Xray Scattering from WDM

Thomson Scattering in the Average-Atom Approximation

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Computational Challenges in WDM

Outline

1. Average-Atom
2. Thomson Scattering
   - Elastic Scattering by Ions
   - Scattering by Free Electrons
   - Inelastic Scattering by Bound Electrons
3. Applications
   - Hydrogen
   - Beryllium
   - Titanium
   - Tin

Procedure

- Use the average-atom model[1] to describe plasma
  - Input: atomic species (Z, A), density, temperature
  - Output: $\psi_a(r)$, $n_b(r)$, $n_c(r)$, Z_i, μ ...
- Evaluate Thomson scattering[2] with input from A-A
- Applications

[1] Feynman, Metropolis & Teller (1949)
[2] Chihara (2000), Gregori et al. (2003)

Average-Atom Model

Divide plasma into neutral cells that include nucleus and Z electrons

- $\left[\frac{p^2}{2} - \frac{Z}{r} + V\right] \psi_a(\mathbf{r}) = \epsilon_a \psi_a(\mathbf{r})$
- $V(r) = V_{\text{Kohn-Sham}}(n(r), r)$
- $n(r) = n_b(r) + n_c(r)$
- $4\pi r^2 n_b(r) = \sum_{nl} \frac{2(2l+1)}{1+\exp[(\epsilon_{nl}-\mu)/k_B T]} P_{nl}(r)^2$
- $Z = \int_{r<R_{WS}} n(r)\, d^3r$
- Number of equations = $N_b + N_l \times N_\epsilon \sim 500$
- Equations are solved self-consistently

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Example: Al metal T=10eV

$A = 27 \qquad \rho = 2.7\ \text{(gm/cc)} \qquad R_{\text{WS}} = 2.99\ \text{(au)}$

State	W(au)	occ#
1s	-54.591	2.00
2s	-3.388	2.00
2p	-2.019	5.97
N_b		9.97
N_c		3.03

$\mu = -0.0209\ \text{(au)} \qquad Z_i = 2.32$

$n_i = 6.02 \times 10^{22}\ \text{cm}^{-3} \qquad n_e = 1.40 \times 10^{23}\ \text{cm}^{-3}$

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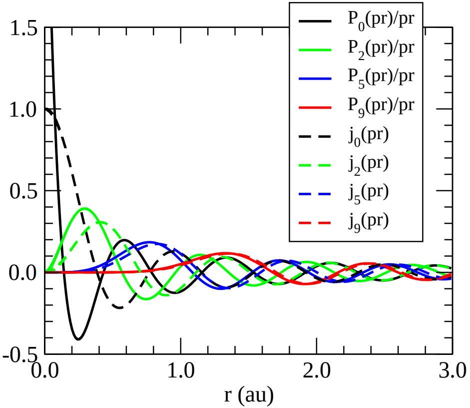
Al metal T=10eV, continued

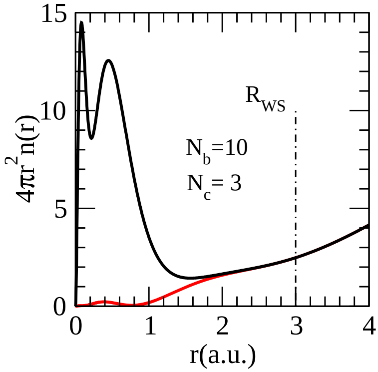
n_l	$V(r)$	V=0	Δ
n_0	0.630	0.601	0.029
n_1	1.132	0.838	0.294
n_2	0.859	0.533	0.326
n_3	0.285	0.236	0.049
n_4	0.089	0.081	0.008
n_5	0.024	0.023	0.001
n_6	0.006	0.005	0.000
n_7	0.001	0.001	0.000
n_8	0.000	0.000	0.000
N_c	3.026	2.318	0.708

