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X-ray Thomson scattering predictions from an average atom model

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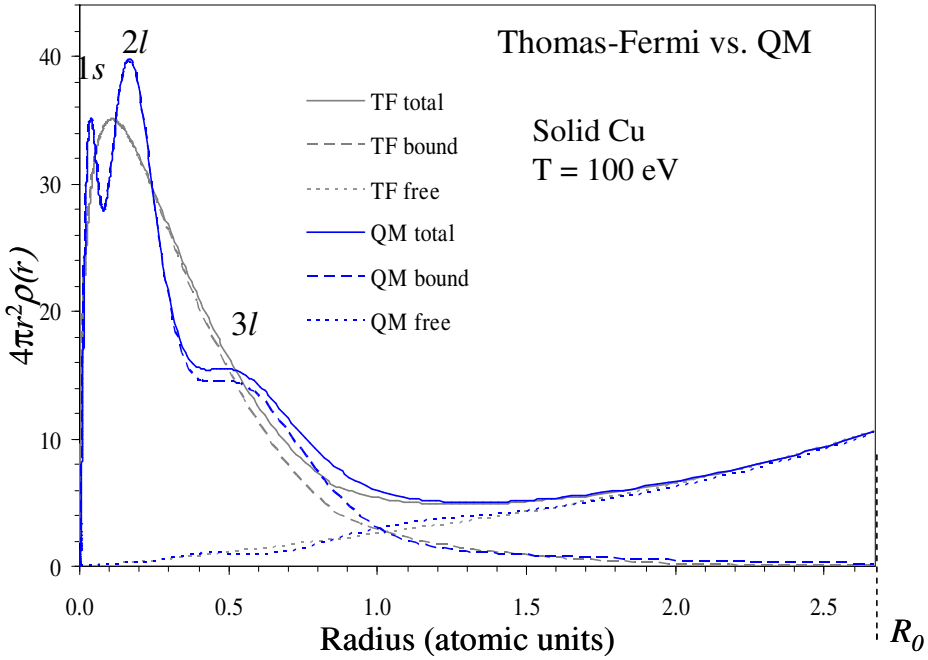
Self-consistent-field average-atom models are widely used for EOS [1,2] and, recently, opacities [3]

The model used in this work, MuZe [4], is a non-relativistic version of Inferno/Purgatorio [1,2], which solves for bound ($\varepsilon < 0$) and continuum ($\varepsilon > 0$) wavefunctions within a self-consistent electrostatic potential V(r) (here Kohn-Sham exchange is used rather than T-dependent Vxc).



Similar in spirit to self-consistent field codes based on Thomas-Fermi fluid models, quantum mechanical average atom SCF models give reasonable representations of bound states, pressure ionization, and deviations from ideal densities of states.

SCF models ensure consistency between the shielded ion potential V(r) and the electron wavefunctions, whose temperature-dependent occupations are governed by Fermi statistics.

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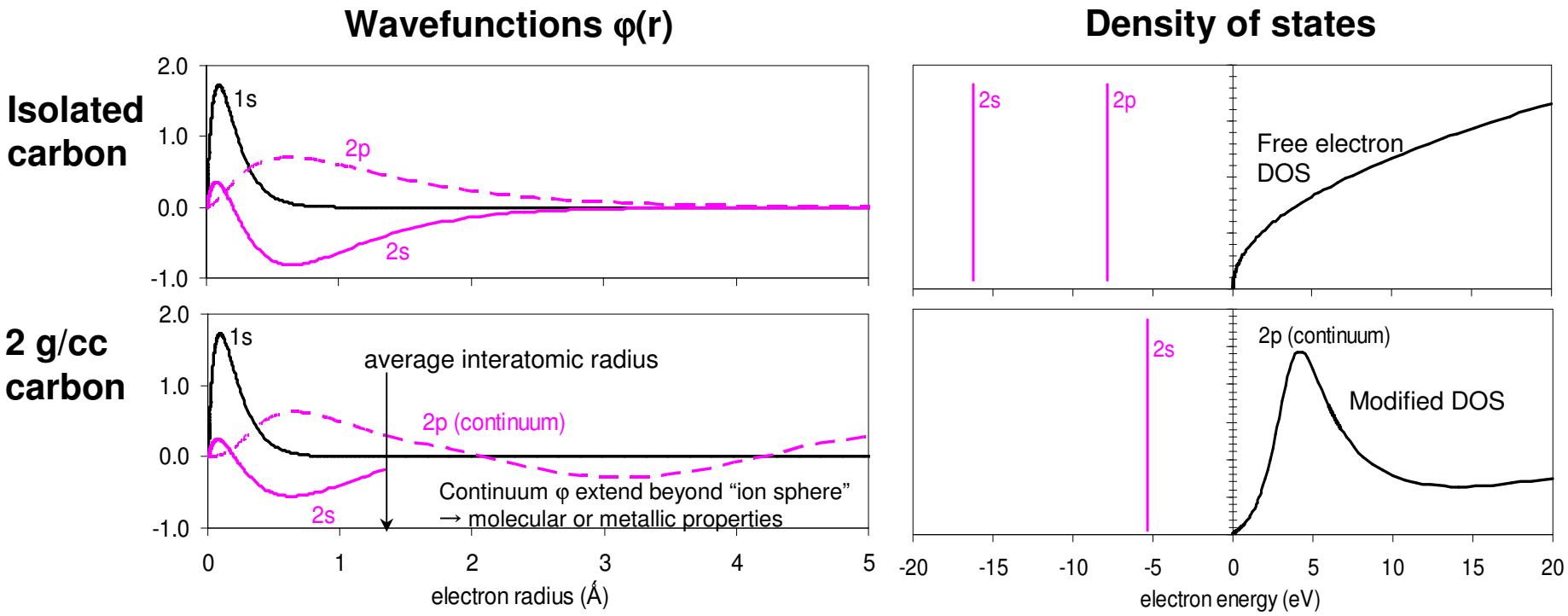
Increasing densities modify the wavefunctions of quantum mechanical average atom models

As ions get closer together, the occupied valence orbitals of neighboring ions interact, leading to phenomena such as density broadening, continuum lowering, and pressure ionization.



