Xray Dispersion and Scattering in the Average-Atom Model of a Plasma

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- Average-Atom & Static Conductivity (Ziman)
- Kubo-Greenwood Formula (Infrared Catastrophe)
- “Proper” Static Limit & Conductivity Sum Rule
- Applications: Anomalous Dispersion of Xray – Compton Scattering
Average Atom & Static Conductivity

## Average-Atom Model of a Plasma

Plasma composed of neutral spheres containing a nucleus $|e|Z$ and $Z$ electrons floating in a “jellium” sea. The radius of each sphere is the $R = \left(\frac{3\Omega}{4\pi}\right)^{1/3}$. (Based on Temperature-Dependent Fermi-Thomas Model, by Feynman, Metropolis, & Teller - 1949)

\[
\left(\frac{p^2}{2m} - \frac{Z}{r} + V\right) u_a(r) = \epsilon_a u_a(r)
\]

\[
V(r) = \int d^3 r' \frac{\rho(r')}{|r' - r|} + V_{\text{exc}}(\rho)
\]

\[
4\pi r^2 \rho(r) = \sum_{nl} \frac{2(2l + 1)}{1 + \exp[(\epsilon_{nl} - \mu)/kT]} P_{nl}(r)^2
\]

\[
Z = \int_{r<R} \rho(r) \, d^3 r = \int_0^R 4\pi r^2 \rho(r) \, dr
\]
**Example**

Aluminum: density $0.27 \text{ gm/cc}$  \( T = 5 \text{ eV} = 10 \times \text{solar surface temperature} \)
\( R = 6.44 \text{ a.u.}, \mu = -0.3823 \text{ a.u.} \)

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Al: density 0.27 gm/cc, $T = 5$ eV
Phase-Shifts & Scattering

Al: density 0.27 gm/cc, \( T = 5 \) eV

\[
f(\theta) = \frac{1}{2i\rho} \sum_l (e^{2i\delta_l} - 1) P_l(\cos \theta), \quad \sigma_{el}(\theta) = |f(\theta)|^2
\]
Transport Cross Section and Conductivity

Classical Drude Formula: \( \sigma = n e^2 \tau / m \), where \( n \) is free electron density and \( \tau \) is mean time between collisions. Generally:

\[
\tau_p = \frac{\Lambda_p}{v} \quad \text{(relaxation time)} \quad \Lambda_p = \frac{\Omega}{\sigma_{tr}(p)} \quad \text{(mean free path)}
\]

\[
\sigma_{tr}(p) = \int (1 - \cos \theta) \sigma_{el}(\theta) \, d\Omega \quad \text{(transport cross section)}
\]

Conductivity obtained as a “thermal average” of Drude Formula:

\[
\sigma = \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^2 \tau_p \quad \text{(Ziman formula)}
\]
Comparison with Experiment

Linear Response and Conductivity

Consider an applied electric field:

\[ E(t) = F \hat{z} \sin \omega t \quad A(t) = \frac{F}{\omega} \hat{z} \cos \omega t \]

The time dependent Schrödinger equation becomes

\[
\left[ T_0 + V(n, r) - \frac{eF}{\omega} v_z \cos \omega t \right] \psi_i(r, t) = i \frac{\partial}{\partial t} \psi_i(r, t)
\]

The current density is

\[ J_z(t) = \frac{2e}{\Omega} \sum_i f_i \langle \psi_i(t) | v_z | \psi_i(t) \rangle \]
Kubo-Greenwood

- Linearize $\psi_i(r, t)$ in $F$
- Evaluate the response current: $J = J_{\text{in}} \sin(\omega t) + J_{\text{out}} \cos(\omega t)$
- Determine $\sigma(\omega)$: $J_{\text{in}}(t) = \sigma(\omega) E_z(t)$

Result:

$$\sigma(\omega) = \frac{2\pi e^2}{m^2 \omega \Omega} \sum_{ij} (f_i - f_j) |\langle j | \mathbf{\epsilon} \cdot \mathbf{p} | i \rangle|^2 \delta(E_j - E_i - \omega),$$

which is an average-atom version of the Kubo$^1$-Greenwood$^2$ formula.

