Investigation of X-Ray Thomson Scattering Using a Statistical Approach

SAND2014-17235PE

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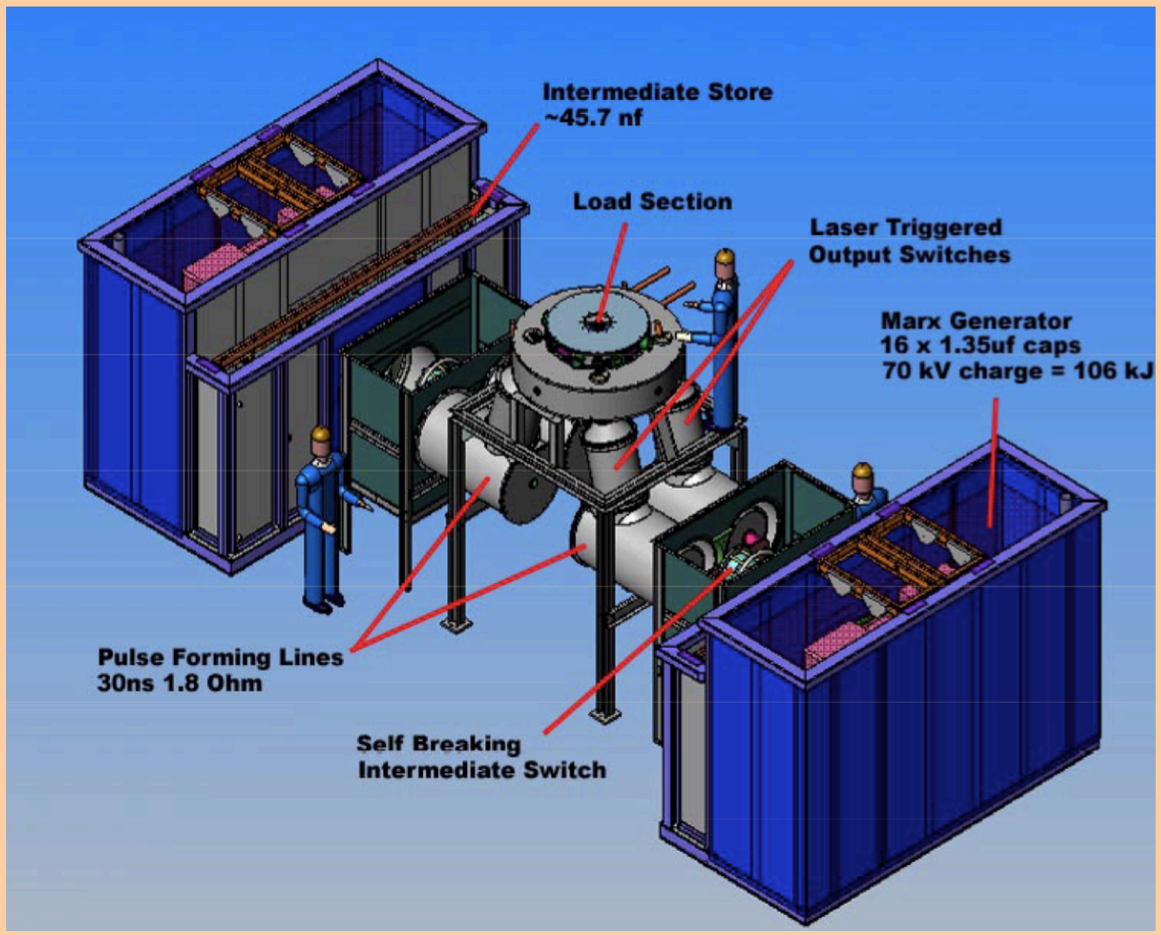
Cornell University
Laboratory of
Plasma Studies