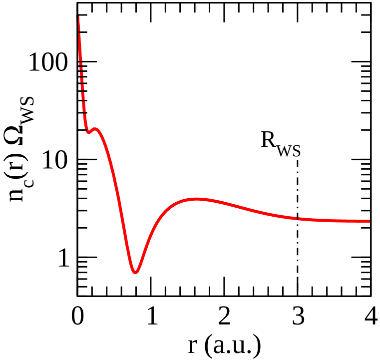
Al metal T=10eV, continued

Continuum Wave Functions



Al metal T=10eV, continued





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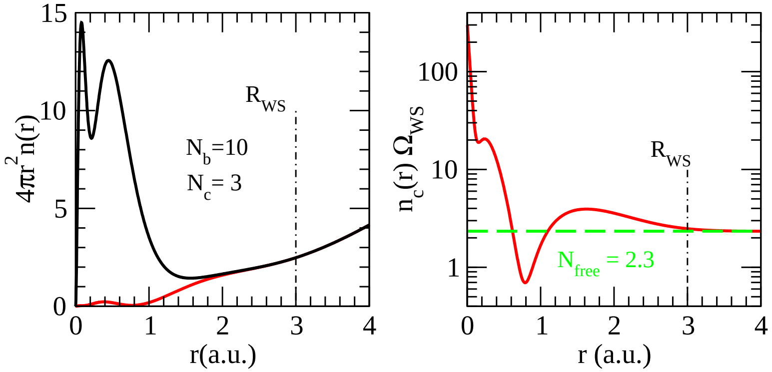
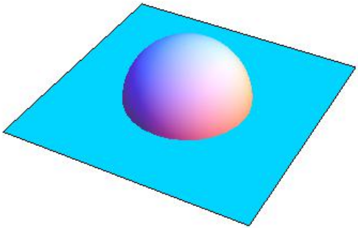
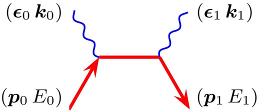


Wigner-Seitz Sphere in Electron-Ion Jellium



A simplified picture that emerges is of a single neutral average atom floating in a uniform sea of Z_i free electrons per cell balanced by an equal but opposite distributed positive ionic charge.

Thompson Scattering



\+ Exchange of photons

In nonrelativistic limit, this leads to

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

with $k = |\boldsymbol{k}_0 - \boldsymbol{k}_1|$, $\omega = \omega_0 - \omega_1$, where $S(k,\omega)$ is the *dynamic structure function* of the plasma.

Dynamic Structure Function

The *dynamic structure function* $S(k, \omega)$ of a plasma can be decomposed into three parts:[3]

[3] Chihara (2000)

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2. $S_{ee}(k,\omega)$ scattering by free electrons.
3. $S_{\mathrm{B}}(k,\omega)$ inelastic scattering by bound electrons.

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Elastic Scattering by Ions

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

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

- $f(k) + q(k) = 4\pi \int_0^{R_{WS}} r^2 [n_b(r) + n_c(r)]\, j_0(kr)\, dr$

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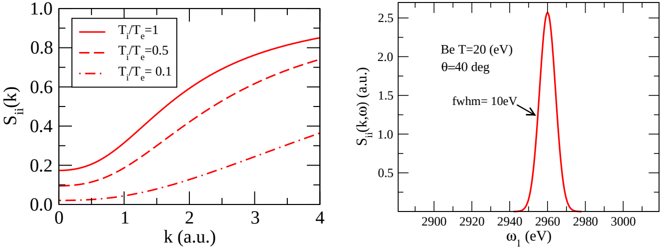


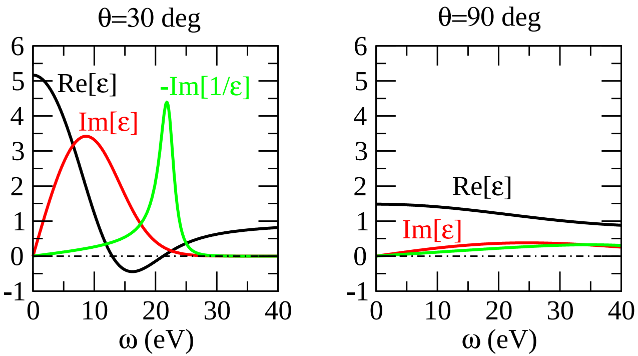
Scattering by Free Electrons

$$S_{ee}(k,\omega) = -\frac{1}{1-\exp(-\omega/k_B T)}\frac{k^2}{4\pi n_e}\Im\left[\frac{1}{\varepsilon(k,\omega)}\right]$$

