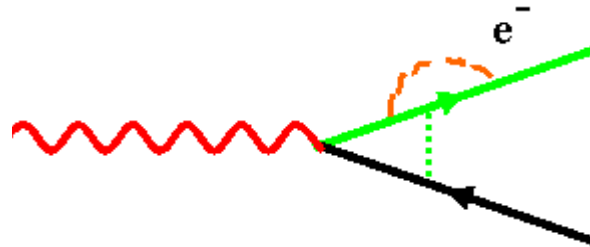


# III. Inelastic losses and many-body effects in x-ray spectra

J. J. Rehr



# Inelastic losses and many-body effects in x-ray spectra

- **TALK:**

- I. Introduction**

- Many-body effects in XAS**

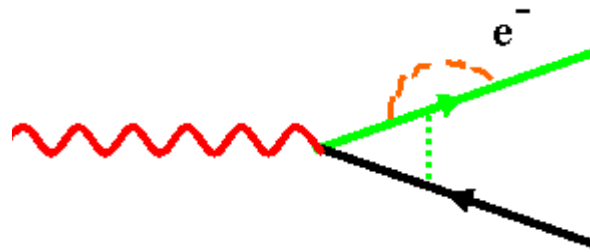
- II. Inelastic losses  
& satellites**

- Cumulant expansion  
beyond GW**

- III. Particle-hole theory: BSE  
Particle-hole cumulant**

- Intrinsic, extrinsic losses  
and interference**

# I. Introduction:



## Key many-body effects

- **Core-hole effects** ----- **Excitonic effects, Screening**
- **Self-energy  $\Sigma(E)$**  ----- **Mean-free path, energy shifts**
- **Phonons, disorder** ----- **Debye-Waller factors**
- **Excitations** ----- **Inelastic losses & satellites**

“ You can judge a many-body theory  
by how it treats the satellites. ”

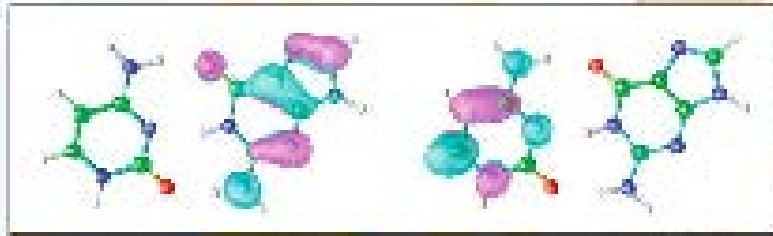
Lars Hedin (1995)

# COMPTES RENDUS DE L'ACADÉMIE DES SCIENCES

Année 2009  
Fascicule 6

Julien Jorès, Acad.  
1201 10 2009

## PHYSIQUE



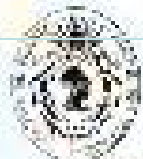
### *Theoretical Spectroscopy* L. Reining, (Ed, 2009)

#### DOSSIER

Theoretical spectroscopy / Spectroscopie théorique

Guest editor / Rédacteur en chef invité :

Luca Reining



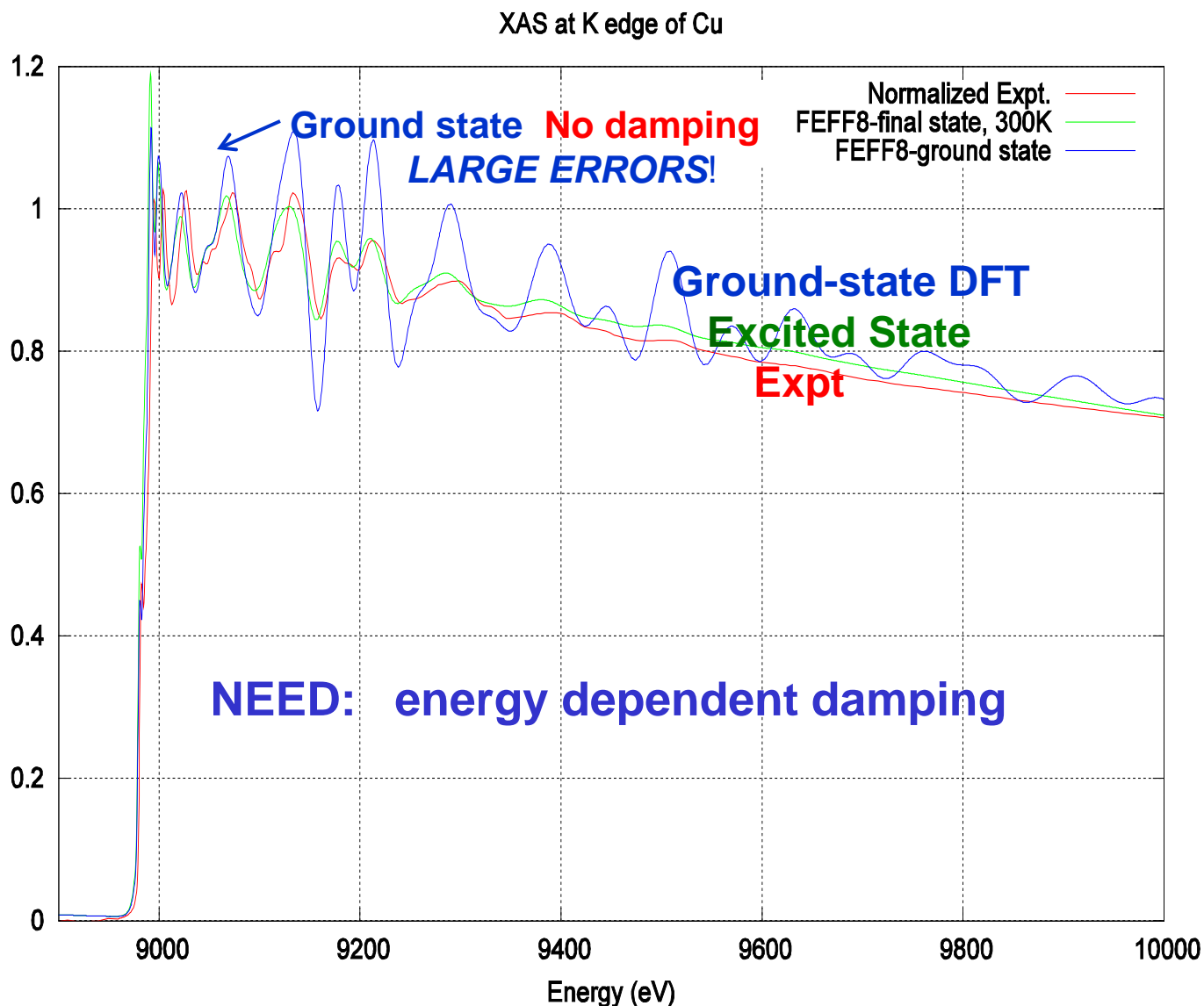
ACADÉMIE DES SCIENCES — PARIS

## Mini-review

### Quasi-particle theory of XAS

JJR et al., Comptes Rendus  
Physique **10**, 548 (2009)

# Motivation: Failure of ground-state DFT in XAS; need for inelastic losses



# Starting point for core-XAS calculations: Quasi-particle final state Green's function

~~Golden rule for XAS via Wave functions~~

~~$$\mu(E) \sim \sum_f |\langle i | \hat{\epsilon} \cdot \mathbf{r} | f \rangle|^2 \delta(E - E_f)$$~~



**Paradigm shift:**

**Golden rule via Green's Functions  $G = 1/(E - h' - \Sigma)$**

$$\mu(E) \sim -\frac{1}{\pi} \text{Im} \langle i | \hat{\epsilon} \cdot \mathbf{r}' G(\mathbf{r}', \mathbf{r}, E) \hat{\epsilon} \cdot \mathbf{r} | i \rangle$$

Final state  $h'$  includes core-hole **AND**  
energy dependent self energy  $\Sigma(E)$

# Many-pole GW Self-energy $\Sigma(E)^*$

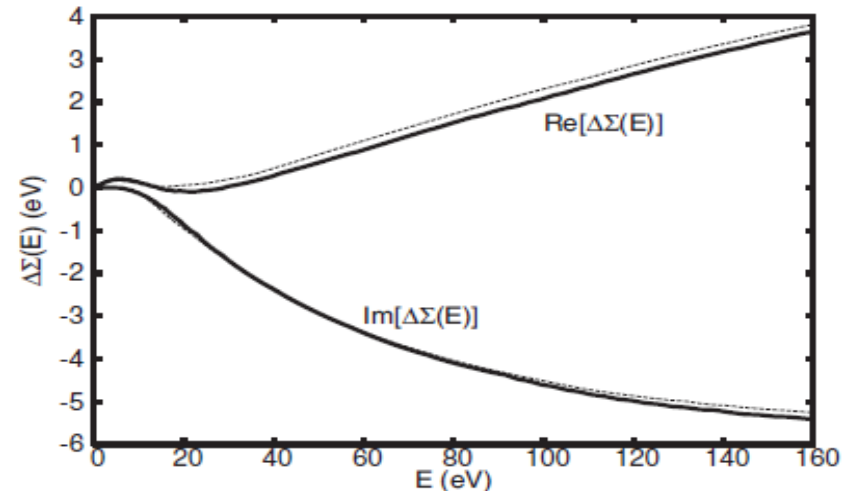
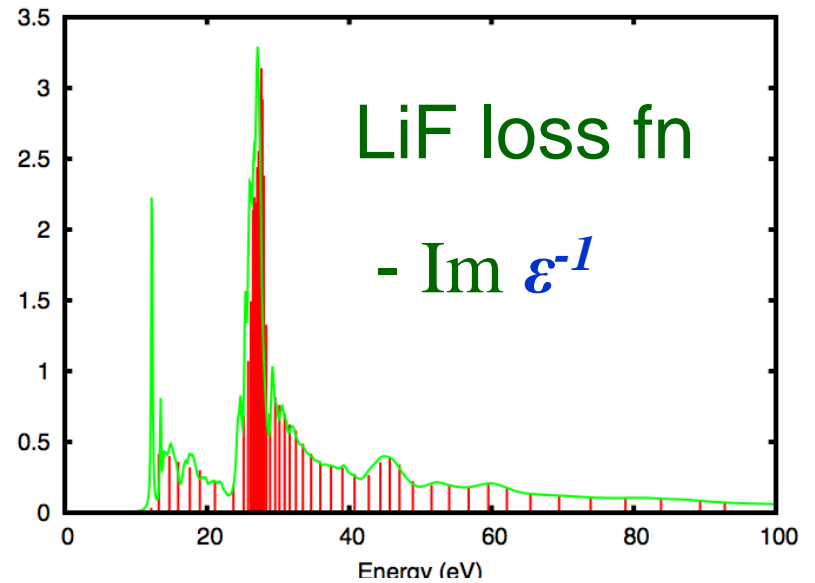
Efficient GW approximation for  
“**Extrinsic Losses**”