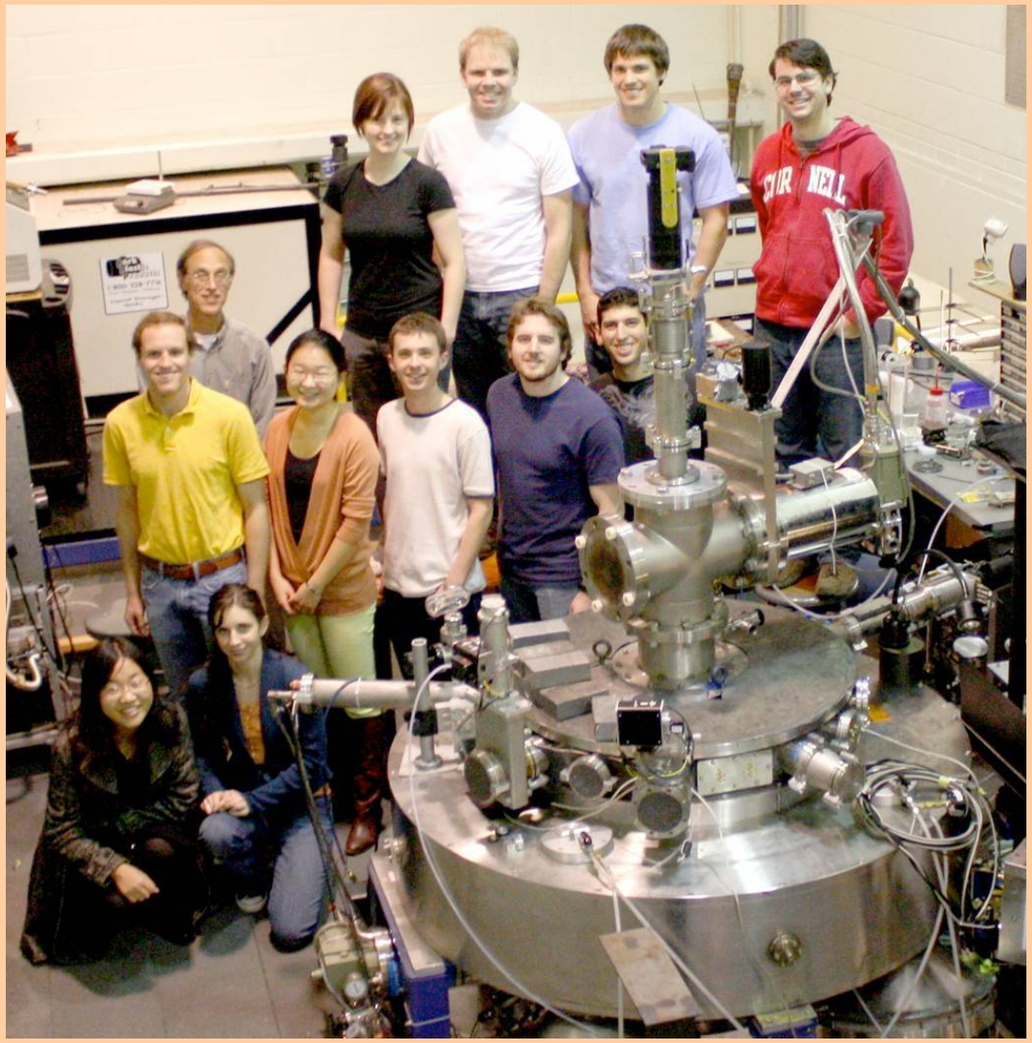
National Nuclear Security Administration

Sandia National Laboratories

Cornell's Lab of Plasma Studies is collecting XRTS data

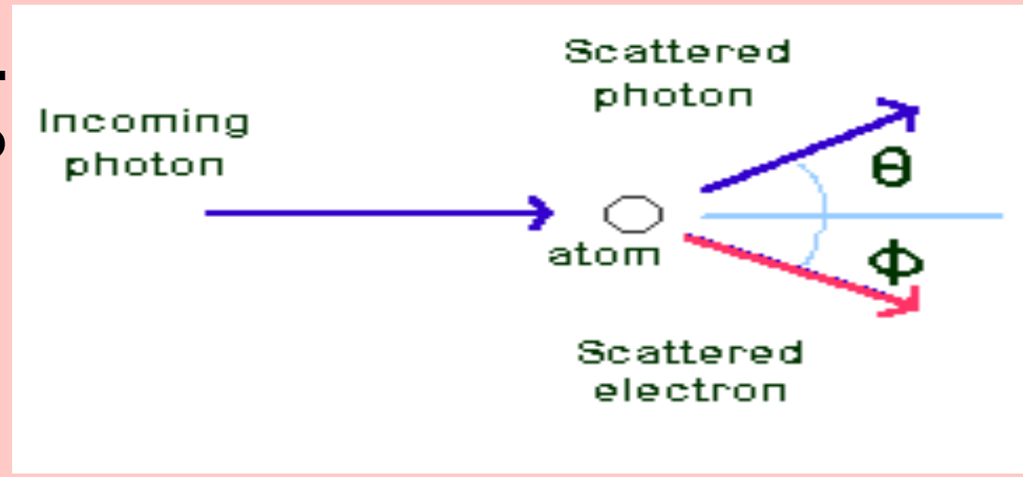
The Cornell Beam Research Accelerator – COBRA – 1 MA, ~ 100 ns





J. B. Greenly, et al. Rev. Sci. Instrum. **79**, 073501 (2008).

X-Ray Thomson Scattering (XRTS)



- The differential scattering cross-section is given by:

$$\frac{d\sigma}{d\omega_1 d\Omega} = |\epsilon_0 \cdot \epsilon_1|^2 \, r_0^2 \, \frac{\omega_1}{\omega_0} \, S(k,\omega)$$

-The structure factor can be split into three pieces:

1.) a piece due to scattering from electrons comoving with the ions

$$|f(k) + q(k)|^2 S_{ii}(k)\,\delta(\omega)$$

2.) a piece due to scattering from "free" electrons $S_{ee}(k,\omega)$

3.) a piece due to scattering from bound electrons $S_B(k,\omega)$

- This work is focused on the scattering from "free" electrons.