Random-Phase Approximation for Dielectric function $\varepsilon(k,\omega)$:

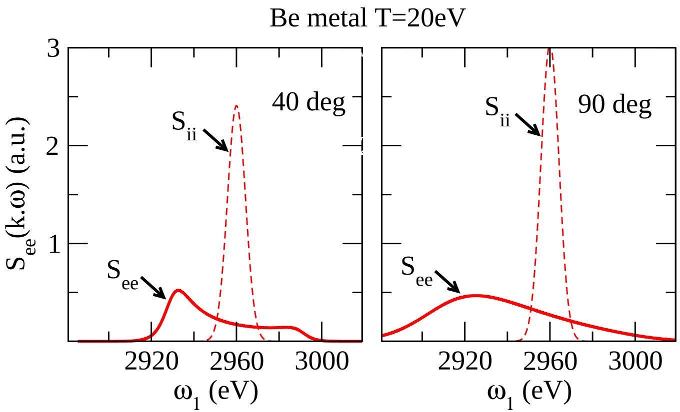
$$\varepsilon(k,\omega) = 1 + \frac{4}{\pi k^2}\int_0^\infty \frac{p^2}{1+\exp[(p^2/2-\mu)/k_B T]}dp$$
$$\int_{-1}^{1} d\eta \left[\frac{1}{k^2-2pk\eta+2\omega+i\nu} + \frac{1}{k^2+2pk\eta-2\omega-i\nu}\right],$$

Dielectric Functions for Be metal T=10eV



$\varepsilon(k, \omega)$ for $\omega_0 = 2690$eV, with $\omega = \omega_0 - \omega_1$.

Example: $S_{ee}(k, \omega)$ for Be metal



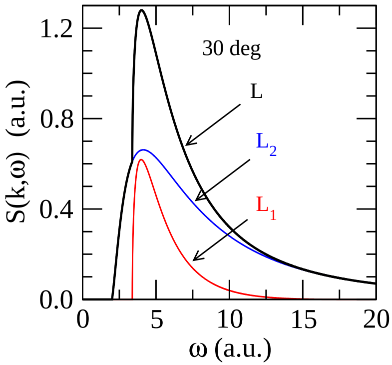
Inelastic Scattering from Bound Electrons

Plane-Wave Final States

$$S_{nl}(k,\omega) = \int \frac{p\,d\Omega_p}{(2\pi)^3} \left[\sum_m \left| \int d^3r\, e^{i\boldsymbol{q}\cdot\boldsymbol{r}}\, \psi_{nlm}(\boldsymbol{r}) \right|^2_{E_p=\omega+E_{nl}} \right]$$