Sum of plasmon-pole models  
matched to loss function

$$\Sigma(E) = iGW = \Sigma' - i\Gamma$$

$$W = \epsilon^{-1} v$$

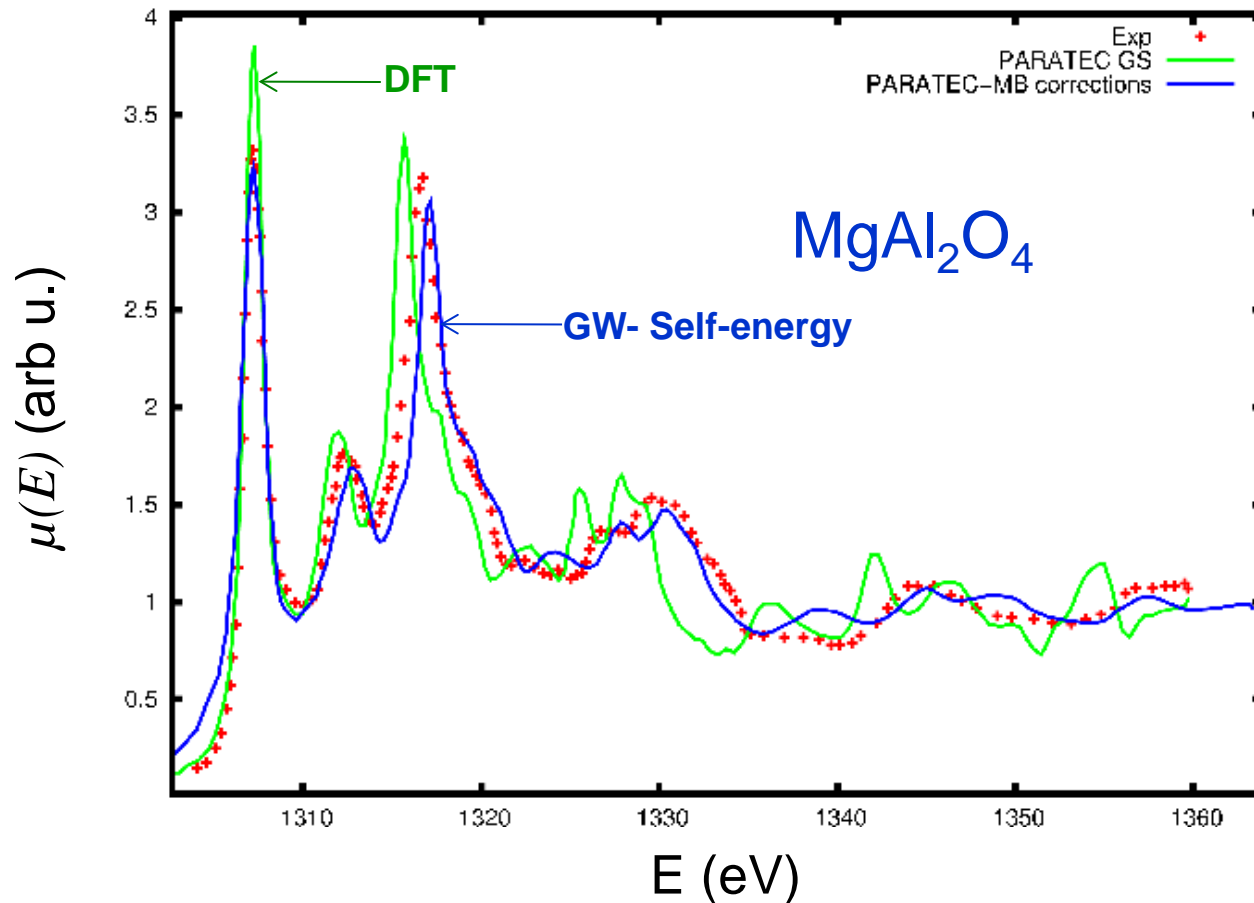
Extension of Hedin-Lundqvist  
GW plasmon-pole model



\* J.J. Kas et. al, Phys Rev B **76**, 195116 (2007)

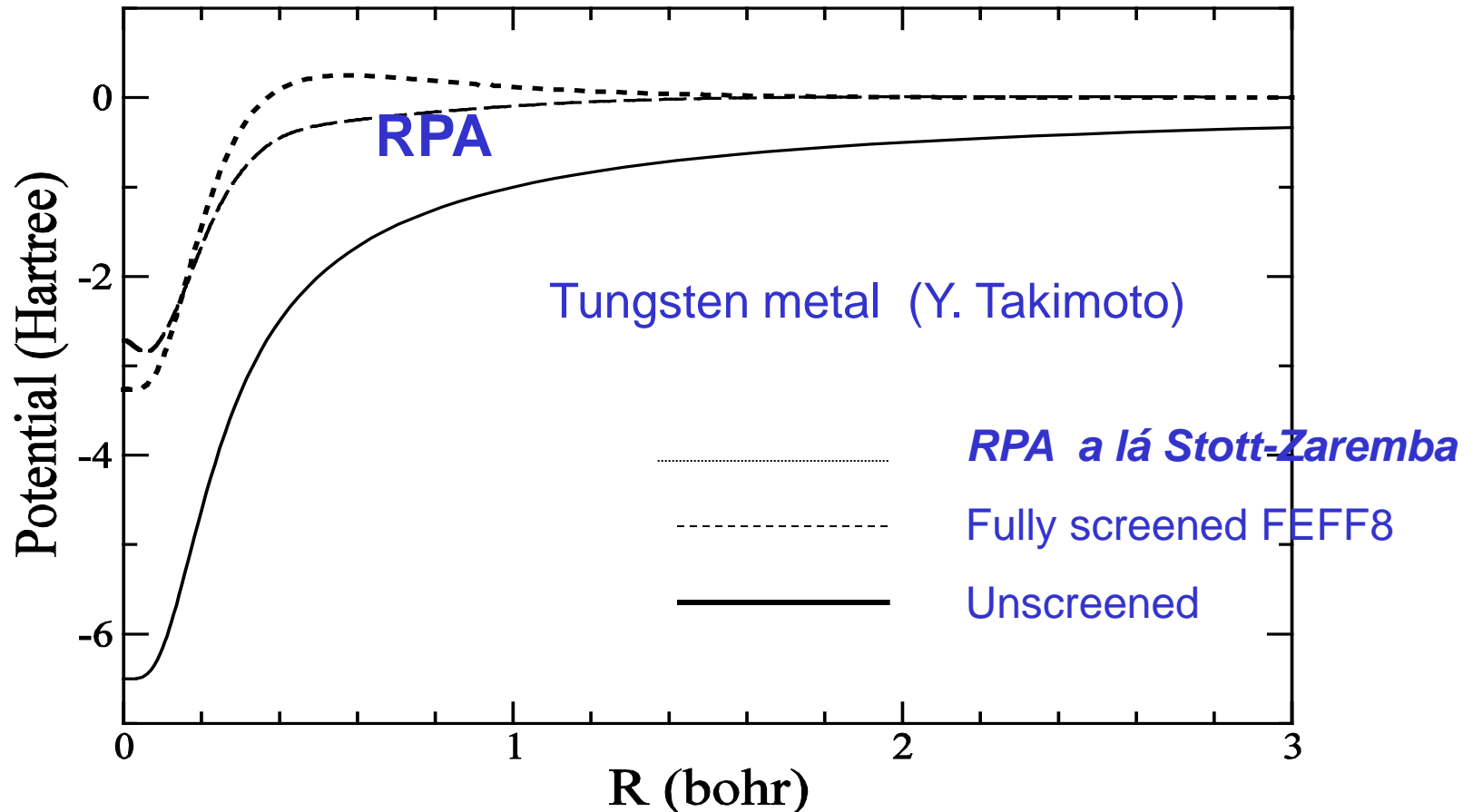


# Self-energy fixes systematic shifts & broadening due to self-energy in XAS



\* J. J. Kas, J. Vinson, N. Trcera, D. Cabaret, E. L. Shirley, and J. J. Rehr, *Journal of Physics: Conference Series* **190**, 012009 (2009)

# Core-hole potential - RPA $W$



*cf.* Screened core hole  $W$  in Bethe-Salpeter Eq

Improves on final state rule,  $Z+1$ , half-core hole

# Phonon effects: Debye Waller factors in XAS

*An Initio* Determination of Extended X-Ray Absorption Fine Structure Debye-Waller Factors\*

$$e^{-2\sigma^2 k^2}$$

Fernando D. Vila, G. Shu, and John J. Rehr  
Department of Physics, University of Washington, Seattle, WA 98195

H. H. Rossner and H. J. Krappe  
Hahn-Meitner-Institut Berlin, Glienicker Strasse 100, D-14109 Berlin, Germany  
(Dated: August 23, 2005)

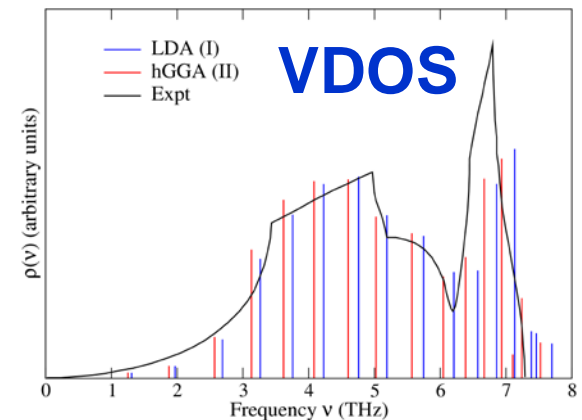


$$\sigma^2 = \frac{\hbar}{\mu_i} \int_0^\infty \rho(\omega^2) \coth \frac{\beta \hbar \omega}{2} d\omega$$

$$\begin{aligned} \rho(\omega^2) &= \langle Q_i | \delta(\omega^2 - D) | Q_i \rangle \\ &= \{6\text{-step Lanczos recursion}\} \end{aligned}$$