These phenomena manifest in EOS, transport, and spectroscopic data, with details dependent on model assumptions (symmetry, exchange potentials, boundary conditions…)

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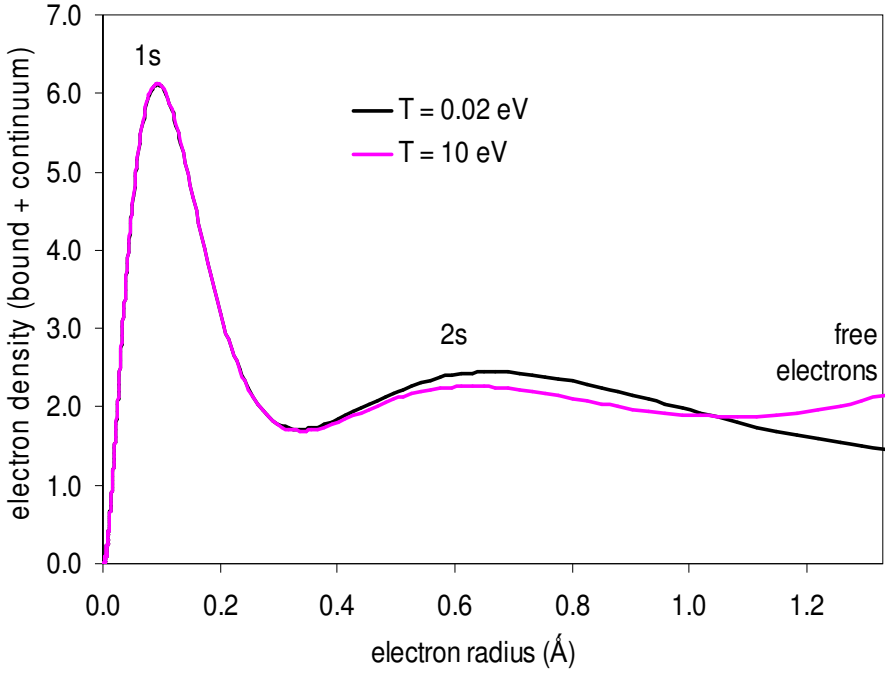
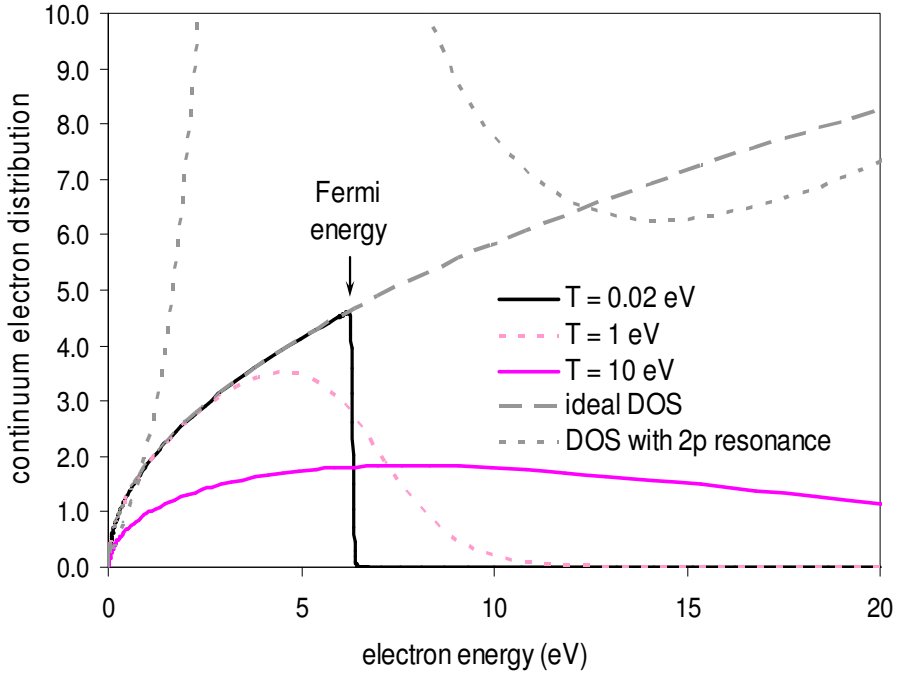
Thermal effects modify the electronic properties predicted with average atom models

Increasing temperatures move more electrons into the continuum, modifying the potential felt by the remaining bound electrons and softening the Fermi edge of the electron distribution.

electron density in 2 g/cc carbon



Free electron population distributions



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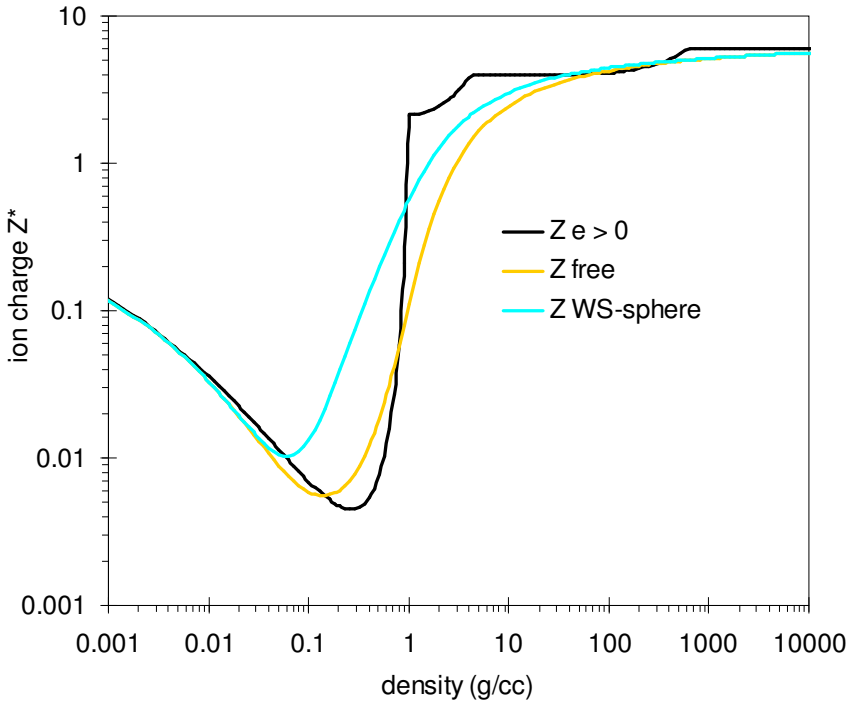
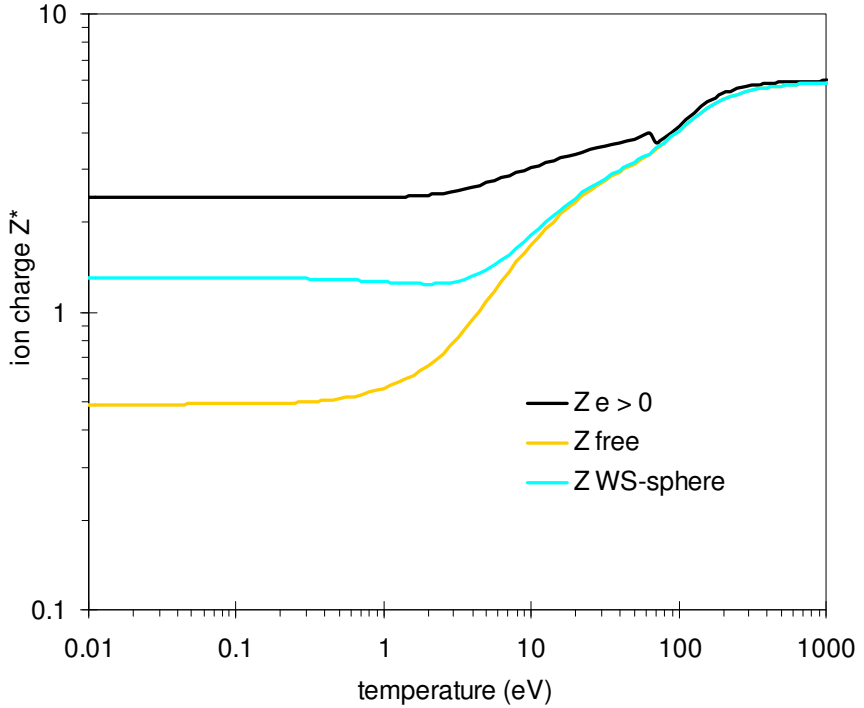
The average ion charge Z* is not uniquely defined