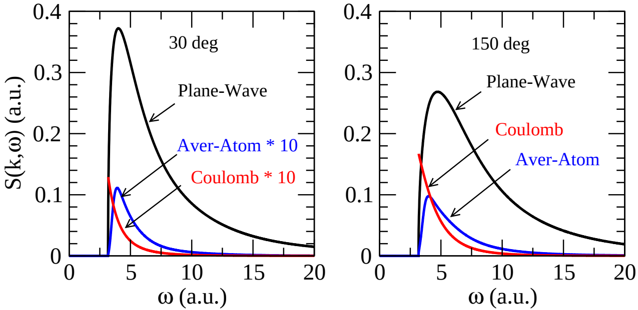
Example: Al 5eV

Plane-Wave Final State



Example: Be 10eV
Average-Atom Final State

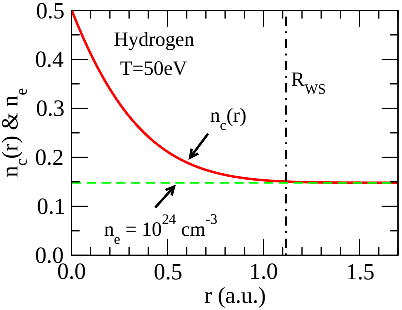
$$S_{nl}(k,\omega) = \int \frac{p\, d\Omega_p}{(2\pi)^3} \sum_m \left| \int d^3r\, \psi_p^\dagger(\boldsymbol{r})\, e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\, \psi_{nlm}(\boldsymbol{r}) \right|^2_{Ep=\omega+E_{nl}} .$$

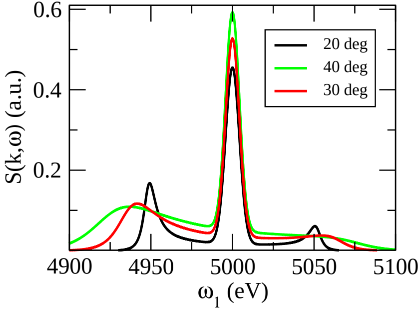


Applications:

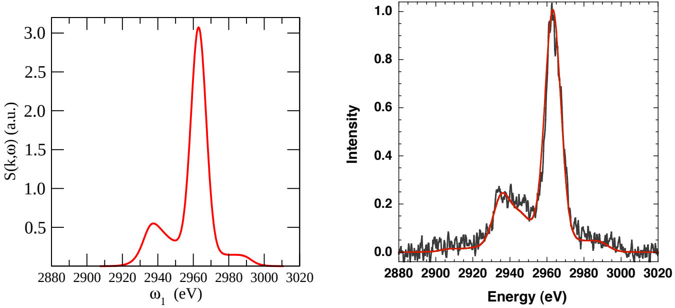
- Hydrogen (high density $n_e = 10^{24}$ cm^{-3})
- Beryllium (light element with available experimental data)
- Titanium (intermediate atomic weight element)
- Tin (heavy metal with interesting bound-state features)

Hydrogen: T = 50eV





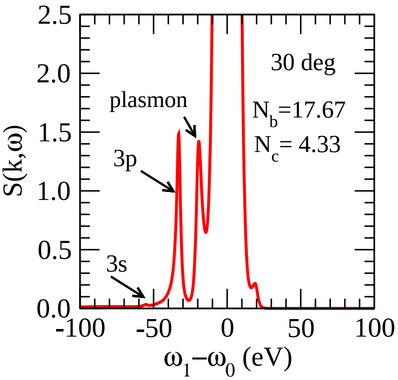
Beryllium: Comparison with Experiment

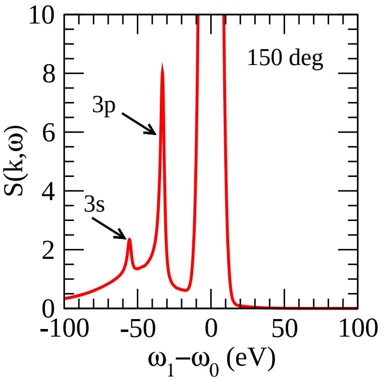


Average-Atom model for xray scattering by Be metal ($T = 18$ eV, $n_e = 1.8 \times 10^{23}$) compared with measurement.[4] $\omega_0 = 2963$ eV & $\theta = 40^\circ$.

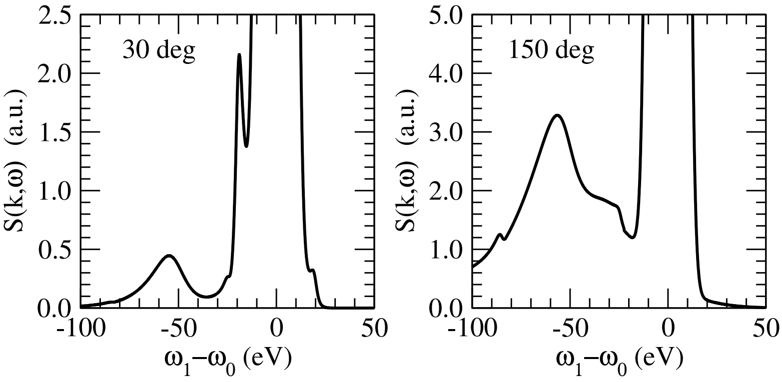
[4] S. H. Glenzer & T. Doeppner, private communication