**D** dynamical matrix < **ABINIT**

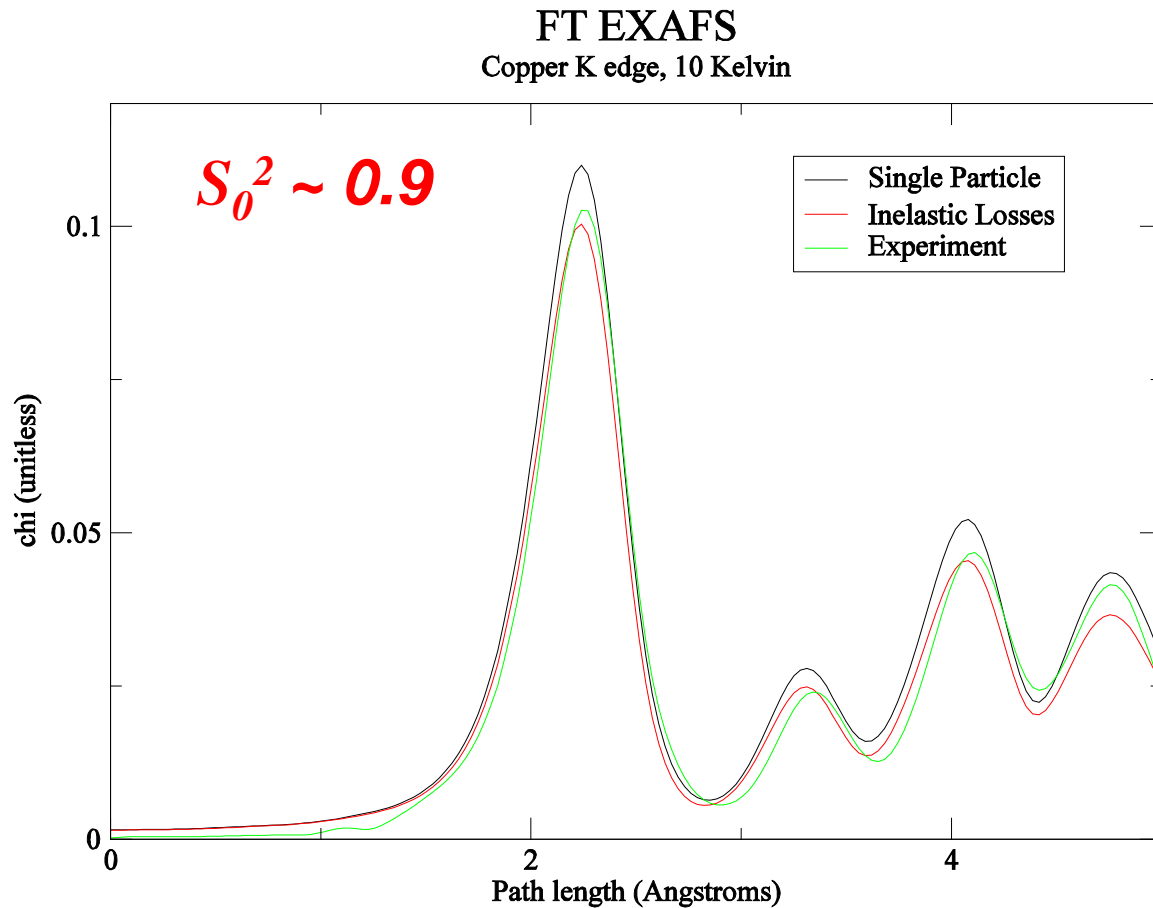
Many pole model  
for phonons



\*Phys. Rev. B **76**, 014301 (2007)

# **PROBLEM:** Amplitude discrepancy in EXAFS

Observed fine structure smaller than QP theory



## II. Inelastic losses and satellites

Q How to treat losses *beyond* the GW-quasi-particle approximation ?

Approach: Improved Green's function  $G(E)$  including satellites in spectral function

$$A(\omega) = (1/\pi) \text{Im } G(E)$$

*Two methods: GW + Dyson Eq.  
Cumulant expansion*

# Which Green's function ?

**GW + Dyson** vs **Cumulant\***

**GW**

$$G(\omega) = G_0 + G_0 \Sigma G$$

$$\Sigma^{GW} = iGW$$

$$W = \epsilon^{-1}v$$

**No vertex**  $\Gamma = 1$

**Cumulant**

$$G(t) = G_0(t) e^{C(t)}$$

$$C \sim \text{Im } \Sigma^{GW}$$

**Implicit vertex**

\*Recent review and new derivation, see J. Zhou et al. J. Chem. Phys. 143, 184109 (2015).

# Answer: XPS expt: Cumulant wins

Phys Rev Lett **77**, 2268 (1996)

## Multiple Plasmon Satellites in Na and Al Spectral Functions from *Ab Initio* Cumulant Expansion

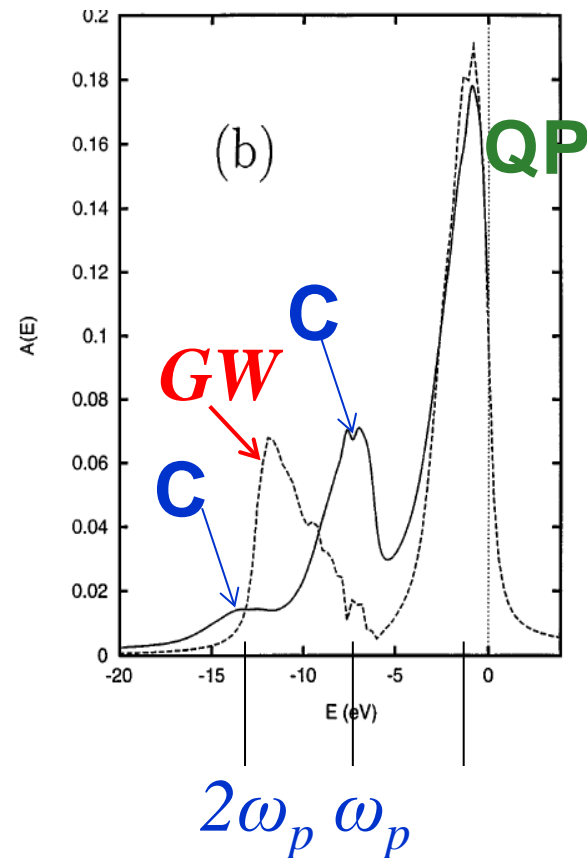
F. Aryasetiawan,<sup>1,2</sup> L. Hedin,<sup>1</sup> and K. Karlsson<sup>3</sup>

Quasi-particle peaks of **both**  
**GW** and **C** agree with XPS expt

**GW fails for satellites: only one**  
**satellite at wrong energy**

**Cumulant model agrees with**  
**experiment: multiple satellites**  
 $\omega_p$  apart

Na XPS



# Reviews & references for cumulant Green's fn

J. Phys.: Condens. Matter 11 (1999) R489–R528

## On correlation effects in electron spectroscopies and the *GW* approximation

Lars Hedin

Department of Theoretical Physics, Lund University, Sölvegatan 14A, 223 62 Lund, Sweden

THE JOURNAL OF CHEMICAL PHYSICS 143, 184109 (2015)

## Dynamical effects in electron spectroscopy

Jianqiang Sky Zhou,<sup>1,2,a)</sup> J. J. Kas,<sup>2,3</sup> Lorenzo Sponza,<sup>4</sup> Igor Reshetnyak,<sup>1,2</sup> Matteo Guzzo,<sup>5</sup> Christine Glorgetti,<sup>1,2</sup> Matteo Gatti,<sup>1,2,6</sup> Francesco Sottile,<sup>1,2</sup> J. J. Rehr,<sup>2,3</sup> and Lucia Reining<sup>1,2</sup>

<sup>1</sup>Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM-IRAMIS, Université Paris-Saclay, F-91128 Palaiseau, France

<sup>2</sup>European Theoretical Spectroscopy Facility (ETSF)

<sup>3</sup>Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA

<sup>4</sup>Department of Physics, King's College London, London WC2R 2LS, United Kingdom

<sup>5</sup>Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany

<sup>6</sup>Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, BP 48, F-91192 Gif-sur-Yvette, France



# Why does it work: Quasi-boson approximation

**IDEA:** Neutral excitations - plasmons, phonons, etc. can be represented as **bosons**

**Theorem:**\* Cumulant representation of core-hole Green's function is EXACT for electrons coupled to bosons

\*D. C. Langreth, *Phys. Rev. B* **1**, 471 (1970)

**Corollary:** also valid for valence with recoil approximation.

**Physics:\*\*** GW approximation describes an electronic-polaron: electrons coupled to density fluctuations modeled as bosons

\*\*B. I. Lundqvist, *Phys. Kondens. Mater.* **6** 193 (1967)

# Cumulant expansion properties

$$G_k(t) = e^{i\epsilon_k^0 t} e^{C(t)}$$

$$C(t) = \int d\omega' \beta(\omega') \frac{e^{i\omega' t} - i\omega' t - 1}{\omega'^2}$$

Landau formula for  $C(t)$

Excitation spectra (GW  $\Sigma$ )

$$\beta_k(\omega) = \frac{1}{\pi} |\text{Im} \Sigma_k(\omega + \epsilon_k)|$$

Spectral Function

$$A_k(\omega) = \int \frac{dt}{2\pi} e^{i(\omega - \epsilon_k)t} \exp \left\{ \int d\omega' \beta(\omega') \frac{e^{i\omega' t} - i\omega' t - 1}{\omega'^2} \right\}$$

\*For diagrammatic expansion of higher order terms, see e.g.  
O. Gunnarsson et al., Phys. Rev. B **50**, 10462 (1994)

# cf. Retarded Cumulant Approximation\*

PHYSICAL REVIEW B 90, 085112 (2014)

## Cumulant expansion of the retarded one-electron Green function

J. J. Kas,<sup>1,\*</sup> J. J. Rehr,<sup>1,2,†</sup> and L. Reining<sup>3,2,‡</sup>

<sup>1</sup>Department of Physics, University of Washington, Seattle, Washington 98195, USA

<sup>2</sup>European Theoretical Spectroscopy Facility (ETSF)

<sup>3</sup>Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, F-91128 Palaiseau, France