Several plausible definitions: All continuum electrons with $\varepsilon > 0$?
Only “free” electrons in plane-wave states? Electrons on the surface of the ion sphere?

Various Z* in 1 eV carbon



Z* in 2g/cc carbon



Many quantities are parameterized in terms of Z* (transport coefficients, structure factors) but different definitions give Z* that vary by factors of a few or more…

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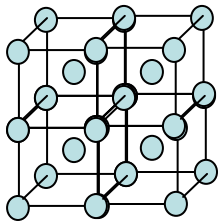
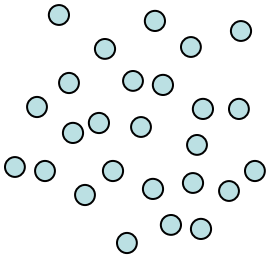
In strongly coupled systems ($E^{Coulomb} > E^{thermal}$), ion properties must also be considered

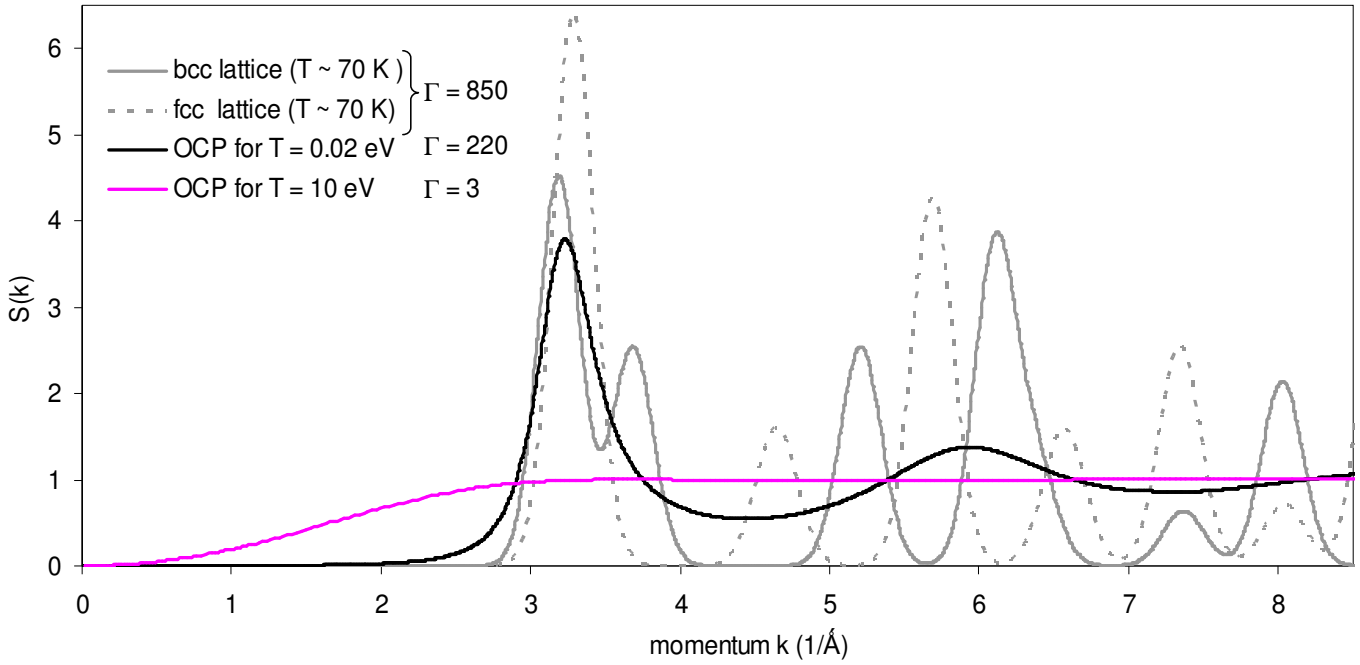
In classical hot plasmas with $\Gamma_{ii} \sim Z^{*2}/TR << 1$, the probability of finding another ion in any direction is g(r) ~ 1, so S(k), the Fourier transform of 1-g(r), is ~1 everywhere. In more strongly coupled systems with $\Gamma_{ii} > 1$, g(r) and S(k) vary to reflect (incipient) lattice structure.

