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

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Collaborators:
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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 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 $R = (3\Omega/4\pi)^{1/3}$. (Based on Temperature-Dependent Fermi-Thomas Model, by Feynman, Metropolis, & Teller - 1949)

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

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

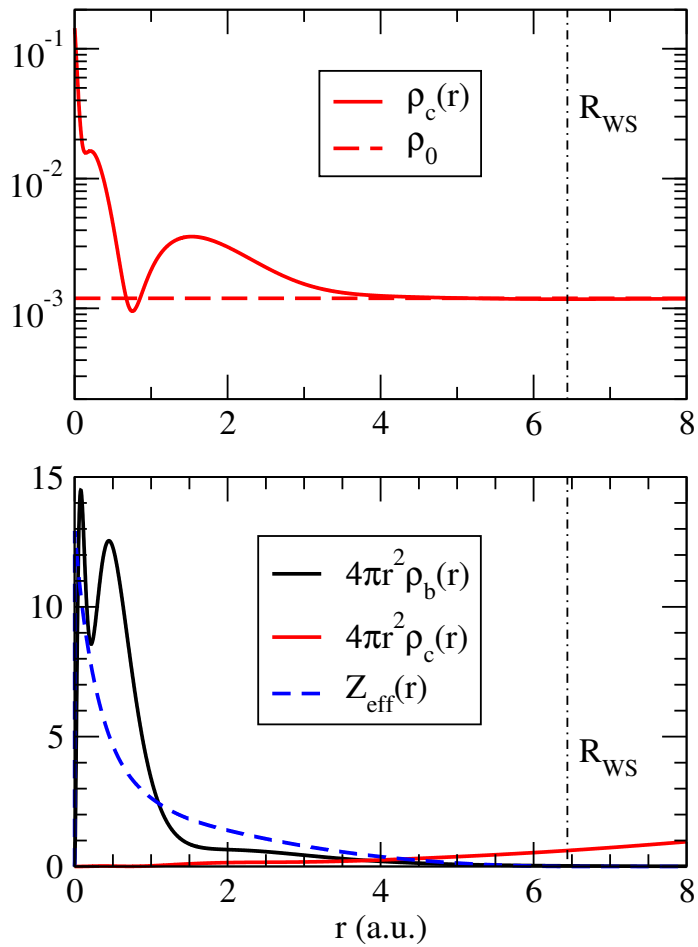
$$4\pi r^2 \rho(r) = \sum_{nl} \frac{2(2l+1)}{1 + \exp[(\epsilon_{nl} - \mu)/kT]} P_{nl}(r)^2$$

$$Z = \int_{r<R} \rho(r)\, d^3r \equiv \int_0^R 4\pi r^2 \rho(r)\, dr$$

Example

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

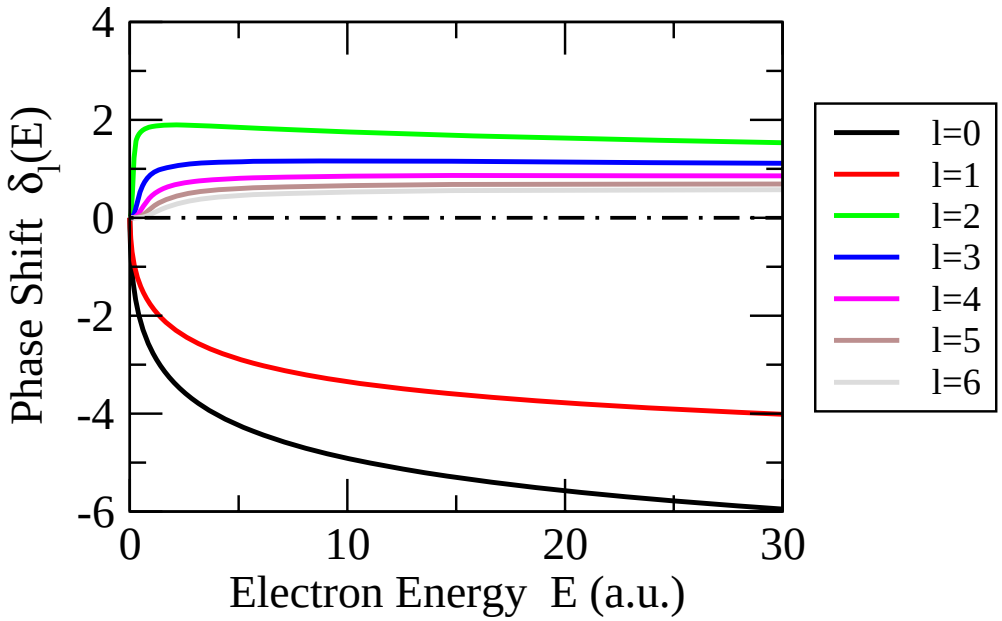
Bound States			Continuum States			
State	Energy	$n(l)$	l	$n(l)$	$n_0(l)$	$\Delta n(l)$
$1s$	-55.189	2.0000	0	0.1090	0.1975	-0.0885
$2s$	-3.980	2.0000	1	0.2149	0.3513	-0.1364
$2p$	-2.610	6.0000	2	0.6031	0.3192	0.2839
$3s$	-0.259	0.6759	3	0.2892	0.2232	0.0660
$3p$	-0.054	0.8300	4	0.1514	0.1313	0.0201
			5	0.0735	0.0674	0.0061
			6	0.0326	0.0308	0.0018
			7	0.0132	0.0127	0.0005
			8	0.0049	0.0048	0.0001
Nbound		11.5059	Nfree	1.4941	1.3404	0.1537