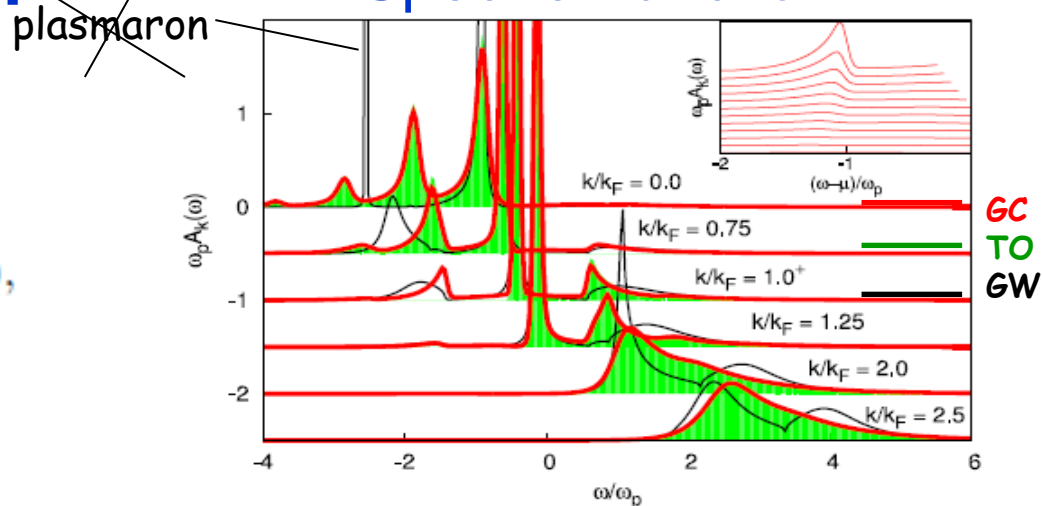
## Retarded GF formalism

$$G_k^R(t) = -i\theta(t)e^{-i\epsilon_k^{HF}t}e^{\tilde{C}_k^R(t)},$$

$$\tilde{C}_k^R(t) = \int d\omega \frac{\beta_k(\omega)}{\omega^2} (e^{-i\omega t} + i\omega t - 1),$$

$$\beta_k(\omega) = \frac{1}{\pi} |\text{Im} \Sigma_k^R(\omega + \epsilon_k)|,$$

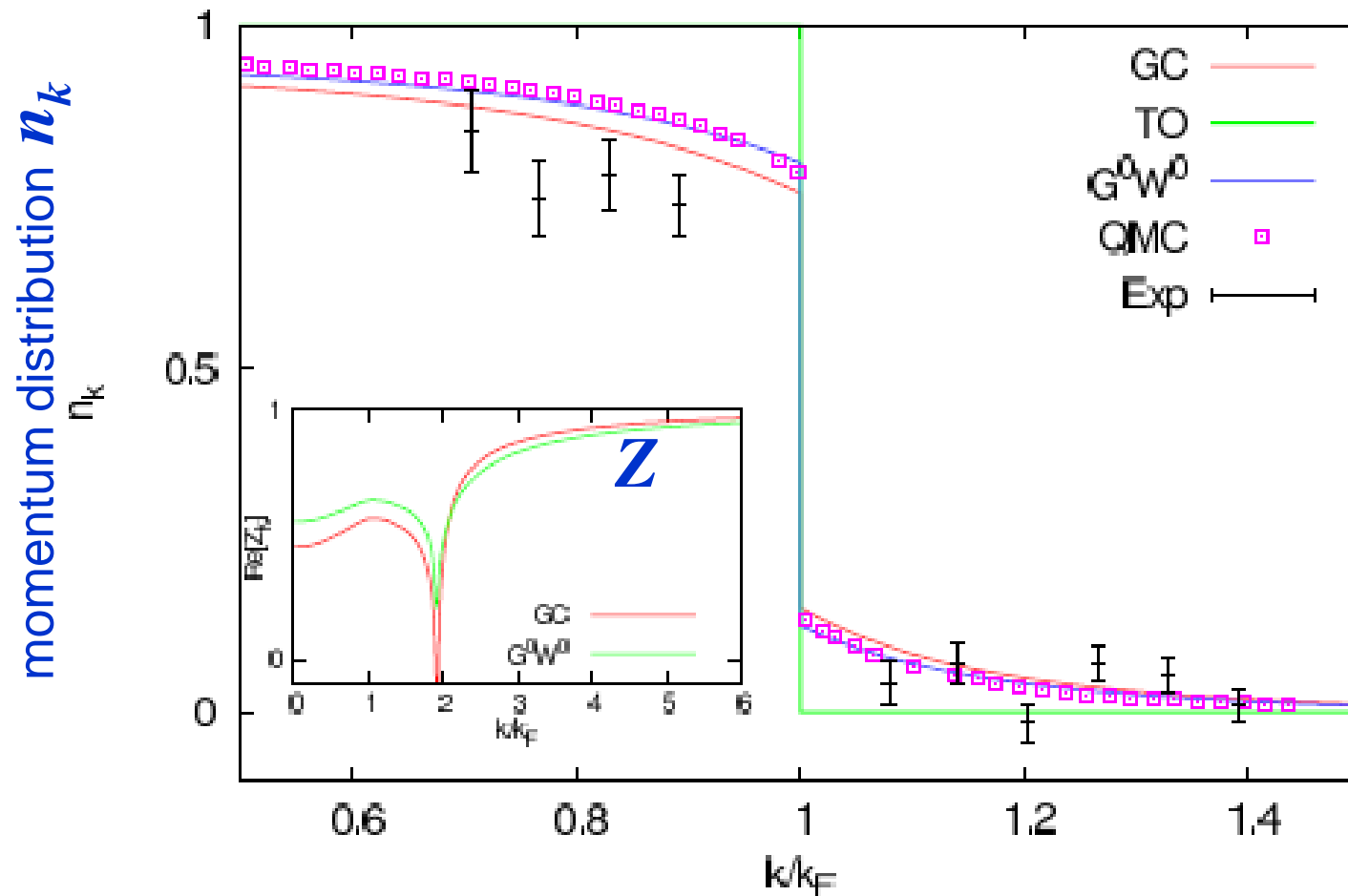
## Spectral function



Retarded cumulant builds in particle-hole symmetry

# Electron-gas quasi-particle properties

Retarded cumulant has good  $n_k$  and  $Z$ ,  
& pretty good correlation energies



# Example: Multiple satellites in XPS of Si

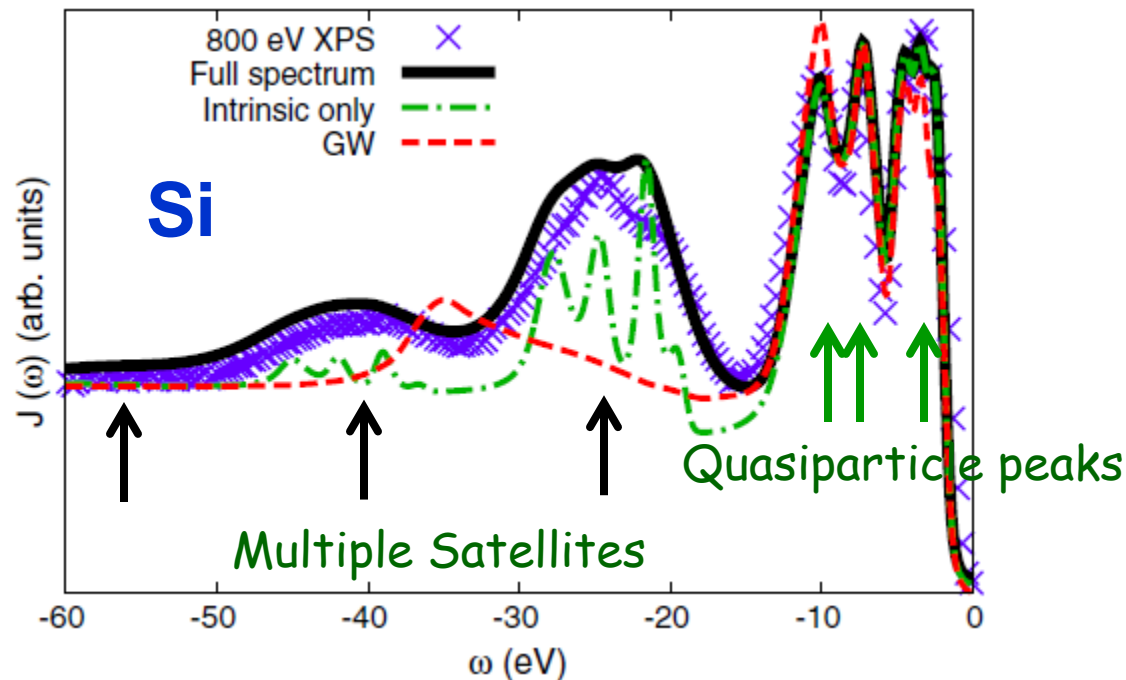
PRL 107, 166401 (2011)

PHYSICAL REVIEW LETTERS

week ending  
14 OCTOBER 2011

## Valence Electron Photoemission Spectrum of Semiconductors: *Ab Initio* Description of Multiple Satellites

Matteo Guzzo,<sup>1,2,\*</sup> Giovanna Lani,<sup>1,2</sup> Francesco Sottile,<sup>1,2</sup> Pina Romaniello,<sup>3,2</sup> Matteo Gatti,<sup>4,2</sup> Joshua J. Kas,<sup>5</sup>  
John J. Rehr,<sup>5,2</sup> Mathieu G. Silly,<sup>6</sup> Fausto Sirotti,<sup>6</sup> and Lucia Reining<sup>1,2,†</sup>



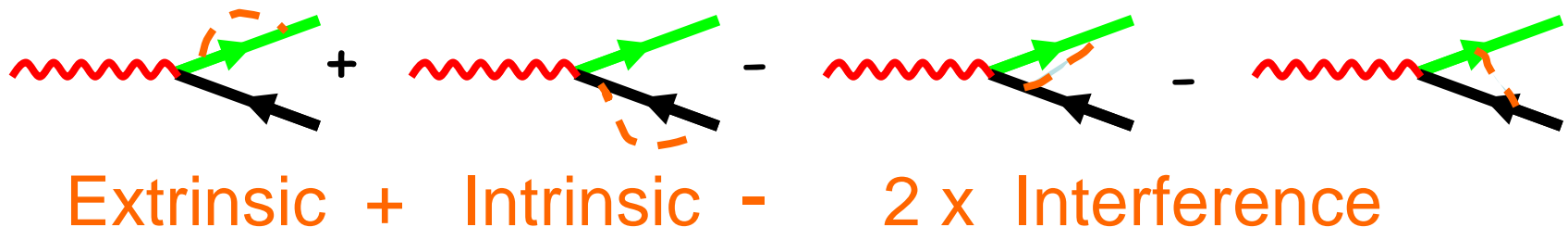
Lucia Reining

**Problems** GW: only one broad satellite at wrong position  
C: position ok but intensity too small

# III. Particle-hole cumulant theory

Q: How to calculate *all* inelastic losses and satellites in x-ray spectra ?

**Problem:** Single-particle cumulant in XPS (or XAS) only has intrinsic (or extrinsic) losses and ignores interference: Need to include all losses.