J. Chihara, J. Phys.: Condens. Matter 12, 231 (2000)

Current Methods to Compute $S_{ee}(k,\omega)$

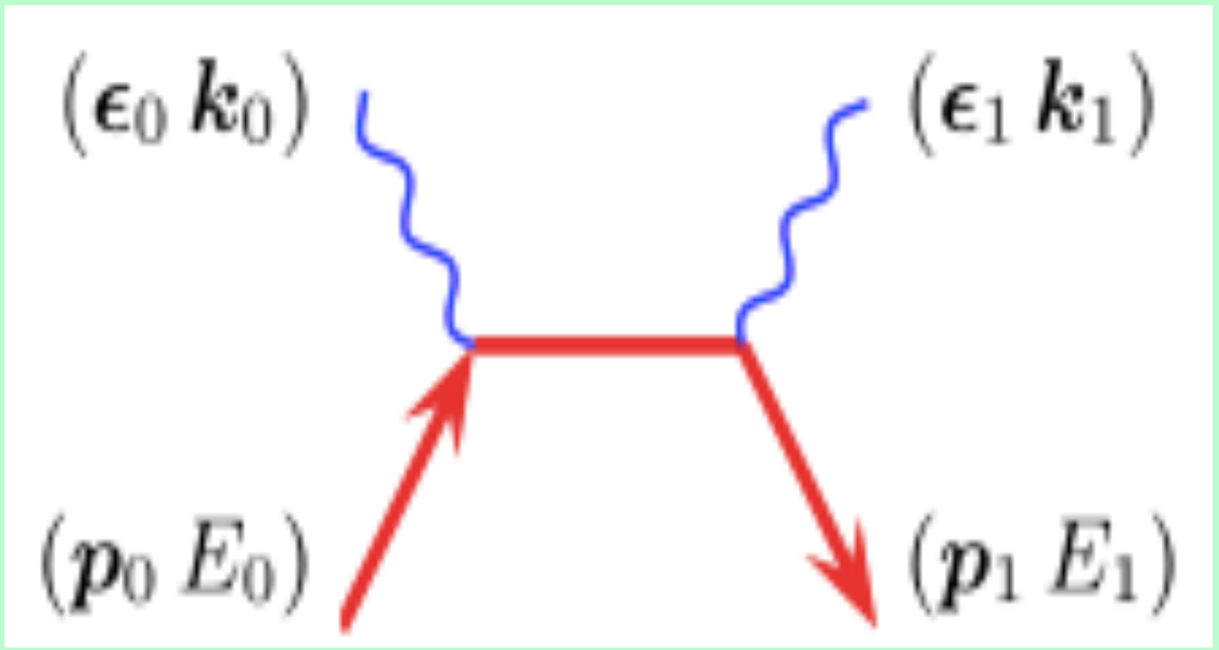
- **Plane Wave Form Factor Approximation -** widely used in the WDM XRTS community, but has a fundamental inaccuracy in that it uses plane waves continuum states.

- **Impulse Approximation -** assumes large energy transfer relative to the initial state binding energy. It is a reasonable approach at finite temperatures, but requires knowing binding energies independently and breaks down for low energy transfer.

- **Average-Atom Approach** –Uses Average-atom wave functions for bound states and plane waves for "free" states.