Cold lattice (bcc)



Hot plasma





The structure factor plays an important role in scattering and bulk transport calculations. In our single-center average atom model, we use an OCP S(k) dependent on the ill-defined Z*

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The widely-used approach of Chihara [5,(6,7)] splits x-ray Thomson Scattering signals according to Z*

$$\frac{d^2\sigma}{d\Omega d\omega} = \sigma_T \frac{k_1}{k_0} S(k,\omega),$$

where σ_T is the usual Thomson cross section and $S(k,\omega)$ the total dynamic structure factor defined as

$$S(k,\omega) = \frac{1}{2\pi N}\int e^{i\omega t}\langle \rho_e(\mathbf{k},t)\rho_e(-\mathbf{k},0)\rangle dt,$$

with $\langle \cdots \rangle$ denoting an ensemble average and

$$\rho_e(\mathbf{k},t) = \sum_{s=1}^{Z_A N} \exp[i\mathbf{k}\cdot\mathbf{r}_s(t)]$$

$$S(k,\omega) = |f_I(k)+q(k)|^2 S_{ii}(k,\omega) + Z_f S^0_{ee}(k,\omega) + Z_c \int \tilde{S}_{ce}(k,\omega-\omega')S_s(k,\omega')d\omega'.$$

$$f_I(k) = \int_0^R 4\pi r^2 \rho_b(r)\frac{\sin kr}{kr} dr$$

$$q(k) = \sqrt{Z_f}\frac{S_{ei}(k)}{S_{ii}(k)}$$

This approach requires reliable calculations of multiple structure factors (See, Sce, Sii) along with ion form factors f(k) and the weakly-bound screening term q(k).
The predictions are fundamentally parameterized by Z_f (Z*).

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We propose an alternative approach for *non-collective* scattering based on average atom wavefunctions

Eisenberger [8] and Platzman [9] define the bound-free scattering term as an integral over (hydrogenic) bound electron wavefunctions $\langle\varphi_b|e^{i\mathbf{k}.\mathbf{r}}|\varphi_f\rangle$; Sahoo *et al*. implement this in [7], W.R. Johnson [10] uses the same approach to reproduce the free-free Compton scattering cross section and derives bound-free scattering signals for average-atom $\varphi_b \sim P(r)Y_{lm}$ and $\varphi_f \sim e^{i\mathbf{p}.\mathbf{r}}$

$$\frac{d\sigma}{d\Omega_1 d\omega_1} = \left(\frac{d\sigma}{d\Omega_1}\right)_{\mathrm{Th}} \left(\frac{\omega_1}{\omega_0}\right) \sum_{i,f} |M_{fi}|^2 \delta(\epsilon_f - \epsilon_i - \omega)$$

where

$$M_{fi} = \langle f|e^{i\mathbf{k}\cdot\mathbf{r}}|i\rangle,$$

Our approach follows Johnson for the bound-free scattering, weighting the signals by the initial bound-state occupations, and extends the calculation to treat
a) free-free scattering as $\langle\varphi_c|e^{i\mathbf{k}.\mathbf{r}}|\varphi_f\rangle$ weighted by DOS*$f(\varepsilon)$,
b) elastic (bound-bound) scattering as occupation-weighted $\langle\varphi_b|e^{i\mathbf{k}.\mathbf{r}}|\varphi_b\rangle$
-- thus treating scattering from all electrons on an equal footing.*

*So far, "true" elastic scattering is calculated for bound-bound processes only.
All other scattering processes are based on an initial electron wavefunction and a free-wave final state.
The <free/cntm | M | free > scattering signals are integrated over energy, partial waves, and radius (to Rws) and occasionally appear to be ill-normalized.

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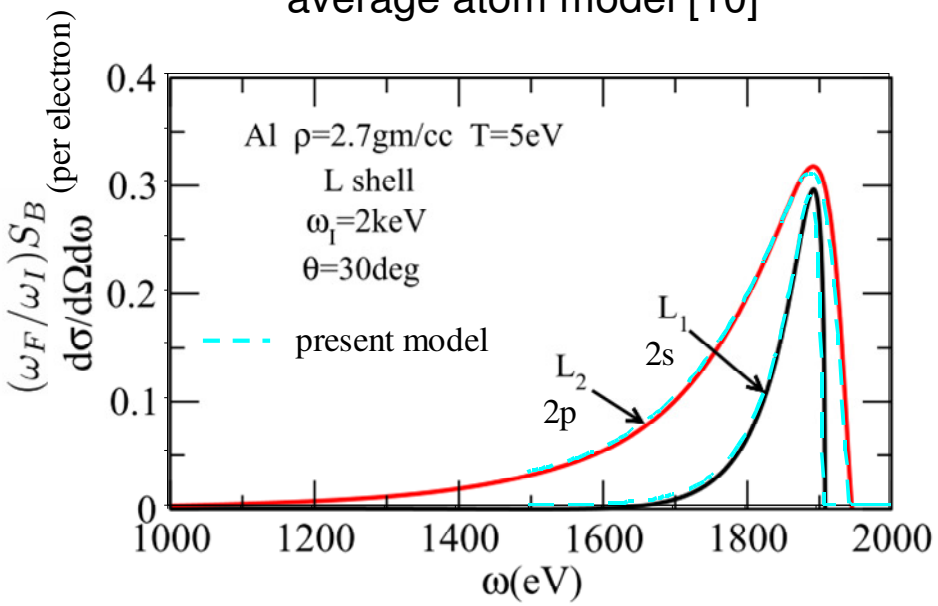
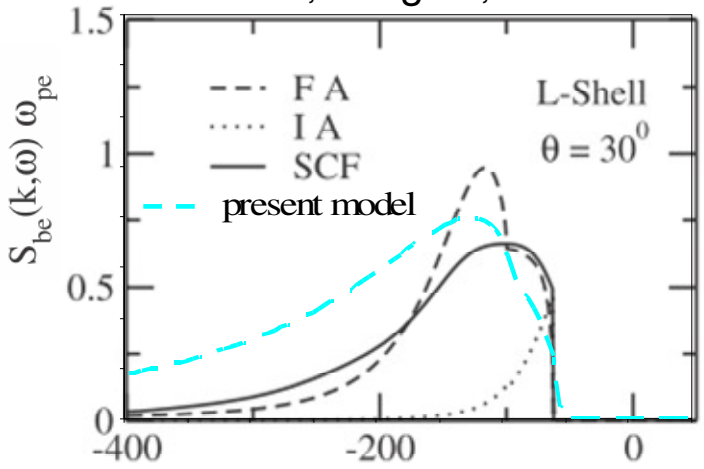
Our implementation agrees with previous work for the bound-free scattering features in WD Al

Comparison with W.R. Johnson average atom model [10]



Comparison with Sahoo *et al.* [7] (scaled intensity)
Al 5 eV, 2.7 g/cc, θ = 30°



Sahoo *et al.* (Slater exchange) predict that 3s electrons are bound; Johnson and MuZe models (Kohn-Sham) predict those states to be in the continuum. A similar difference in φ_{2l} may account for the longer "tails" on L-shell predicted by MuZe in the right-hand plot.