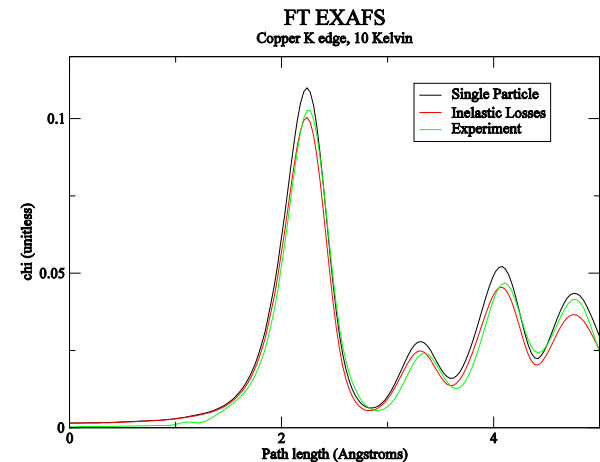
# Hedin suggestion: quasi-boson method with intrinsic, extrinsic and interference

Explanation of XAFS many-body amplitude factor:\*  $\chi_{exp} = \chi_{th} * S_0^2$

EXTRINSIC AND INTRINSIC PROCESSES IN EXAFS  
Lars Hedin, Dept of Theoretical Physics, University of Lund, Sweden

Physica B 158 (1989) 344-346  
North-Holland, Amsterdam

The importance of correlation effects in spectroscopies like EXAFS and photoemission is well recognized. The two main mechanisms are shake-off (in which we include shake-up) when the photoelectron is created, and energy loss of the propagating electron. Shake-off is clearly impossible at threshold, due to lack of energy. For photoemission often the "Spicer three-step model" is used, (1) creation of the photoelectron (including shake-off), (2) propagation to the surface (including losses), and (3) passage through the surface (including losses). Langreth [1] has pointed out that one should add the amplitudes for (2) and (3), and not, as in the Spicer model, convolute their squares, the probabilities. This effect is important primarily at threshold.

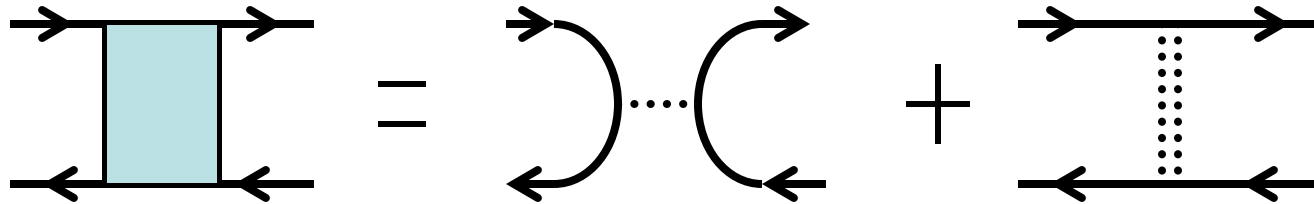


\* J.J. Rehr, E.A. Stern, R.L. Martin, and E.R. Davidson, Phys. Rev. B 17,560 (1978)

# Starting point: GW/BSE

## Particle-hole Green's function w/o satellites

$$-\text{Im } \epsilon^{-1}(\mathbf{q}, \omega) = \frac{4\pi}{q^2} \text{Im} \langle \Psi_0 | \hat{D}^\dagger \frac{1}{E_0 + \omega - \hat{H} + i\gamma} \hat{D} | \Psi_0 \rangle$$



**Ingredients:** Particle-Hole Hamiltonian

$$H = h_e - h_h + V_{eh} \quad h_{e/h} = \epsilon_{nk} + \Sigma_{nk}$$

$\Sigma$  GW self-energy

$$V_{eh} = V_x + W \quad \text{Particle-hole interaction}$$



# OCEAN: core-level GW/BSE code

PHYSICAL REVIEW B 83, 115106 (2011)

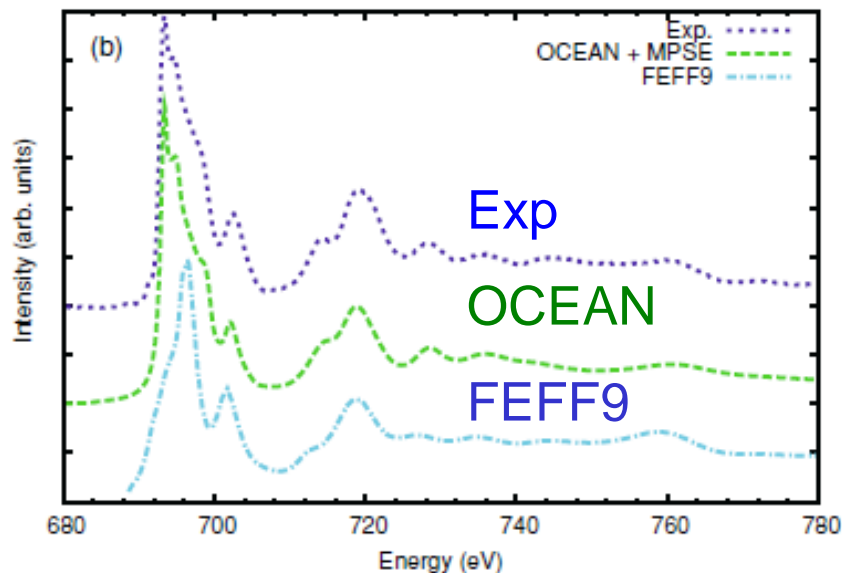
## Bethe-Salpeter equation calculations of core excitation spectra

J. Vinson, J. J. Rehr, and J. J. Kas

*Department of Physics, University of Washington, Seattle, Washington 98195, USA*

E. L. Shirley

*National Institute of Standards and Technology (NIST), Gaithersburg, Maryland 20899, USA*



\*Obtaining Core Excitations  
from ABINIT and NBSE

PW-PP + PAW  
+ MPSE + NBSE

\*J. Vinson et al. Phys. Rev. B83, 115106 (2011)

# Particle-hole cumulant in XPS\*

Europhys J. B **85**, 324 (2012)

## Plasmon Satellites in Valence-band Photoemission Spectroscopy

Ab Initio study of the photon-energy dependence in semiconductors

Matteo Guzzo<sup>1,2</sup>, Joshua J. Kas<sup>3</sup>, Francesco Sottile<sup>1,2</sup>, Mathieu G. Silly<sup>4</sup>, Fausto Sirotti<sup>4</sup>, John J. Rehr<sup>3</sup>, and Lucia Reining<sup>1,2</sup>

$$\langle J_k(\omega) \rangle = \sum_i |M_{ik_0}|^2 \int_0^\infty e^{-a} \int_{-\infty}^\infty e^{i(\omega_0 - \epsilon_k + \epsilon_i)t} \\ \times \exp \left[ \int \gamma_{ik}(\omega) (e^{-i\omega t} - 1) d\omega \right] dt dz_c$$

**Kernel  $\gamma(\omega)$  with extrinsic, intrinsic and interference terms**

$$\gamma_{ik}(\omega) = \sum_{\mathbf{q}} |g_{\mathbf{q}}|^2 \delta(\omega - \omega_{\mathbf{q}}) = \gamma_i^{int} + \gamma_k^{ext} + \gamma_{ik}^{inf}$$

\*L. Hedin, J. Michiels, and J. Inglesfield, Phys. Rev. B **58**, 15 565 (1998).

# Quasi-boson method for particle-hole GF\*

- Excitations:  $H_v = \sum_n \omega_n a_n^\dagger a_n$   $V^n \rightarrow -\text{Im } \varepsilon^{-1}(\omega_n, q_n)$
- Electrons:  $h' = \sum_k \epsilon_k c_k^\dagger c_k$  **fluctuation potentials\***
- e-boson coupling  $V_{pv} = \sum_{nkk'} [V_{kk'}^n a_n^\dagger + (V_{kk'}^n)^* a_n] c_k^\dagger c_{k'}$
- Core-hole-boson coupling:  $V_{vc} = -\sum_n V_{bb}^n (a_n^\dagger + a_n)$

Partition contributions into Intrinsic + Extrinsic + Interference

$$\gamma_K(\omega) = \sum_q \left| V^q \tilde{g}(\omega - \omega_q) - \frac{V_{cc}^q}{\omega_q} \right|^2 \delta(\omega - \omega_q) = \gamma_c(\omega) + \gamma_k(\omega) + \gamma_{ck}(\omega)$$

\* L. Hedin, J. Michiels, and J. Inglesfield, Phys. Rev. B 58, 15 565 (1998)

# Example: Satellites in XPS of Si again

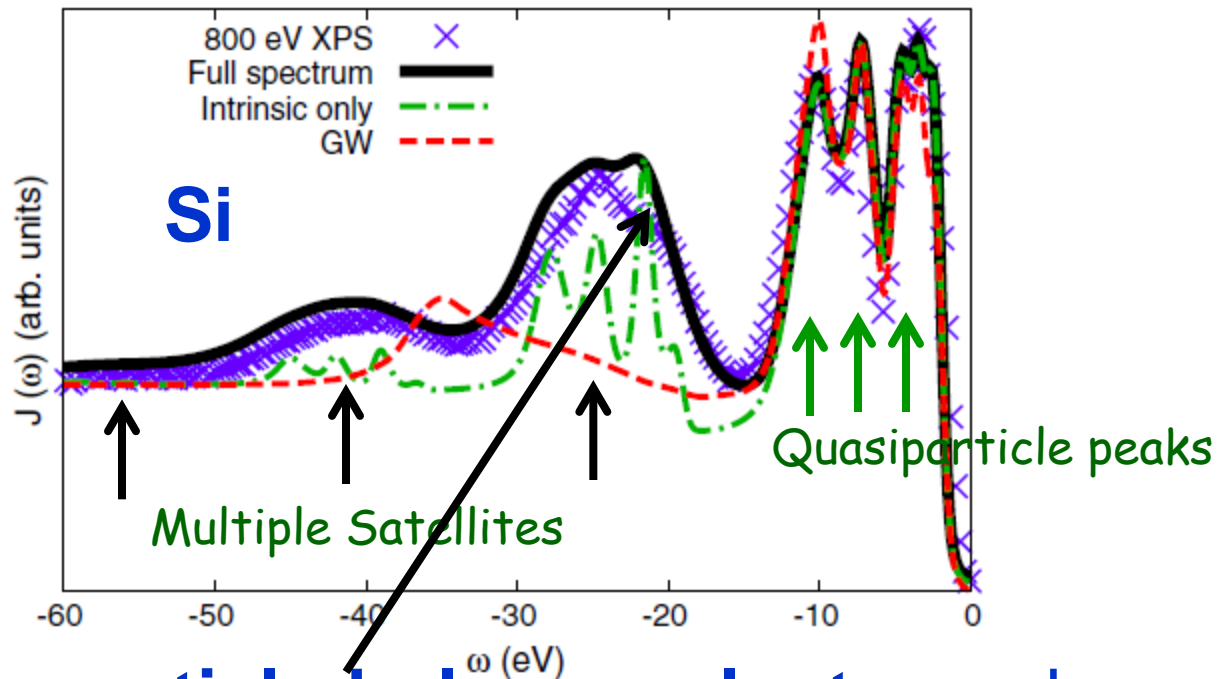
PRL 107, 166401 (2011)