Johnson, W. R. *Thomson scattering in the average-atom approximation (2012).*

Statistical Approach to Computing Scattering



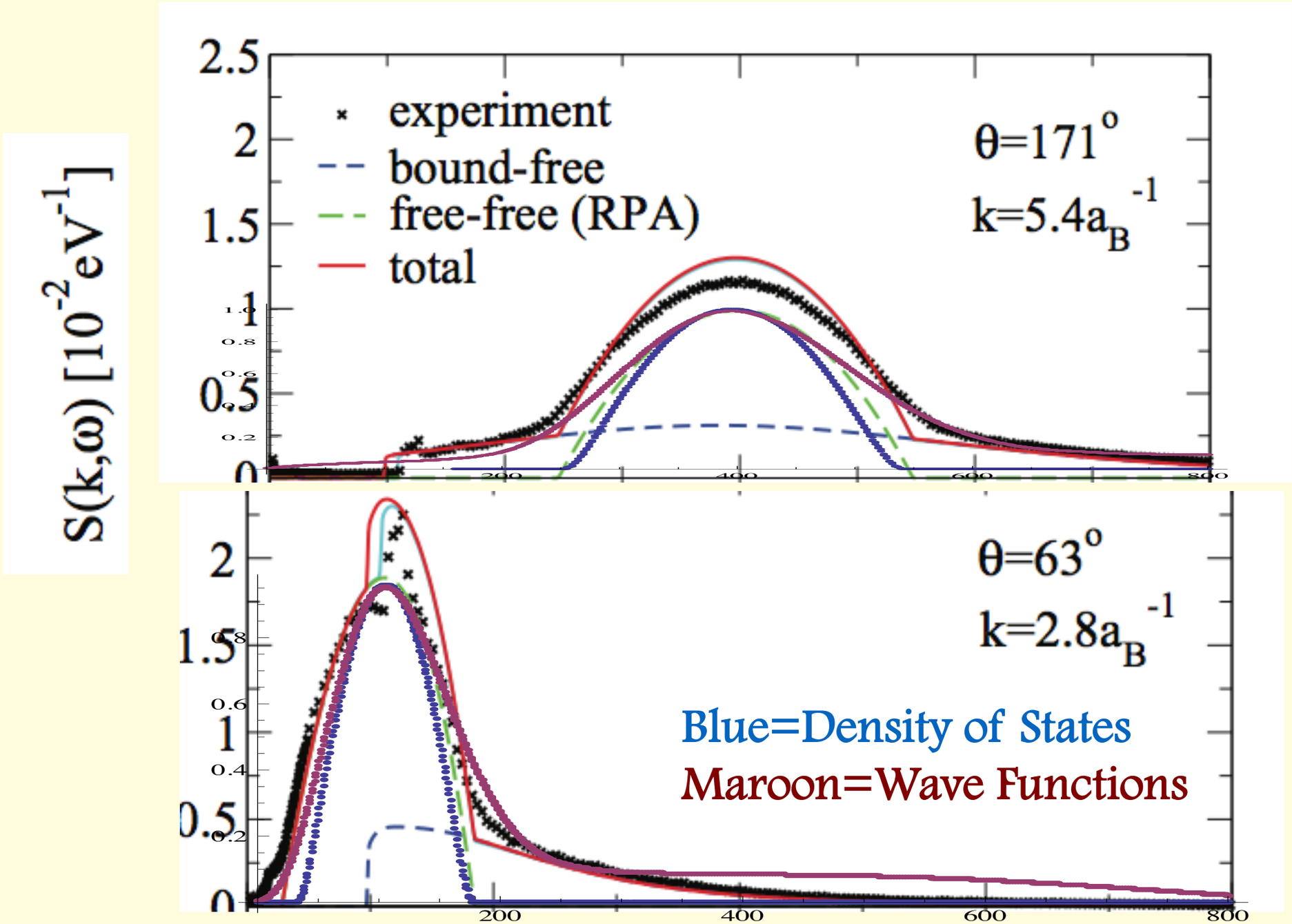
Use conservation of energy and momentum

$$E\gamma + Ei = E\gamma' + Ef$$

$$\vec{p}\gamma + \overrightarrow{pi} = \vec{p}\gamma' + \overrightarrow{pf}$$

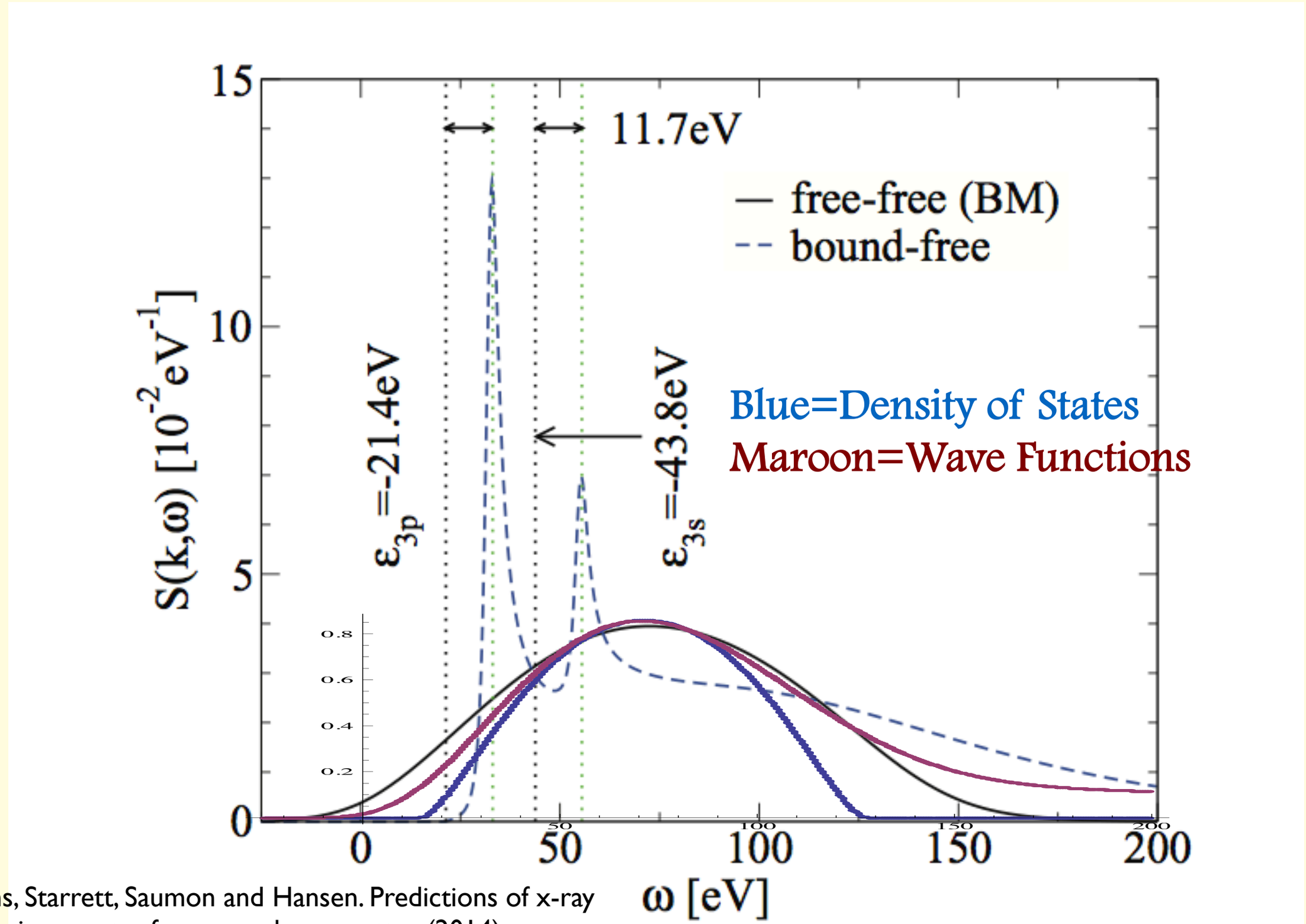
Method: Solve energy and momentum equations for an arbitrary electron velocity and weight each velocity by its likelihood of occurrence based on its momentum-space wave function or its density of states.