Titanium metal (Z=22) at T = 10 eV, ω_0 = 2960 eV





Tin (Z=50) at T = 10 eV, ω_0 = 2960 eV



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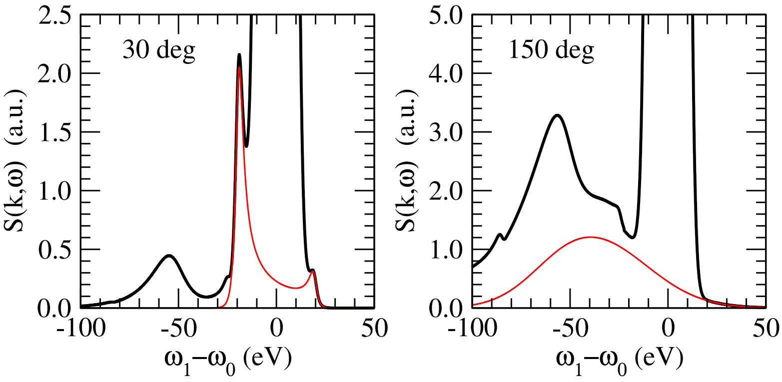

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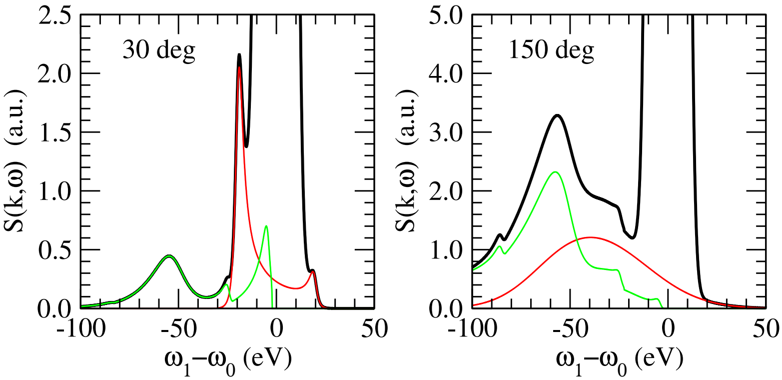

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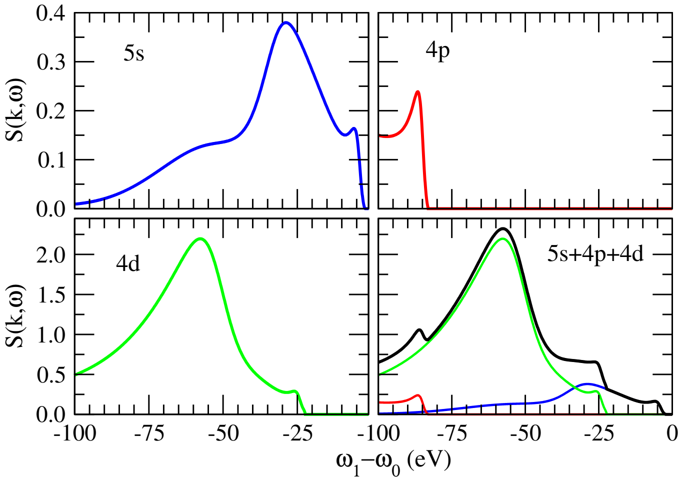

Summary:

- A-A model is used to study Xray scattering from WDM.
- Scattering from bound-states easily accommodated

To be done:

- Improve the treatment of $S_{ii}(k)$ (hypernetted chains? or molecular dymamics?)
- Go beyond RPA and include correlation corrections to $S_{ee}(k, \omega)$

References

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