PHYSICAL REVIEW LETTERS

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Matteo Guzzo,<sup>1,2,\*</sup> Giovanna Lani,<sup>1,2</sup> Francesco Sottile,<sup>1,2</sup> Pina Romaniello,<sup>3,2</sup> Matteo Gatti,<sup>4,2</sup> Joshua J. Kas,<sup>5</sup> John J. Rehr,<sup>5,2</sup> Mathieu G. Silly,<sup>6</sup> Fausto Sirotti,<sup>6</sup> and Lucia Reining<sup>1,2,†</sup>



**Success for particle-hole cumulant: good agreement only if extrinsic and interference terms are included**

# Particle-hole cumulant in XAS\*

PHYSICAL REVIEW B **94**, 035156 (2016)

## Particle-hole cumulant approach for inelastic losses in x-ray spectra

J. J. Kas,<sup>1</sup> J. J. Rehr,<sup>1</sup> and J. B. Curtis<sup>2</sup>

<sup>1</sup>*Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA*

<sup>2</sup>*Department of Physics, University of Rochester, Rochester, New York 14927, USA*

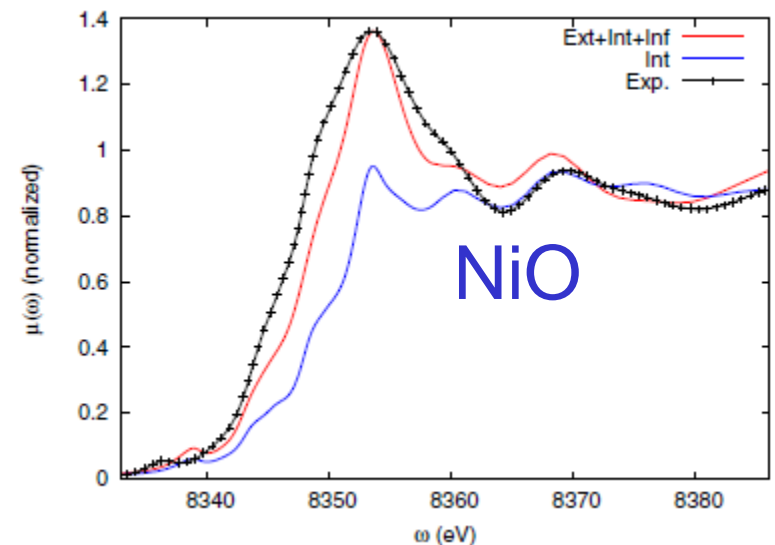
$$\tilde{G}_K(t) = \tilde{G}_K^0(t)e^{\tilde{C}_K(t)}$$

$$\tilde{C}_K(t) = \int d\omega \gamma_K(\omega)(e^{i\omega t} - i\omega t - 1)$$

$$\tilde{C}_K(t) = C_c(t) + C_k(t) + C_{ck}$$

All losses in particle-hole spectral function  $A_K$

$$\mu(\omega) = \int d\omega' \tilde{A}_K(\omega')\mu_K(\omega - \omega')$$



\* cf. L. Campbell, L. Hedin, J. J. Rehr, and W. Bardyszewski, Phys. Rev. B **65**, 064107 (2002)

# Theory of many-body amplitude factor

- Many-body XAS  $\approx$  Convolution

$$\begin{aligned}\mu(\omega) &= \int_0^\infty d\omega' \tilde{A}(\omega, \omega') \mu_{qp}(\omega - \omega') \\ &\equiv \langle \mu_{qp}(\omega) \rangle \approx \mu_{qp}(\omega) S_0^2(\omega)\end{aligned}$$

- Explains crossover: **adiabatic**  $S_0^2(\omega) = 1$   
to sudden transition  $S_0^2(\omega) \approx 0.9$

$$|g_q|^2 = |g_q^{ext}|^2 + |g_q^{intrin}|^2 - 2 g_q^{ext} g_q^{intrin}$$

Interference reduces loss!

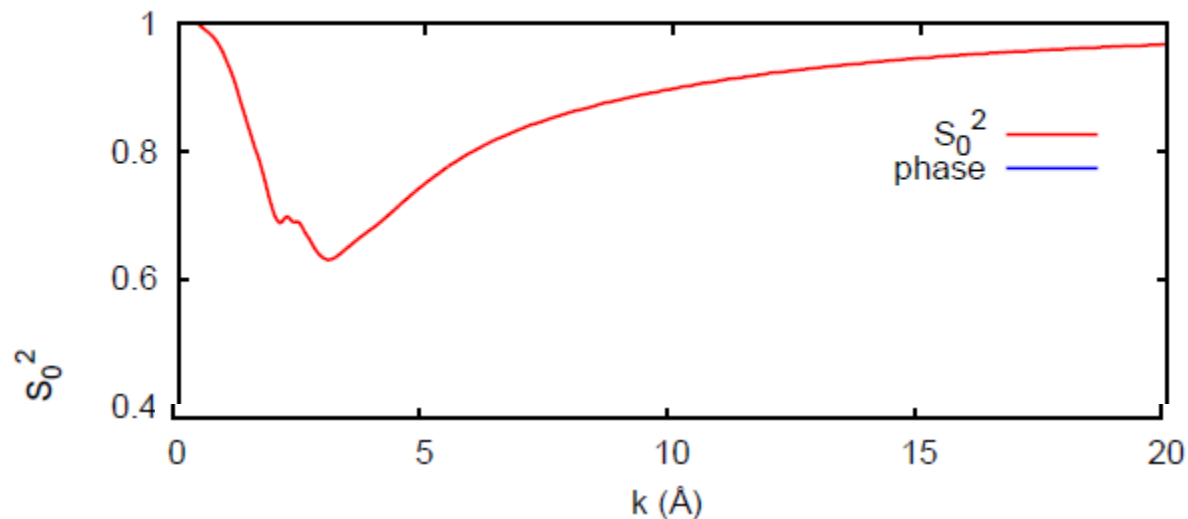
# Many-body amplitude factor $S_0^2$

MS Nano Proceedings, Springer (in press 2017)

## Cumulant approach for inelastic losses in x-ray spectra

John J. Rehr and Joshua J. Kas

$$S_0^2(R) = \int_0^\omega d\omega' \tilde{A}(\omega, \omega') e^{i2[k(\omega - \omega') - k(\omega)]R}$$



# Intrinsic losses: real-time TDDFT cumulant

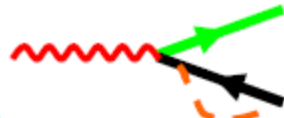
PHYSICAL REVIEW B 91, 121112(R) (2015)

Real-time cumulant approach for charge-transfer satellites in x-ray photoemission spectra

J. J. Kas,<sup>1</sup> F. D. Vila,<sup>1</sup> J. J. Rehr,<sup>1</sup> and S. A. Chambers<sup>2</sup>

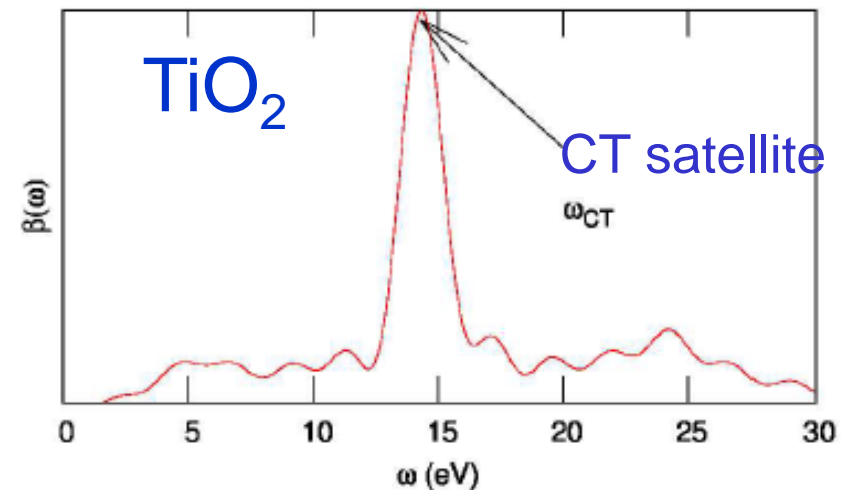
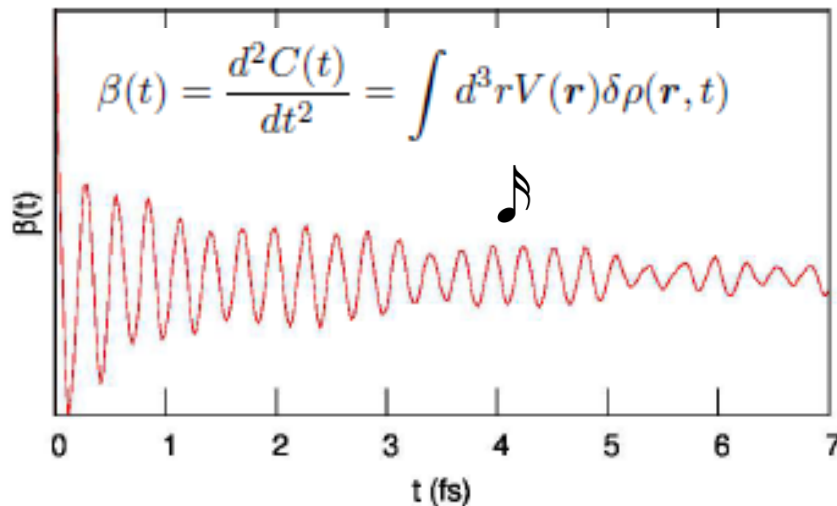
<sup>1</sup>Department of Physics, University of Washington, Seattle, Washington 98195-1560, USA

<sup>2</sup>Physical Sciences Division, Pacific Northwest National Laboratory, Richland, Washington 99352, USA



## Langreth cumulant in time-domain\*

$$C(t) = \sum_{\mathbf{q}, \mathbf{q}'} V_{\mathbf{q}}^* V_{\mathbf{q}'} \int d\omega S(\mathbf{q}, \mathbf{q}', \omega) \frac{e^{i\omega t} - i\omega t - 1}{\omega^2} = \int d\omega \beta(\omega) \frac{e^{i\omega t} - i\omega t - 1}{\omega^2}$$