Comparison of Method to an Experiment on Solid Beryllium at Ambient Conditions collected at a scattering energy of 9890 eV and to Souza's model.



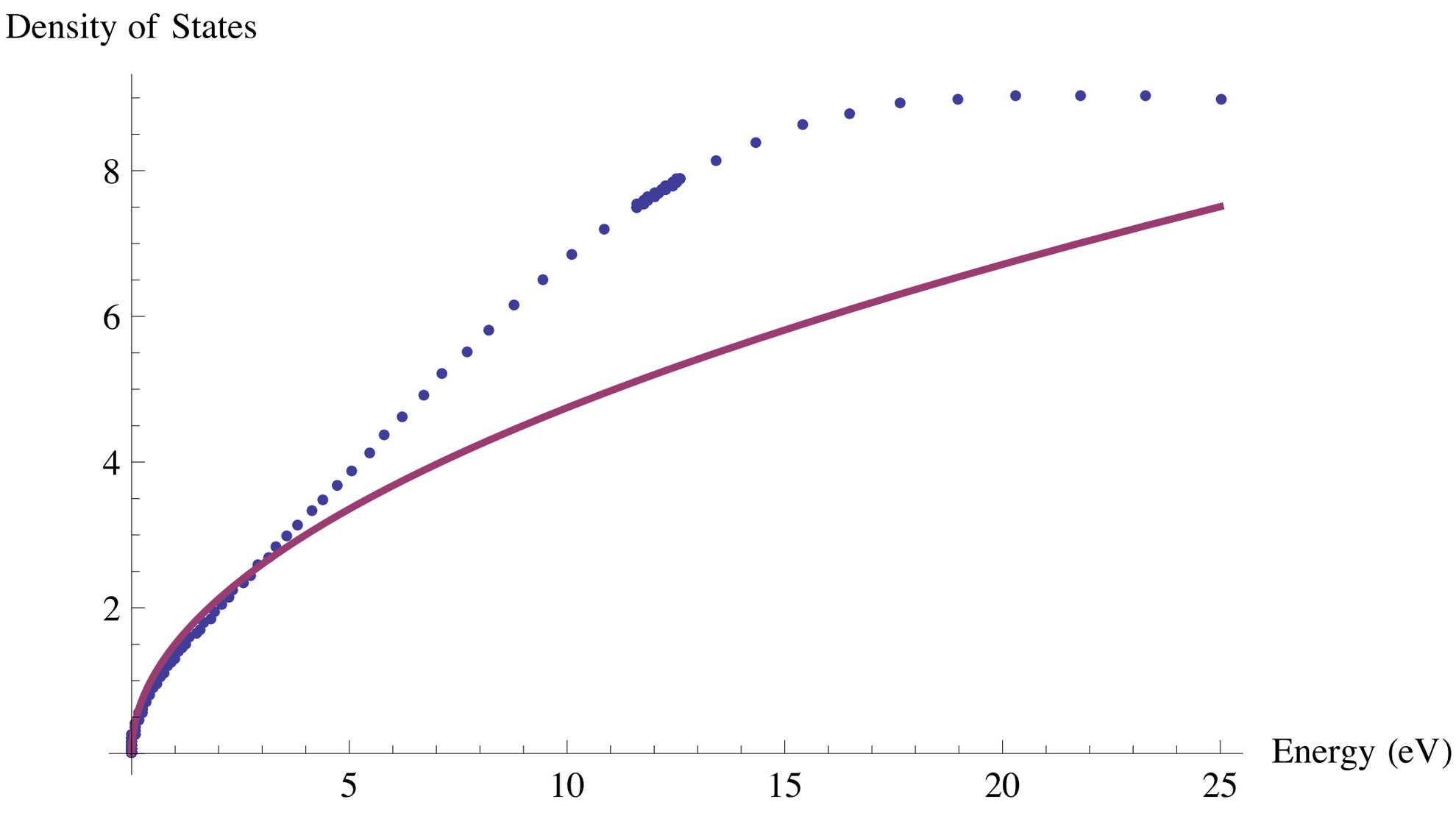
Souza, Perkins, Starrett, Saumon and Hansen. Predictions of x-ray scattering spectra for warm dense matter (2014).

Comparison of Method to Souza's Model on Warm Dense Titanium at 5 eV and 4.51 g/cm^3 with a probe energy of 4750 eV and collected at an angle of 130^o.



