sigma} e^{-i\mathbf{Q}\cdot\mathbf{r}_j} \frac{\langle i|d_{j\sigma}|n\rangle\langle n|d^{\dagger}_{j\sigma}|i\rangle}{E_i - \tilde{E}^{N+1}_n + \omega + i\Gamma} \right|^2 \tag{3}$$

$$= \left| \sum_{j\sigma} e^{-i\mathbf{Q}\cdot\mathbf{r}_j} \int_0^{\infty} e^{-(i\omega+\Gamma)t} \langle i|d_j e^{-i\mathcal{H}_1(j)t} d^{\dagger}_j e^{-i\mathcal{H}_0 t}|i\rangle dt \right|^2, \tag{4}$$

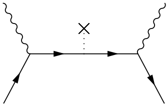
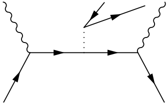
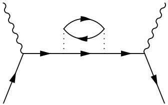
$$\sum_n \frac{|n\rangle\langle n|\ldots|i\rangle}{E_i - \tilde{E}^{N+1}_n + \omega + i\Gamma} = \sum_n \int_0^{\infty} e^{(E_i - \tilde{E}^{N+1}_n + \omega + i\Gamma)it} |n\rangle\langle n|\ldots|i\rangle dt \tag{5}$$

$$= \int_0^{\infty} e^{i\omega - \Gamma t} e^{-iH_j t} \cancelto{1}{\sum_n |n\rangle\langle n|} \ldots e^{iH_0 t}|i\rangle dt \tag{6}$$

Summary of REXS Experiments

- Abbamonte, Science (2002). REXS at O K resonance. Observed thin-film interference.
- Wilkins, PRL (2003). Magnetic REXS in manganites.
- Wilkins, PRL (2003) and Dhesi, PRL (2004). Orbital order in manganites.
- Abbamonte, Nature (2004). Hole crystal in $Sr_{14}Cu_{24}O_{41}$.
- Abbamonte, Nature Physics (2005). First direct evidence of cuprate CDW. Proposed spatially-modulated Mottness to explain second peak. Related: Fink, PRB (2009) with LESCO.
- Schussler-Langeheine, PRL (2005); Nazarenko, PRL (2006); Herrero-Martin, PRB (2006); CDW in other correlated systems.
- Ghiringhelli, Science (2012). Incommensurate CDW in YBCO.

Why one can ignore interactions

Diagram	in Words	Contribution to REXS
	elastic scattering	contributes
	inelastic scattering	does not contribute
	self-energy	renormalizes quasiparticles

Relation to Green's function

$$I_{\mathrm{REXS}}(\omega, \mathbf{Q}) \propto \left| \sum_{j,n} e^{-i\mathbf{Q}\cdot\mathbf{r}_j} \frac{\langle i|d_j|n\rangle\langle n|d_j^\dagger|i\rangle}{E_i - \tilde{E}_n^{N+1} + \omega + i\Gamma} \right|^2 \qquad (7)$$

while STM measures local density of states $\mathrm{Im}G(\omega, \mathbf{r}_j)$,

$$\mathrm{Im} \sum_n \left[\frac{\langle i|d_j|n\rangle\langle n|d_j^\dagger|i\rangle}{E_i - E_n^{N+1} + \omega + 0^+ i} + \frac{\langle i|d_j^\dagger|n\rangle\langle n|d_j|i\rangle}{-E_i + E_n^{N-1} + \omega + 0^+ i} \right] \qquad (8)$$

Differences: decay of intermediate state in REXS, intermediate state energy depends on core hole interaction, REXS does not have electron-removal term.