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We have also implemented the "impact approximation" (IA) for scattering among states in the continuum

Eisenberger [8] and Platzman [9] develop a formalism for the impact approximation in which an initial photon interacts with an electron-ion system. The system V(r) evolves only after the scattered photon has departed. In this approximation, the scattering signal is an integral over n_p, the probability of the initial electron having momentum **p** and a delta function:

$$\frac{d\sigma}{d\omega\, d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th}} \frac{\omega_1}{\omega_2} \frac{1}{(2\pi)^3} \times \int \delta\left(\omega - \frac{k^2}{2m} - \frac{\vec{k}\cdot\vec{p}_0}{m}\right) n_{p_0}\, d^3p_0$$

Compton scattering shift

Doppler shift

In the IA for the average atom, we use the continuum DOS and temperature-dependent Fermi functions to assign each initial electron energy a probability n(e); scattering signals for isotropic n(p) are calculated for initial electrons in both ideal ("free") and modified ("continuum") DOS.

The method appears to be so reliable for free electrons that we area-normalize the <f|M|f> and <c|M|f> scattering spectra to the nc(p) and nf(p) IA spectra.

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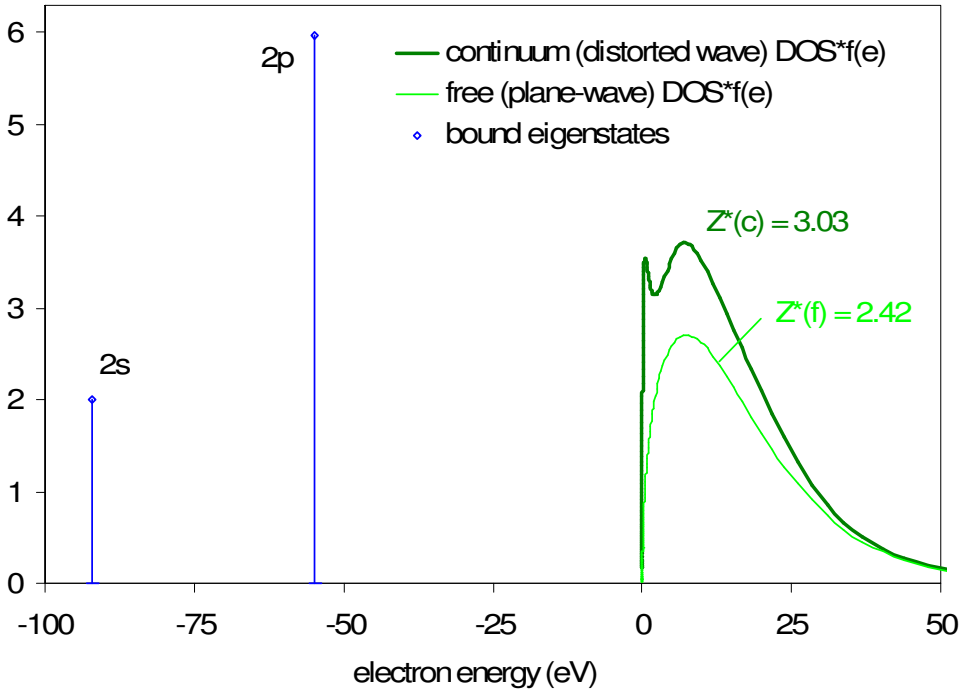
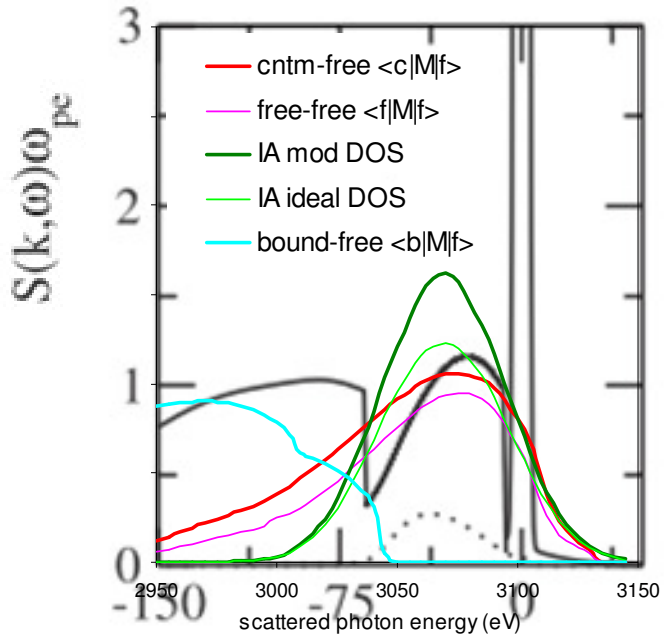
Although Sahoo and MuZe Z* differ by ~2, the overall scattering signals have similar character

Distributions of bound, “continuum” (DW), and “free” (plane wave) electron states in MuZe
Al 10 eV 2.7 g/cc



Comparison with Sahoo *et al.* [7] (scaled): Al 10 eV, 2.7 g/cc, θ = 130°



The $3s^2$ electrons are bound in Sahoo model (Z*~1), unbound in MuZe (Z*~ 3). But the IA free electron feature from MuZe approximately matches the free + M-shell feature from Sahoo *et al.*