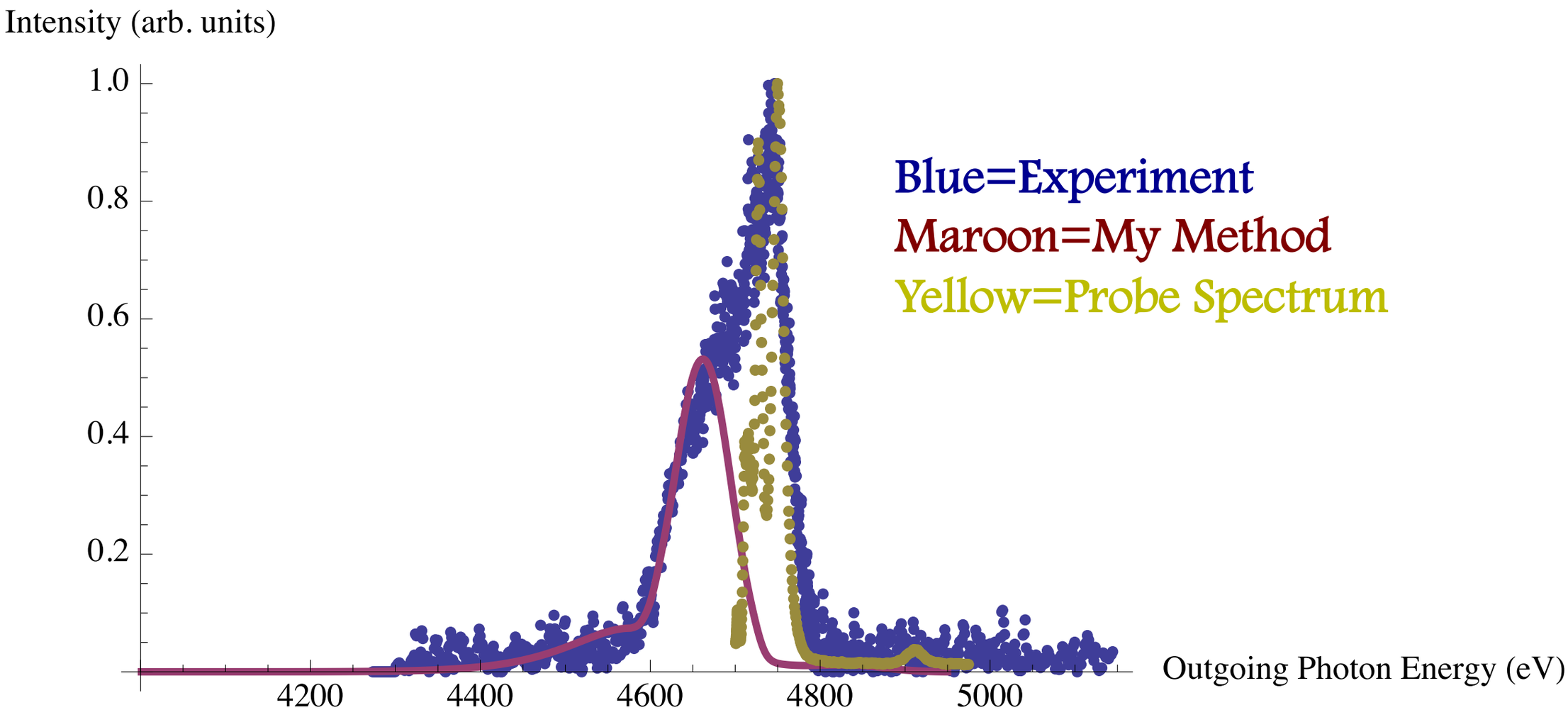
Souza, Perkins, Starrett, Saumon and Hansen. Predictions of x-ray scattering spectra for warm dense matter (2014).

Density of States and Ideal Density of States



Slide comparing to Fourier transform of Bessel Functions or will just overlay bessel on previous plot.

Comparison to an Experiment on COBRA using Ambient Aluminum with a Probe Energy of 4750 eV and Collected at a Scattering Angle of 130^0 by Cad Hoyt from Cornell's Lab of Plasma Studies



Impulse Approximation

The structure factor can be written as:

$$\left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th}} \frac{\omega_1}{\omega_2}\ S(k,\omega) = \left(\frac{d\sigma}{d\Omega}\right)_{\mathrm{Th}} \frac{\omega_1}{\omega_2} \frac{1}{(2\pi)} \int dt e^{i\omega t}$$

$$\times \langle i | e^{iHt} e^{-i\vec{k}\cdot\vec{r}} e^{-iHt} e^{+i\vec{k}\cdot\vec{r}} | i \rangle$$

The Hamiltonian operator ($H=H_o+V$) can be expanded using the Campbell-Baker-Hausdorff theorem:

$$e^{iHt} = e^{iH_0 t} e^{iVt} e^{-[H_0, V]t^2/2} \ldots$$

The essence of the impulse approximation come from

$$\exp\left(-\tfrac{1}{2}[H_0, V]t^2\right) \equiv 1$$

so that all Lie bracket terms vanish.

Future Work

- Expand the Impulse Approximation to improve accuracy.
- Compare with ongoing XRTS experiments at Cornell's Laboratory of Plasma Studies and at Sandia National Laboratories.

