# Thomson Scattering from WDM Average-Atom Approximation

W. R. Johnson, Notre Dame J. Nilsen & K. T. Cheng, LLNL

The cross section for Thomson scattering of x-rays by warm dense matter is studied within the framework of the average-atom model.

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**Thomson Scattering** 

- Elastic Scattering by lons
- Inelastic Scattering by Free Electrons
- Inelastic Scattering by Bound Electrons



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# Average-Atom Model

- Divide plasma into WS cells with a nucleus and Z electrons
- $\left| \frac{p^2}{2} \frac{Z}{r} + V \right| \psi_a(\mathbf{r}) = \epsilon_a \psi_a(\mathbf{r})$
- $V(r) = V_{\mathrm{KS}}(n(r), r)$
- $n(r) = n_b(r) + n_c(r)$
- $4\pi r^2 n_b(r) = \sum_{nl} \frac{2(2l+1)}{1+\exp[(\epsilon_{nl}-\mu)/k_BT]} P_{nl}(r)^2$

• 
$$Z = \int_{r < R_{\rm WS}} n(r) d^3r$$

- Number of equations =  $N_b + N_l \times N_\epsilon \sim 500$
- Equations are solved self-consistently

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# Aluminum Metal





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# Thomson Scattering



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

Elastic Scattering by Ions Inelastic Scattering by Free Electrons Inelastic Scattering by Bound Electrons

# Elastic Scattering by lons

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



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- Modified by Gregori et al. (2006) to include  $T_i \neq T_e$

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Elastic Scattering by Ions Inelastic Scattering by Free Electrons Inelastic Scattering by Bound Electrons

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# Inelastic Scattering by Free Electrons

From Gregori et al. (2003):

$$\mathcal{S}_{ee}(k,\omega) = -rac{1}{1-\exp(-\omega/k_{\scriptscriptstyle B}T)}rac{k^2}{4\pi^2 n_e} {
m Im}\left[rac{1}{arepsilon(k,\omega)}
ight]$$

Random-phase approximation for dielectric function  $\varepsilon(k, \omega)$ :

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

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#### **Dielectric Function**



Scattering from AI metal,  $k_B T = 5 \text{ eV}$ ,  $\omega_0 = 3.1 \text{ keV}$ ,  $\theta = 30^{\circ}$ 

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## Inelastic Scattering by Bound Electrons

$$S_{B}(k,\omega) = \sum_{nl} S_{nl}(k,\omega)$$
$$S_{nl}(k,\omega) = \frac{o_{nl}}{2l+1} \sum_{m} \int \frac{p \, d\Omega_{p}}{(2\pi)^{3}} \left| \int d^{3}r \, \psi_{p}^{\dagger}(r) e^{ik \cdot r} \, \psi_{nlm}(r) \right|_{E_{p}=\omega+E_{nl}}^{2}$$

Plane-wave Approximation:  $\psi_{p}(\mathbf{r}) \approx \mathbf{e}^{i\mathbf{p}\cdot\mathbf{r}}$ 

$$\mathcal{S}_{nl}(k,\omega) = rac{o_{nl}}{\pi k} \int_{|p-k|}^{p+k} q \, dq \, |\mathcal{K}_{nl}(q)|^2, \quad ext{where}$$

$$K_{nl}(q) = \int_0^\infty dr \, r \, j_l(qr) P_{nl}(r).$$





Bound-state contribution to  $S(k, \omega)$  for x-ray scattering from the *K*-shell of Be metal at  $k_{B}T$ =18 eV.

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 Elastic Scattering by lons

 Thomson Scattering
 Inelastic Scattering by Free Electrons

 Application to Aluminum
 Inelastic Scattering by Bound Electrons

#### Comparison with Sahoo et al. Phys. Rev. E 77, 046402 (2008)



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RPWDM-15

## Application to Aluminum



RPWDM-15

Summary:

- AA model is used to study x-ray scattering from WDM.
- Scattering from bound-states easily accommodated.
- Present results disagree with earlier AA results by Sahoo et al. for Al.

To be done:

• Understand why  $T_i/T_e \neq 1$  is needed in  $S_{ii}(k, \omega)$  in some equilibrium cases but not in others?

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Go beyond RPA for S<sub>ee</sub>(k, ω) and include correlation effects.

## References

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