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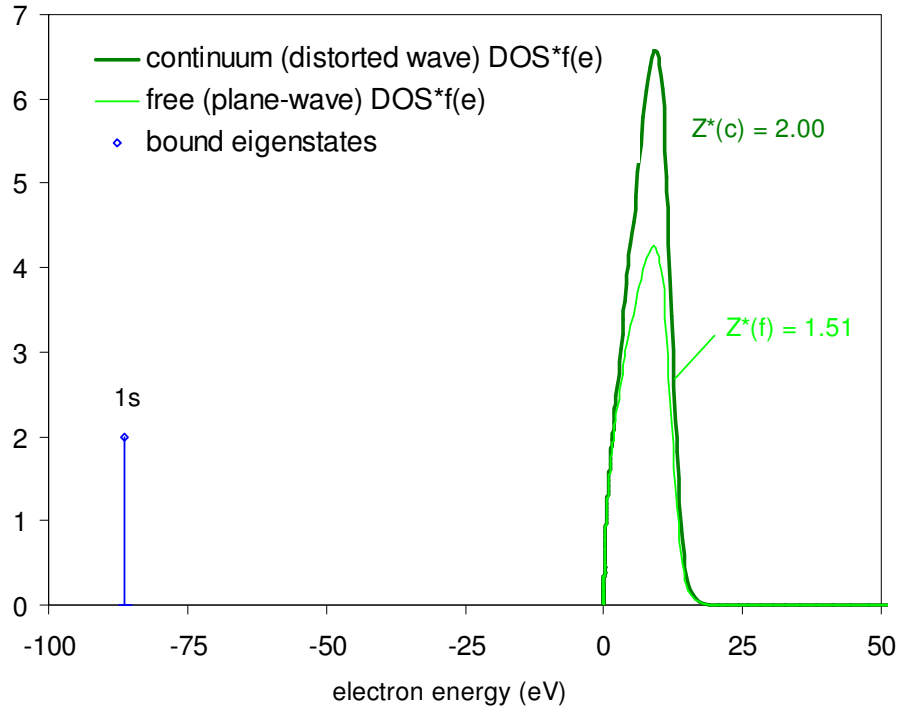
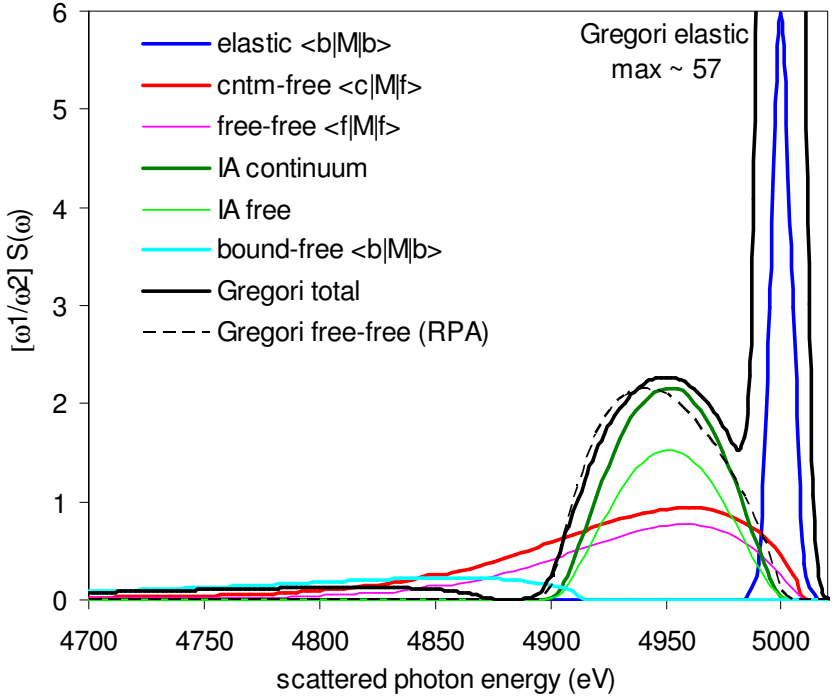
Predicted scattering from cool, solid Be compared with Gregori's SLFC/SOCP model [11]

Distributions of bound, "continuum" (DW), and "free" (plane wave) electron states in MuZe
Be 1 eV, 1.85 g/cc



Gregori's model: Z* = 2, θ = 90° α~0.5,
Both codes have elastic FWHM = 10 eV



-- The bound-free and (RPA/IA) free-free features are in reasonable agreement between codes
-- Static local field corrections are small; the φ-based approach <c|M|f> broadens the free-free signal
-- The elastic feature is ~10x smaller using <b|M|b> than SOCP (Sii ~1.5)

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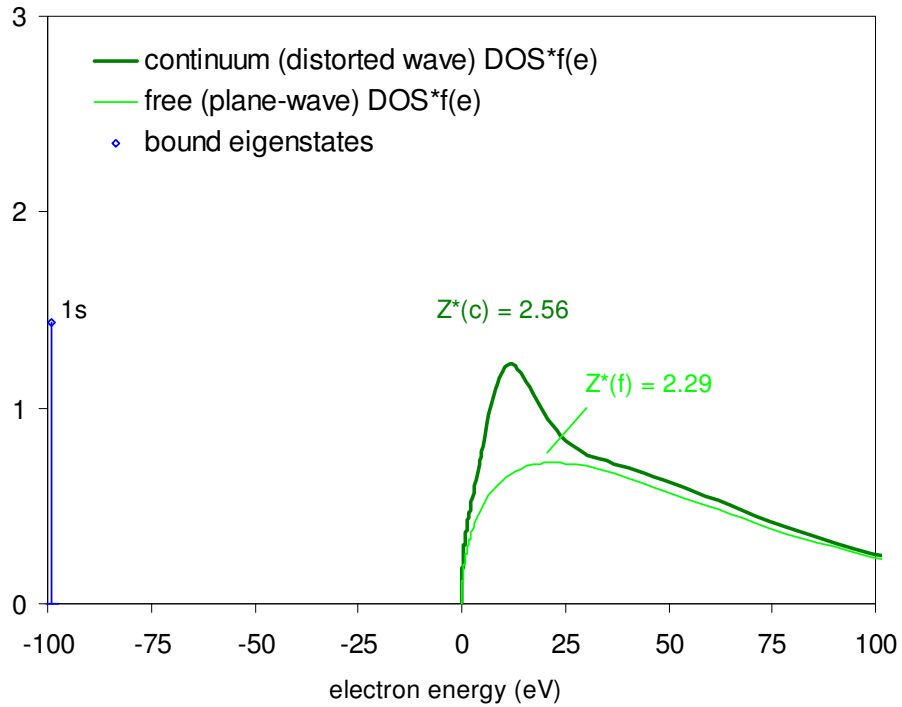
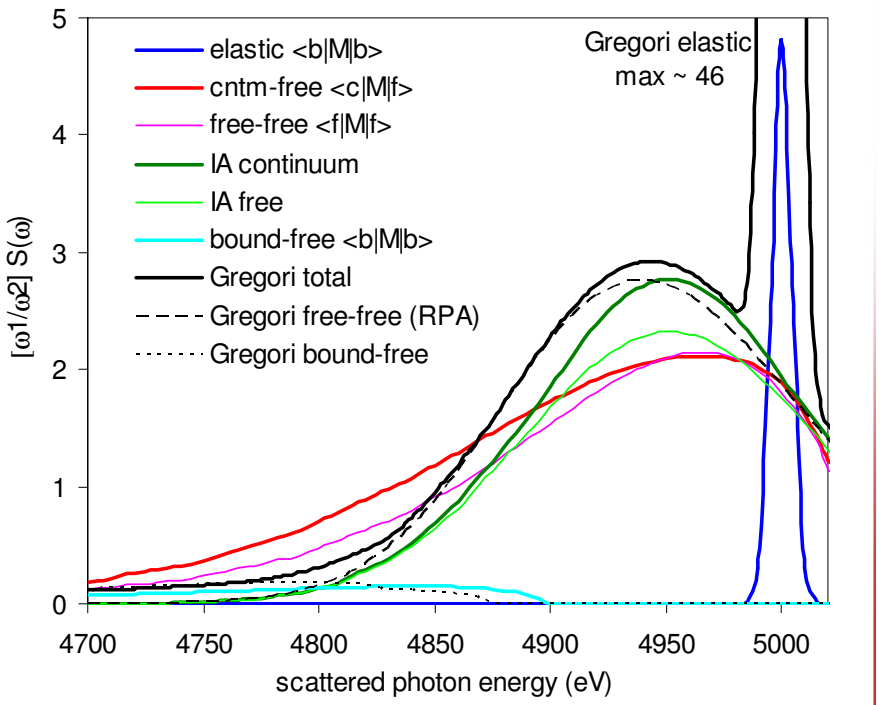
Predicted scattering from warm, solid Be compared with Gregori's SLFC/SOCP model [11]