Acknowledgements

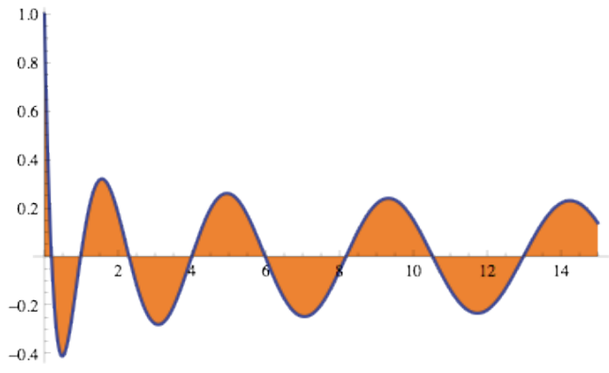
- Stephanie Hansen
- David Hammer
- Cornell Laboratory of Plasma Studies
- Sandia National Laboratories

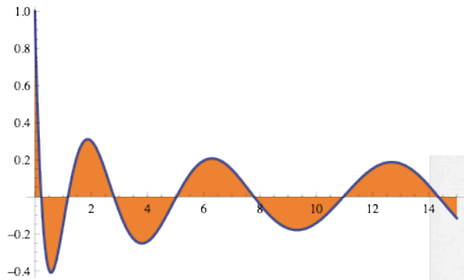
Cornell University
Laboratory of
Plasma Studies

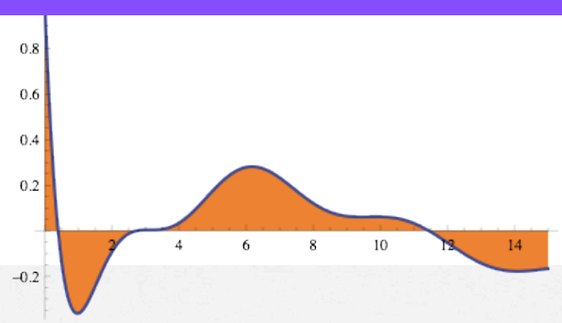
National Nuclear Security Administration

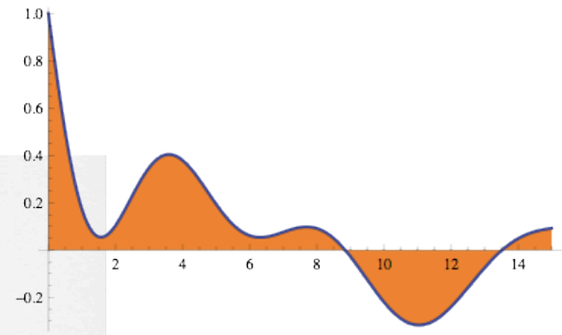
The “free” electrons are not really free.
They are distorted by the atom.