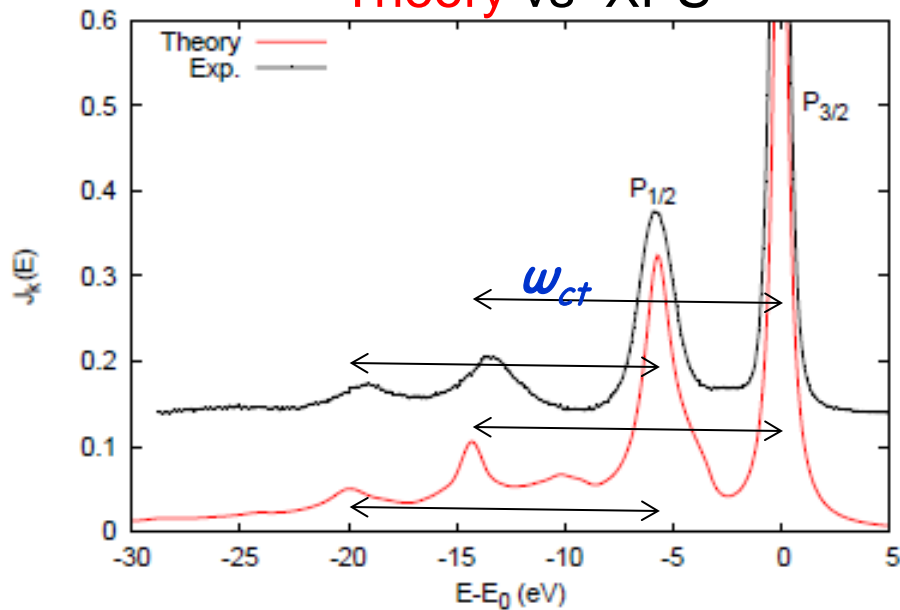
\*D. C. Langreth, Phys. Rev. B 1, 471 (1970)



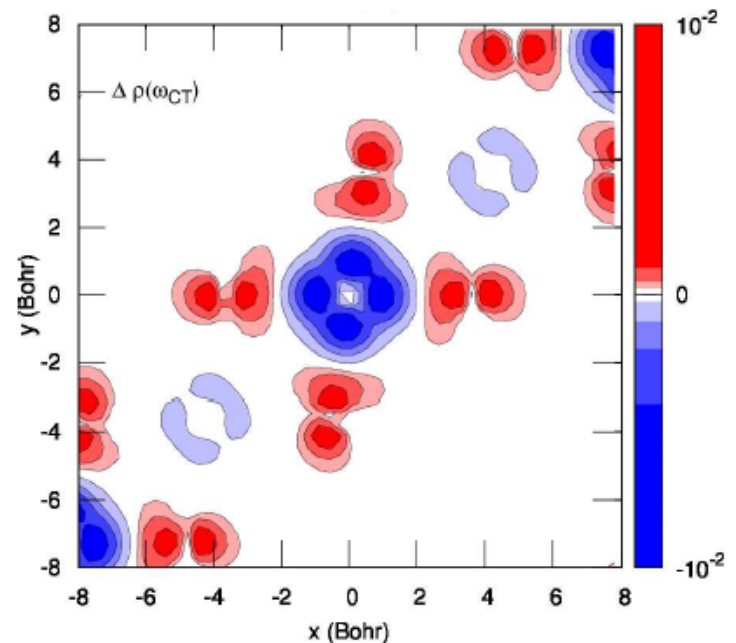
# Satellites and real-space interpretation

## RT TDDFT Cumulant

Theory vs XPS

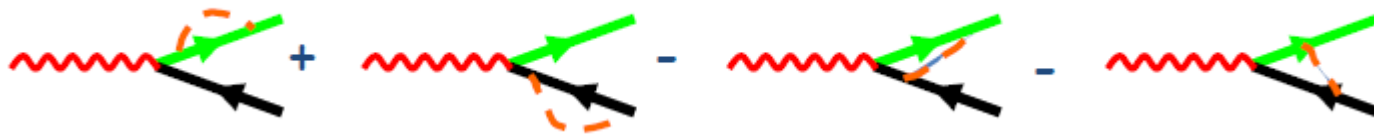


## Charge transfer fluctuations

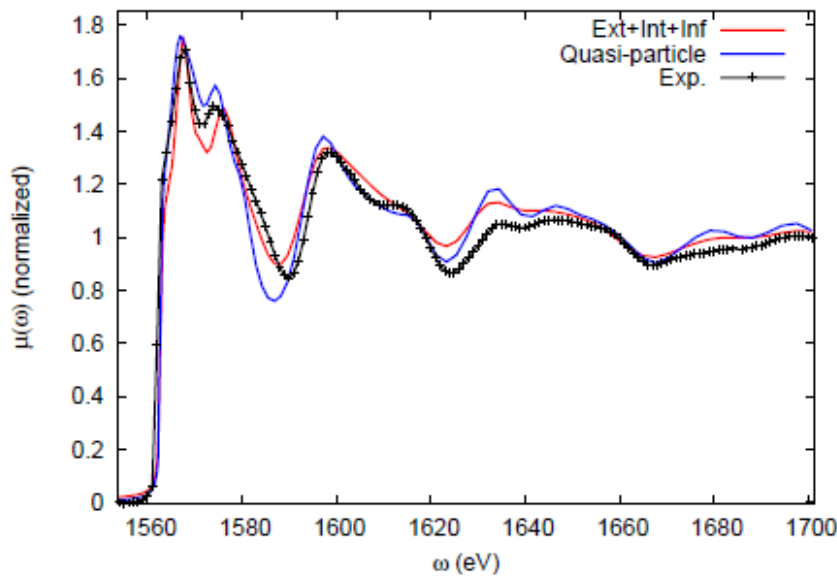


**Interpretation:** satellites arise from **charge density fluctuations** between ligand and metal at frequency  $\sim \omega_{CT}$  due to suddenly turned-on core-hole

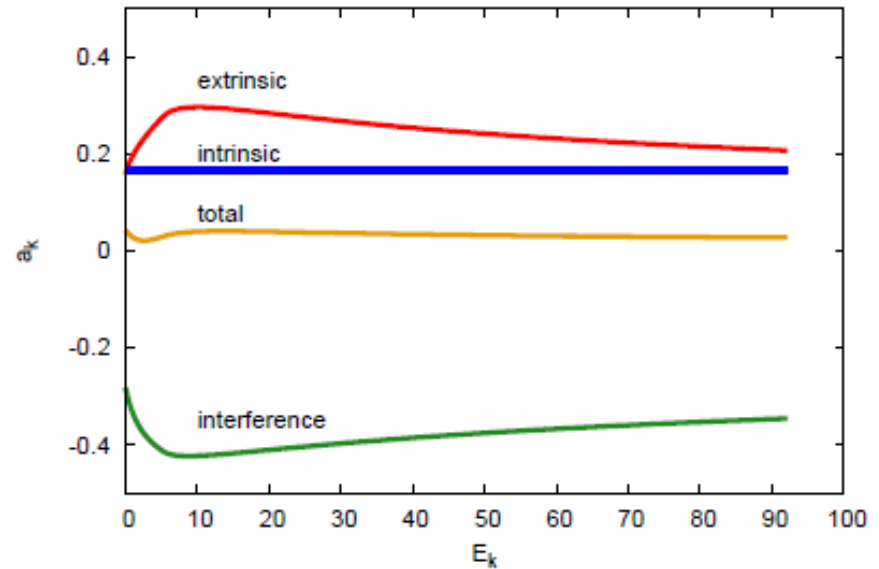
# Extrinsic, intrinsic and interference terms



## XAS of Al



## Satellite strengths



Particle-hole cumulant explains **cancellation** of extrinsic and intrinsic losses at threshold and

crossover:

**adiabatic**

to

**sudden**

approximation

# Examples: high accuracy XPS and XAS

Phys Rev B (in press, 2017)

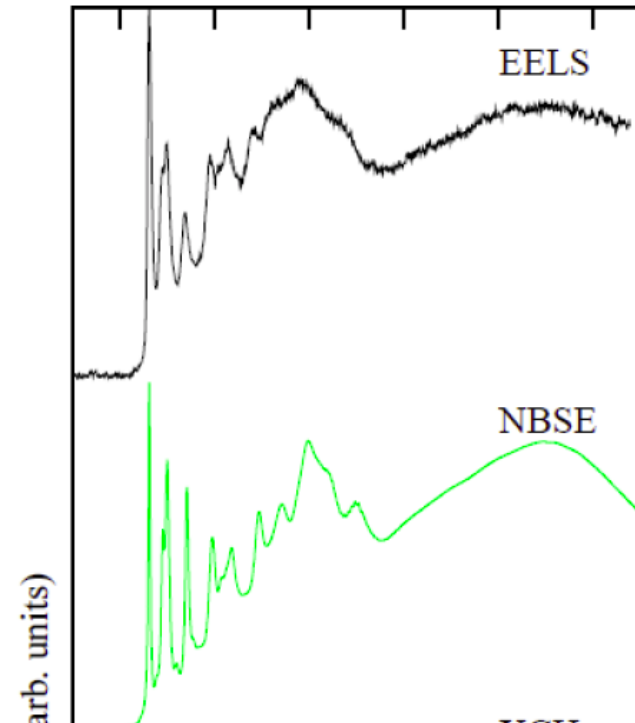
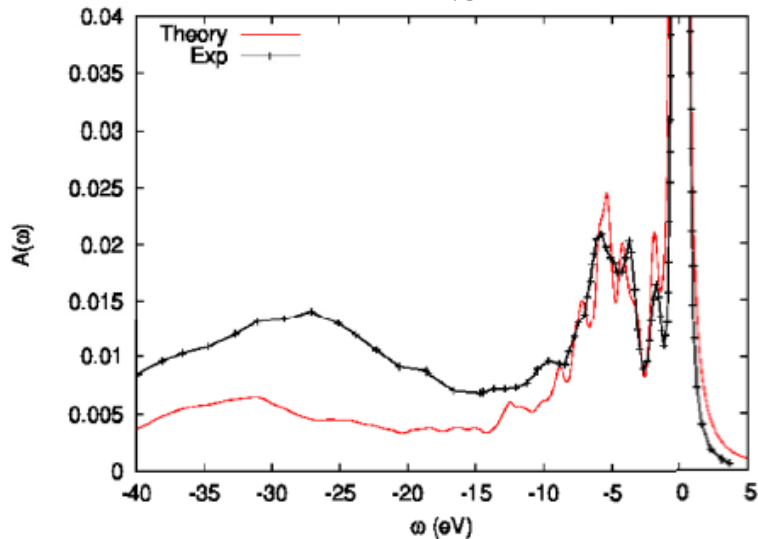
**High-resolution valence and core excitation spectra of solid C<sub>60</sub>**