Distributions of bound, "continuum" (DW), and "free" (plane wave) electron states in MuZe
Be 40 eV, 1.85 g/cc



Gregori's model: Z* = 2.75, θ = 90° α~0.3,
Both codes have elastic FWHM = 10 eV



-- The bound-free and (RPA/IA) free-free features are in reasonable agreement between codes
-- Static local field corrections are small; the φ-based approach <c|M|f> broadens the free-free signal
-- The elastic feature is ~9x smaller using <b|M|b> than SOCP (Sii ~1.0)

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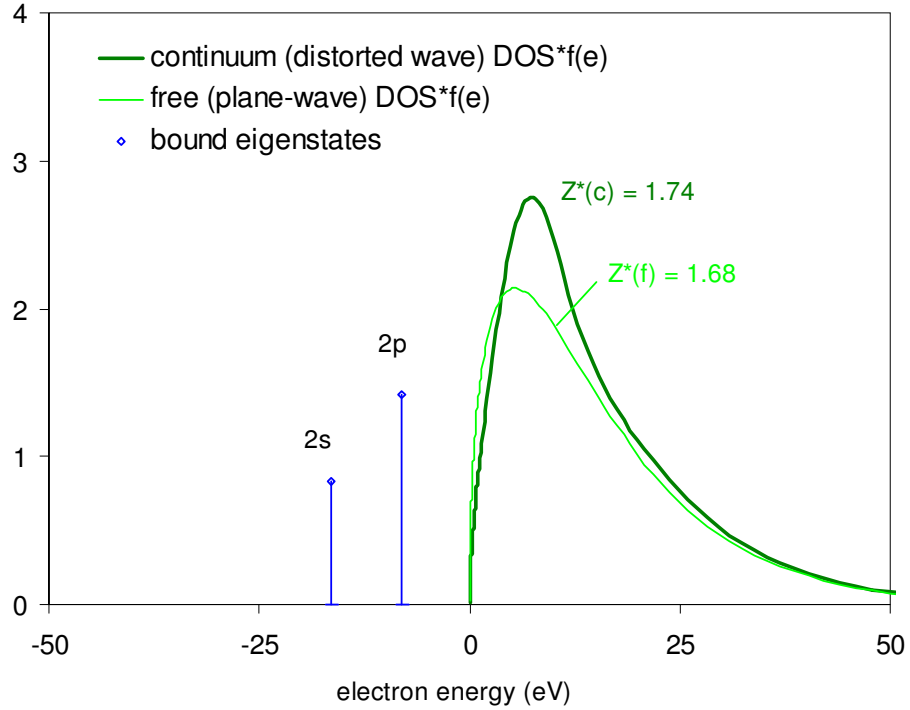
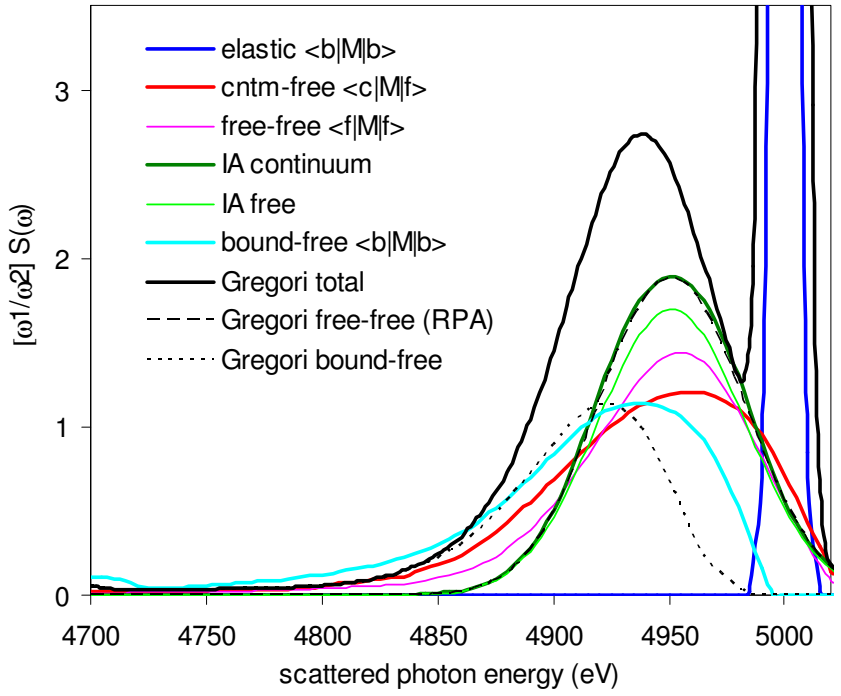
Predicted scattering from warm, expanded C compared with Gregori's SLFC/SOCP model [11]