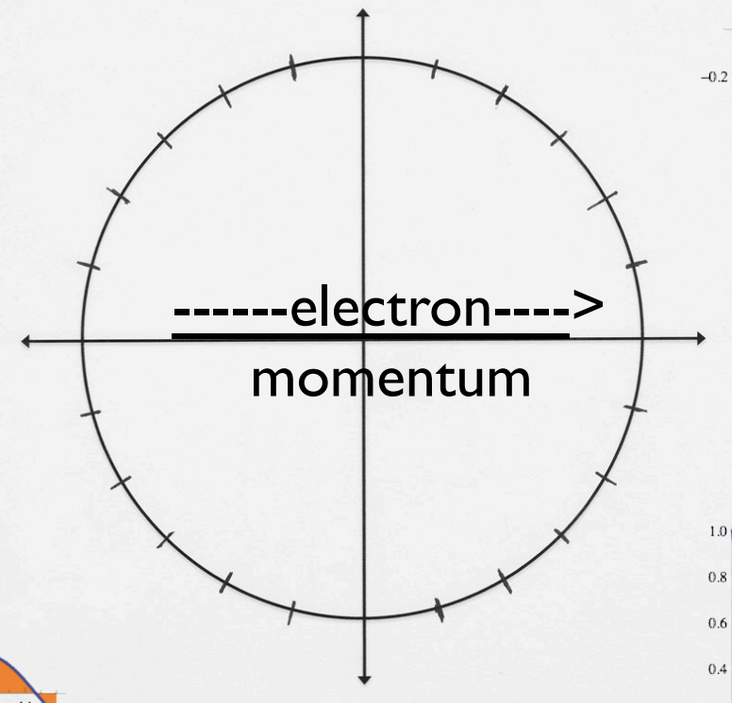
Atom

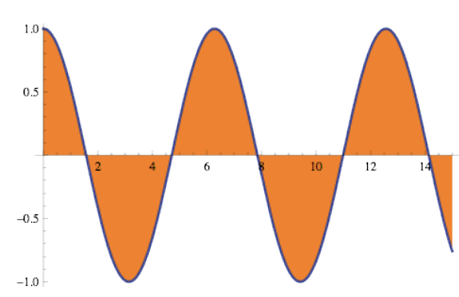


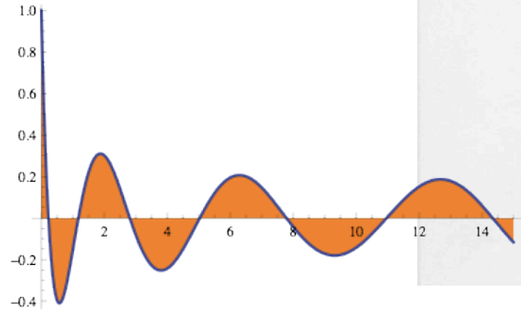


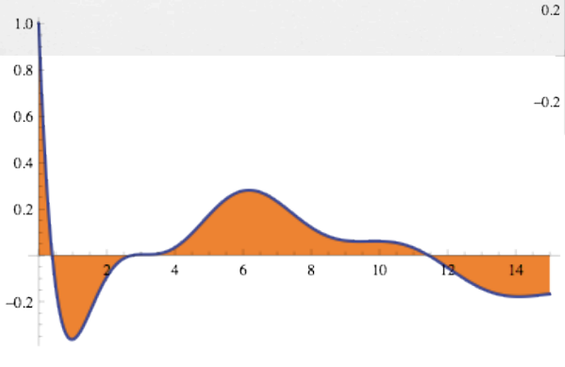


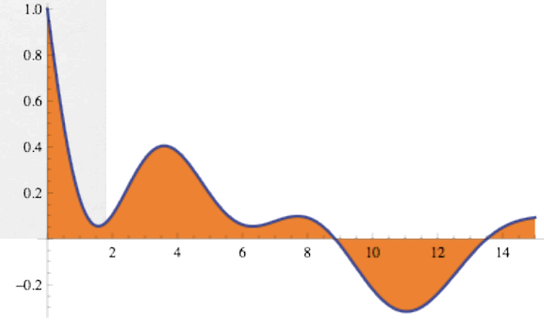












$$|f\rangle = (2\pi/p\alpha)^{1/2}(1-e^{-2\pi/p\alpha})^{-1/2} \times e^{i\vec{p}\cdot\vec{r}} F(i/p\alpha, 1, i(pr - \vec{p}\cdot\vec{r}))$$

High-Resolution Measurements Can Benchmark Theory

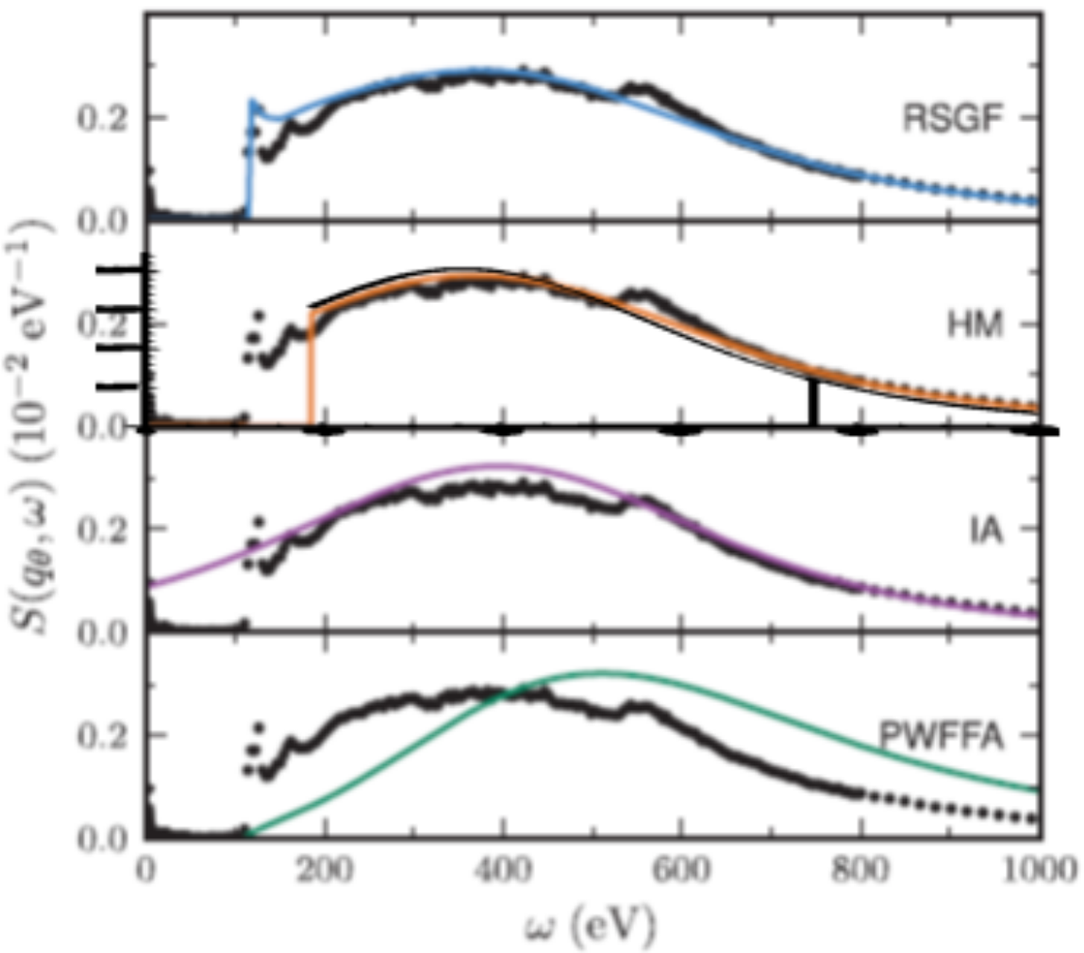


FIG. 2. Comparison of extracted core-shell XRTS with theoretical calculations using the RSGF, the hydrogenic model (HM), impulse approximation (IA), and plane-wave form-factor approximation (PWFFA). The energy transfer ω is the difference between the incident and scattered photon energies. *All calculations are in absolute units.* Vertical guides are shown at the 1*s* binding energy (112 eV) and the free-particle Compton shift (396 eV).

"The information content in the measured XRTS spectra for WDM has been insufficient to alert the experimenters to the presence of an unphysical model for the electronic structure."

Mattern and Siedler. *Theoretical treatments of the bound-free contribution and experimental best practice in X-ray Thomson scattering from warm dense matter* (2013).