**via first-principles calculations and experiment**

F. Fossard, K. Gilmore, G. Hug, J J. Kas, J J Rehr, E L Shirley and F D Vila

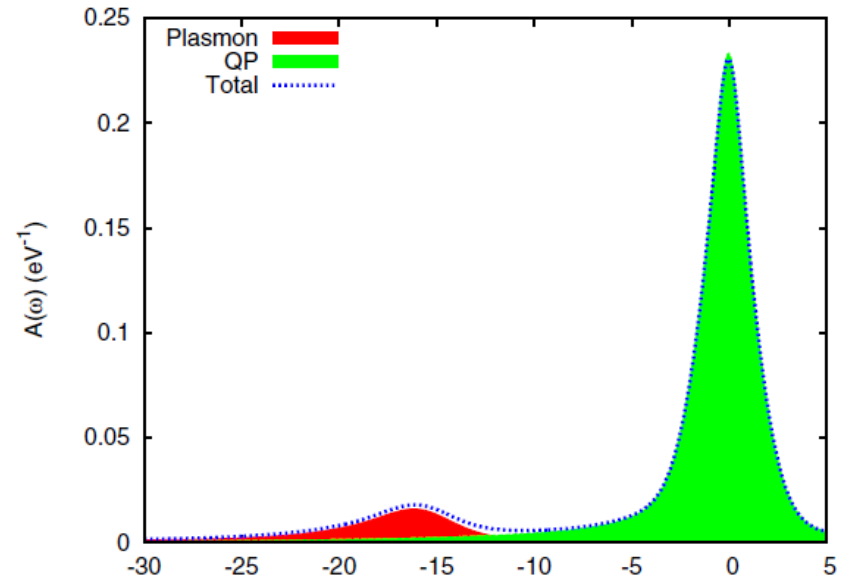
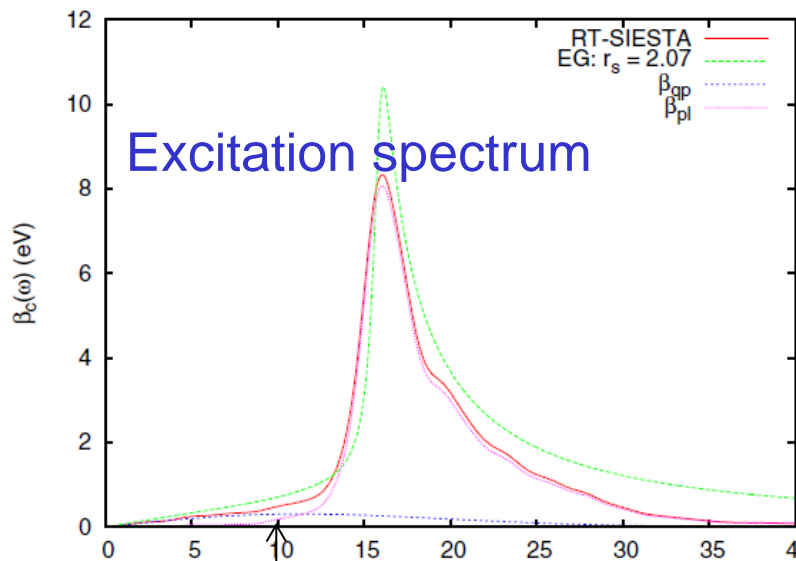
Particle-hole cumulant

RT-TDDFT intrinsic cumulant  
XPS



# X-ray Edge Singularities in metals

Low energy particle-hole excitations in cumulant **explain** edge singularities in XPS and XAS of metals



$$\beta_{ph}(\omega) = \alpha \omega e^{-\omega/\omega_p}$$

$$C_{ph}(t) = -i\alpha\omega_p t - \alpha \ln(1 - i\omega_p t) \quad A_{ph}(\omega) = e^{-a_{pl}} \frac{e^{-\tilde{\omega}/\omega_p}}{\Gamma(\alpha)} \frac{\omega_p^{-\alpha}}{\tilde{\omega}^{1-\alpha}}$$

cf Doniach-Sunjic line-shape in XPS

# Correlated systems

## Standard approximation: Hubbard-model

PHYSICAL REVIEW B **85**, 165123 (2012)

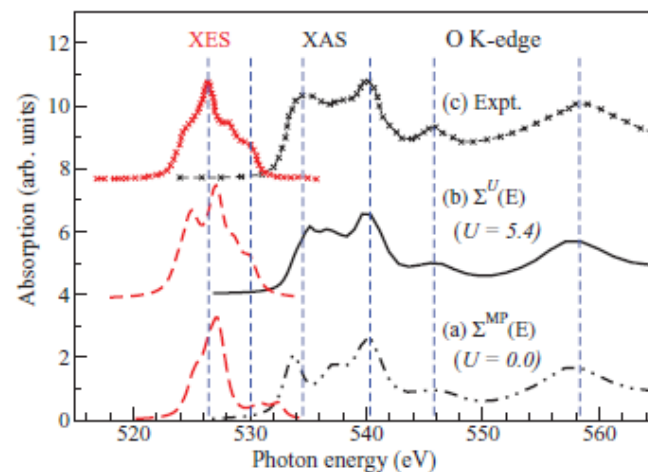
### Hubbard model corrections in real-space x-ray spectroscopy theory

Towfiq Ahmed, J. J. Kas, and J. J. Rehr

O K-edge MnO

Hubbard  $U$  as self-energy correction

$$V^U(\mathbf{r}, E) = V^{SCF}(\mathbf{r}) + \Sigma^{GW}(E) + \Sigma_{lm\sigma}^U(E)$$



cf. H. Jiang, Rinke et al. Phys. Rev. B **82**, 045108 (2010).

# Alternative approach: cumulant

**Question: Does the particle-hole cumulant method work for correlated *d*- and *f*- systems ?**

**Hedin's answer \* **MAYBE****

“Calculation similar to core case ... but with more complicated fluctuation potentials ...

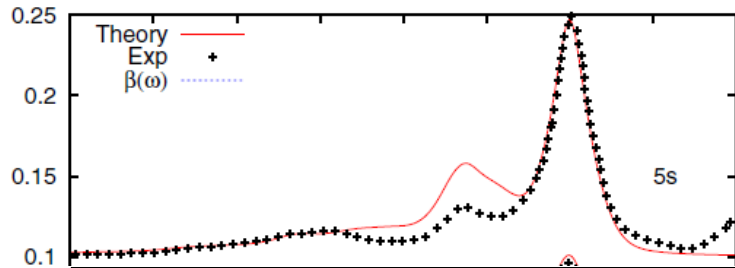
$$V^n \rightarrow -\text{Im } \varepsilon^{-1}(\omega_n, q_n)$$

... not question of principle, but of computational work...”

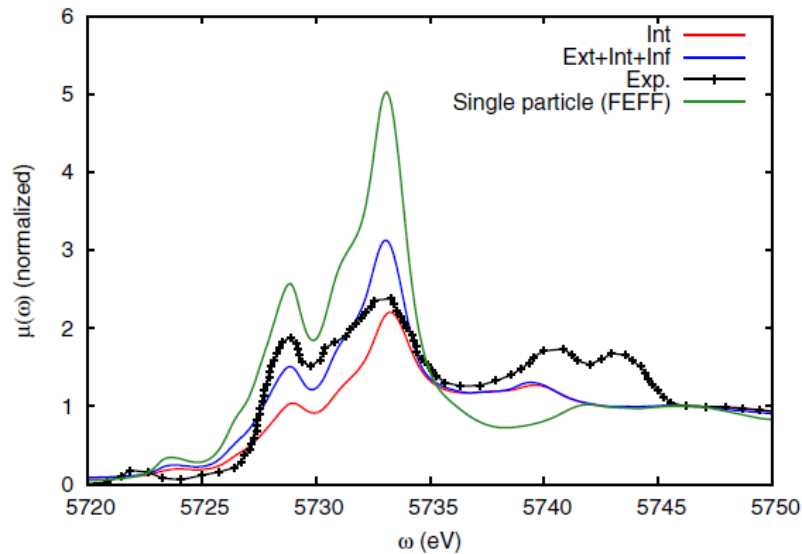
\* L. Hedin, J. Phys.: Condens. Matter **11**, R489 (1999)

# Particle-hole cumulant for $\text{CeO}_2^*$

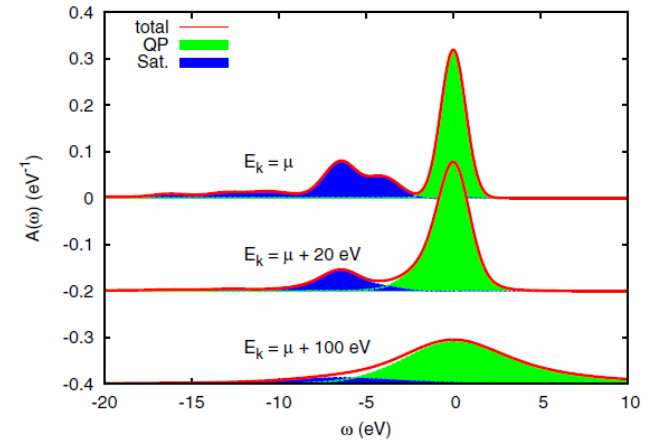
## Ce 5s XPS of $\text{CeO}_2$



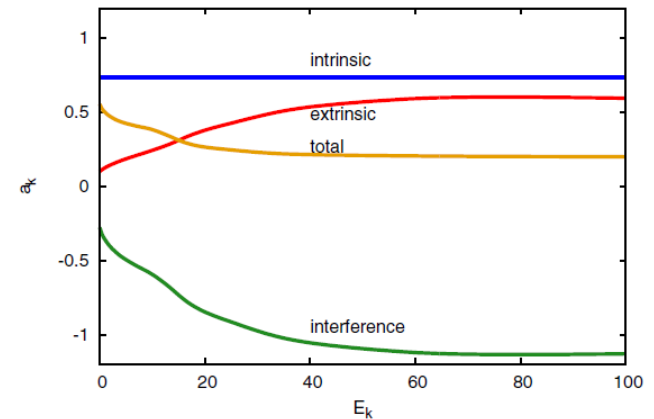
## Ce $L_3$ XAS of $\text{CeO}_2$



## Spectral function



## Spectral weights



\*J. Kas et al. Phys Rev B **94**, 035156 (2016)

# Conclusions

Many-body corrections including self-energy shifts, and inelastic losses, and Debye-Waller factors are essential for quantitative agreement with experimental x-ray spectra

Particle-hole cumulant theory approximation can explain all losses (extrinsic, intrinsic and interference) in x-ray spectra.

All losses can be lumped into a spectral function  $A_K(\omega)$

**AND** *can be added ex post facto*

$$\mu(\omega) = \int d\omega' \tilde{A}_K(\omega') \mu_K(\omega - \omega')$$



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