(n.b. bound-bound, bound-free, free-free contributions)

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Infrared “Catastrophe”

Particle in a potential $V(r)$:

$$\langle p_2 | \epsilon \cdot p | p_1 \rangle = \frac{1}{\omega} (\epsilon \cdot q) V(q)$$

Relation between scattering amplitude and potential

$$f(\theta) = -\frac{m}{2\pi} V(q)$$

Result: (Low-frequency theorem QED)

$$\langle p_2 | \epsilon \cdot p | p_1 \rangle = \frac{2\pi}{m\omega} (\epsilon \cdot q) f(\theta)$$
Infrared Catastrophe

Low-Frequency Kubo-Greenwood

\[
\langle |\langle p_2| \epsilon \cdot p |p_1 \rangle|^2 \rangle_{\text{ave}} \approx \frac{2 (2\pi)^2}{3 m^2 \omega^2} p^2 (1 - \cos \theta) \sigma_{\text{el}}(\theta)
\]

\[
f_1 - f_2 \approx -\omega \frac{\partial f}{\partial E}
\]

Free-free contribution:

\[
\sigma(\omega) \approx \frac{2\pi e^2}{m^2 \Omega} \int \frac{d^3 p_1}{(2\pi)^3} \int \frac{d^3 p_2}{(2\pi)^3} \left(-\frac{\partial f}{\partial E}\right) |\langle p_2| \epsilon \cdot p |p_1 \rangle|^2 \delta(E_2 - E_1 - \omega)
\]

\[
= \frac{2e^2}{3} \int \frac{d^3 p}{(2\pi)^3} \left(-\frac{\partial f}{\partial E}\right) v^2 \frac{1}{\omega^2 \tau_p} \quad \text{(Low-Freq K-G formula)}
\]
\[ \left\langle |\langle p_2|\mathbf{e} \cdot \mathbf{p}|p_1\rangle|^2 \right\rangle_{\text{ave}} \approx \frac{2(2\pi)^2}{3m^2\omega^2} p^2 (1 - \cos \theta) \sigma_{\text{el}}(\theta) \]
\[ f_1 - f_2 \approx -\omega \frac{\partial f}{\partial E} \]

Free-free contribution:

\[ \sigma(\omega) \approx \frac{2\pi e^2}{m^2\Omega} \int \frac{d^3p_1}{(2\pi)^3} \int \frac{d^3p_2}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) |\langle p_2|\mathbf{e} \cdot \mathbf{p}|p_1\rangle|^2 \delta(E_2 - E_1 - \omega) \]
\[ = \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^2 \frac{1}{\omega^2\tau_p} \]  
(Low-Freq K-G formula)

\[ \sigma(0) = \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^2\tau_p \]  
(Ziman formula)
Influence of Collisions on Wave Function

\[ \psi(p, t) \rightarrow \exp \left[ i (p \cdot r - E t) - \frac{t}{\tau_p} \right] \]

Effect\(^3\):

\[ \frac{1}{\omega^2} \rightarrow \frac{1}{\omega^2 + 1/\tau_p^2} \equiv \frac{\tau_p^2}{\omega^2 \tau_p^2 + 1} \]

With this in mind, the low-frequency K-G Formula becomes

\[ \sigma(\omega) = \frac{2 e^2}{3} \int \frac{d^3 p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^2 \frac{\tau_p}{\omega^2 \tau_p^2 + 1} \quad \text{(Modified K-G Formula)} \]

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Comparison of Conductivity Formulas

Aluminum Plasma
T=5eV
0.27 gm/cc

K-G Formula
K-G Low Freq Approx
Modified K-G

Photon Energy (a.u.)
Conductivity (a.u.)
Conductivity Sum Rule

\[ \int_0^\infty \sigma(\omega) d\omega = \frac{\pi e^2}{3} \int \frac{d^3 p}{(2\pi)^3} v^2 \left( - \frac{\partial f}{\partial E} \right) \]

\[ = \frac{e^2 \pi}{3} \int \frac{dE d\Omega}{(2\pi)^3} p^3 m \left( - \frac{\partial f}{\partial E} \right) \]

\[ = e^2 \pi \int \frac{dE d\Omega}{(2\pi)^3} p f(E) \]

\[ = \frac{e^2 \pi}{m} \int \frac{d^3 p}{(2\pi)^3} f(E) = \frac{e^2 \pi}{2m} Z^* \]
Summary of Modified K-G Formula