Distributions of bound, "continuum" (DW), and "free" (plane wave) electron states in MuZe C 10 eV, 0.3 g/cc



Gregori's model: Z* = 1.74, θ = 90° α~0.2, Both codes have elastic FWHM = 10 eV



-- The bound-free and (RPA/IA) free-free features are in very good agreement between codes
-- Including SLFC has minimal effect, but the φ-based approach broadens the "continuum"-free signal (the "free" feature is less affected)
-- The elastic feature is ~4x smaller using <b|M|b> than SOCP (Sii ~1.0)

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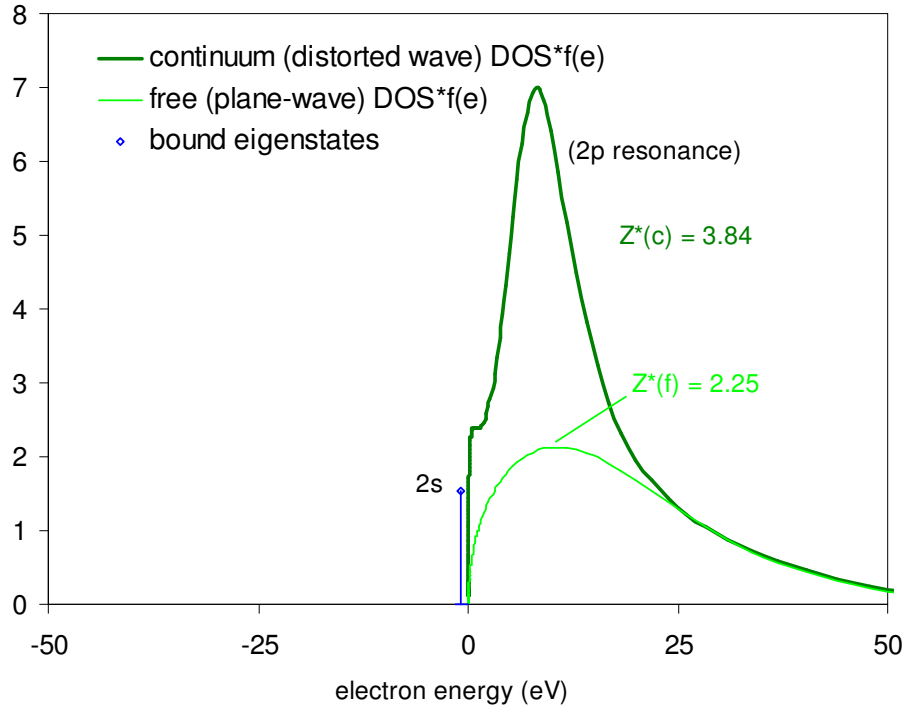
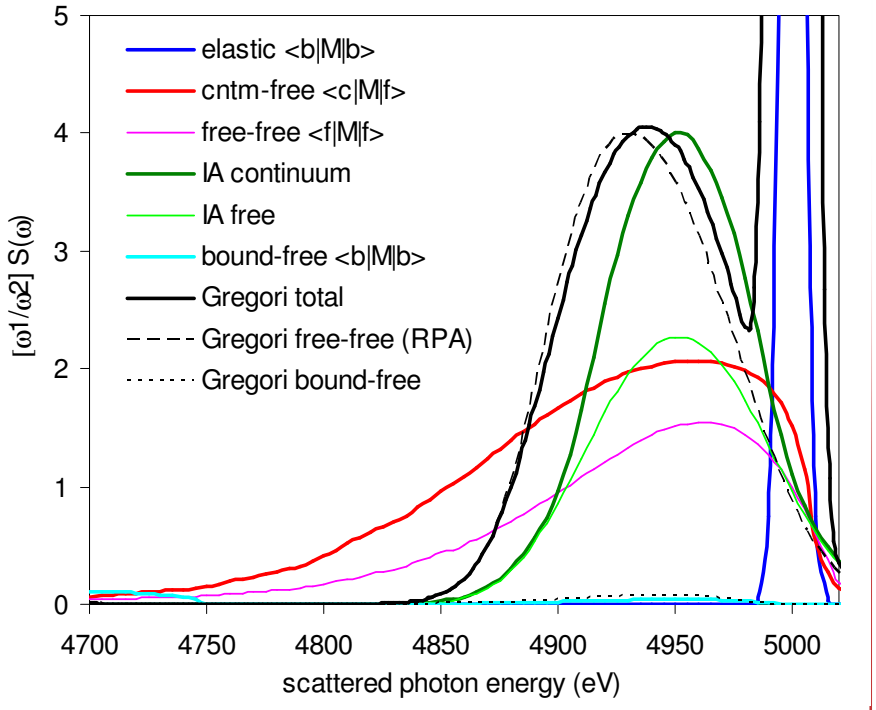
Predicted scattering from warm, near-solid C compared with Gregori's SLFC/SOCP model [11]

Distributions of bound, "continuum" (DW), and "free" (plane wave) electron states in MuZe
C 10 eV, 3 g/cc



Gregori's model: Z* = 3.84, θ = 90° α~0.6,
Both codes have elastic FWHM = 10 eV



-- The bound-free (2s) and (RPA/IA) free-free features are in fair agreement (Ec~48 eV)
-- Both SLFC and the φ-based approach have significant effects on the free-free signal
-- The elastic feature is ~10x smaller using <b|M|b> than SOCP (Sii ~1.2)

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Conclusions & future work

- Treating scattering from all electrons on the same theoretical footing (S~< i |M| f >) removes the uncertainty associated with Z* splitting in the Chihara approach
- For non-collective scattering, the present approach also removes some of the uncertainty caused by the ion-ion structure factor
  caveat: so far, only bound states contribute to its intensity
- There remain some questions:
  - What is the appropriate normalization for <f |M| f> and <c |M| f>?
  - Is the low-energy "tail" on <f |M| f> and <c |M| f> realistic?
  - Is integration on $\Psi(r)$ to Rws sufficient?
  - Is significant error introduced by using plane waves as final states?
  - (related) how much do "weakly free" continuum states contribute to the elastic feature?
  - We include occupancy factors for initial states but do not account for scattering into final electron states that are fully occupied… does the neglected factor matter?
  - Can the present approach be extended to collective scattering?
  - What experiments, published or planned, can test the predictions of the model?

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