- 3s-3p
- 2p-3s
- 2s-3p
- free-free
- bound-bound
- bound-free
- total

- n=3
- n=2

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Dispersion Relations

By Cauchy’s theorem, a function $f(z)$ analytic in the upper half plane that falls off as $1/|z|$ satisfies

$$f(x_0) = \frac{1}{i\pi} \text{P.V.} \left( \int_{-\infty}^{\infty} \frac{f(x)}{x - x_0} \right)$$

Apply to Modified K-G formula for $\text{Re}[\sigma(\omega)]$ to find

$$\text{Im}[\sigma(\omega)] = \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^2 \frac{\omega \tau_p^2}{\omega^2 \tau_p^2 + 1}$$

$\sigma(\omega)$ as an analytic function of $\omega$ is therefore

$$\sigma(\omega) = \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^2 \frac{\tau_p}{1 - i\omega \tau_p}$$
Dielectric Function, Index of Refraction

\[ \varepsilon_r(\omega) = 1 + 4\pi i \frac{\sigma(\omega)}{\omega}, \quad n(\omega) + i\kappa(\omega) = \sqrt{\varepsilon_r(\omega)}. \]

![Graph showing the relationship between photon energy and refractive index and absorption coefficient for a material with temperature T=5eV and density \(\rho=0.27\) gm/cc. The graph illustrates how the refractive index and absorption coefficient vary with photon energy.](image-url)
Laser Interferometry

COMET is a unique table-top X-ray laser user facility

- Long Pulse: 15 J, 600 ps
- Short Pulse: 7.5 J, 0.5 ps
- Beam 3: 1 J, 0.5 ps
- Probe Beam: 0.5 ps 2ω, 3ω

100 fs Oscillator/Pulse Stretcher/Regenerative Amplifier

Pulse Compressor in Vacuum Chamber

Long Pulse Beam

Main Amplifiers
Inward curvature of fringes in RH panel implies $n_{\text{free}} = \sqrt{1 - \frac{\omega_0^2}{\omega^2}} > 1$ which, in turn, implies $n_e < 0$ and $v_{\text{phase}} = c/n_{\text{free}} > c$. (anomalous dispersion)
Comparison with Average-Atom Model

Aluminum plasma with ion density $n_{ion} = 10^{20}/\text{cc}$  

(With Joe Nilsen)
Compton Scattering & LCLS

LCLS (linac coherent light source) at SLAC in Menlo Park, California, is a free-electron laser that generates x-ray pulses at energies between 800eV and 8000eV (15 to 1.5 Å). An end station to study plasma physics is expected to open in the summer of 2011. One principal diagnostic will be Compton scattering.
Compton Scattering

• Classical Thompson Scattering: Photon scattered by a free electron.

\[
\frac{d\sigma}{d\Omega} = r_0^2 \left( \epsilon_1^* \cdot \epsilon_2 \right)^2
\]

• Thompson scattering from an electron in a plasma. (incorrectly referred to as Compton scattering)

\[
\frac{d\sigma}{d\Omega d\omega} = \left( \frac{d\sigma}{d\Omega} \right)_{Th} \left( \frac{\omega_2}{\omega_1} \right) S(\omega, k)
\]

where \( S(\omega, k) \) contains information about the electron distribution in the plasma.

• Average Atom: To be done!
  
  – free-free: Collective effects such as plasma oscillations are expected to give peaks in the energy spectrum at \( \omega_2 = \omega_1 \pm \omega_0 \)
  
  – bound-free: Scattering from bound electrons is expected for scattered photon energy in the range \( 0 \leq \omega_2 \leq E_b \).
This is an example of the final electron energy spectrum for bound-free scattering of a 2keV photon from an aluminum plasma (metallic density and $T = 5$eV) obtained using the average-atom code to describe the bound electron.
Conclusions

- The Kubo-Greenwood formula for $\sigma(\omega)$ applied to the average-atom model diverges as $1/\omega^2$ at low frequencies.
- Including finite relaxation time leads to an approximation for the free-free contribution to $\sigma(\omega)$ that is finite and reduces to the Ziman formula at $\omega = 0$.
- The modified Kubo-Greenwood formula provides a simple and useful approximation for studies of the optical response of plasmas, including anomalous dispersion.
- Average atom model is potentially useful in understanding “Compton” scattering from plasmas; an important diagnostic for upcoming experiments at LCLS. Work remains to be done on this problem!!