Al: density 0.27 gm/cc, $T = 5$ eV

Phase-Shifts & Scattering

Al: density 0.27 gm/cc, $T = 5$ eV



$$f(\theta) = \frac{1}{2ip} \sum_l \left(e^{2i\delta_l} - 1\right) P_l(\cos\theta) \ , \qquad \sigma_{\text{el}}(\theta) = |f(\theta)|^2$$

Transport Cross Section and Conductivity

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

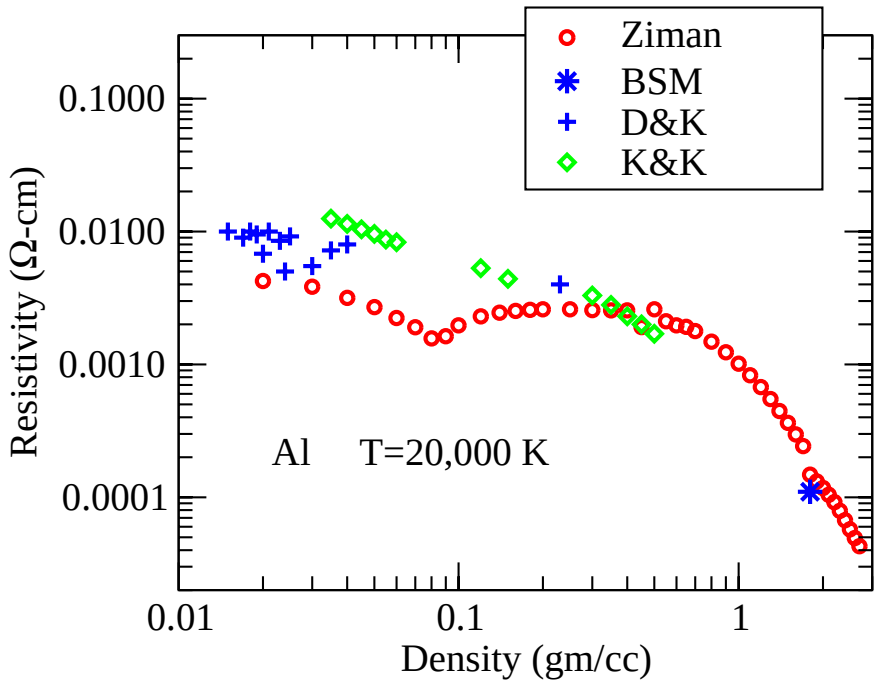
$$\tau_p = \frac{\Lambda_p}{v} \quad \text{(relaxation time)} \qquad \Lambda_p = \frac{\Omega}{\sigma_{\text{tr}}(p)} \quad \text{(mean free path)}$$

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

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



BSM: J. F. Benage, W. R. Shanahan, and M. S. Murillo, Phys. Rev. Letts. **83**, 2953 (1999); D & K: A. W. DeSilva and H.-J. Kunze, Phys. Rev. E**49**, 4448 (1994); K & K: I. Krisch and H.-J. Kunze, Phys. Rev. E**58**, 6557 (1998).

Linear Response and Conductivity

Consider an applied electric field:

$$\boldsymbol{E}(t) = F\hat{\boldsymbol{z}}\ \sin\omega t \qquad \boldsymbol{A}(t) = \frac{F}{\omega}\,\hat{\boldsymbol{z}}\ \cos\omega t$$

The time dependent Schrödinger equation becomes

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

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 $\psi_i(\boldsymbol{r}, t)$ 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:

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

which is an average-atom version of the Kubo[1]-Greenwood[2] formula.

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

[1] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957)

[2] D. A. Greenwood, Proc. Phys. Soc. London **715**, 585 (1958)

Infrared "Catastrophe"

Particle in a potential $V(r)$:

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

Relation between scattering amplitude and potential

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

Result: (Low-frequency theorem QED)

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

Low-Frequency Kubo-Greenwood

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

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

Free-free contribution:

$$\begin{aligned}\sigma(\omega) &\approx \frac{2\pi e^2}{m^2\Omega}\int\frac{d^3p_1}{(2\pi)^3}\int\frac{d^3p_2}{(2\pi)^3}\left(-\frac{\partial f}{\partial E}\right)\left|\langle p_2|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|p_1\rangle\right|^2\delta(E_2-E_1-\omega)\\ &= \frac{2e^2}{3}\int\frac{d^3p}{(2\pi)^3}\left(-\frac{\partial f}{\partial E}\right)v^2\frac{1}{\omega^2\tau_p} \qquad \text{(Low-Freq K-G formula)}\end{aligned}$$

Low-Frequency Kubo-Greenwood

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

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

Free-free contribution:

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

$$= \frac{2e^2}{3}\int\frac{d^3p}{(2\pi)^3}\left(-\frac{\partial f}{\partial E}\right)v^2\frac{1}{\omega^2\tau_p} \qquad \text{(Low-Freq K-G formula)}$$

$$\sigma(0) = \frac{2e^2}{3}\int\frac{d^3p}{(2\pi)^3}\left(-\frac{\partial f}{\partial E}\right)v^2\tau_p \qquad \text{(Ziman formula)}$$

Influence of Collisions on Wave Function

$$\psi(\boldsymbol{p}, t) \to \exp\left[i\left(\boldsymbol{p}\cdot\boldsymbol{r} - Et\right) - \frac{t}{\tau_p}\right]$$

Effect[3]:

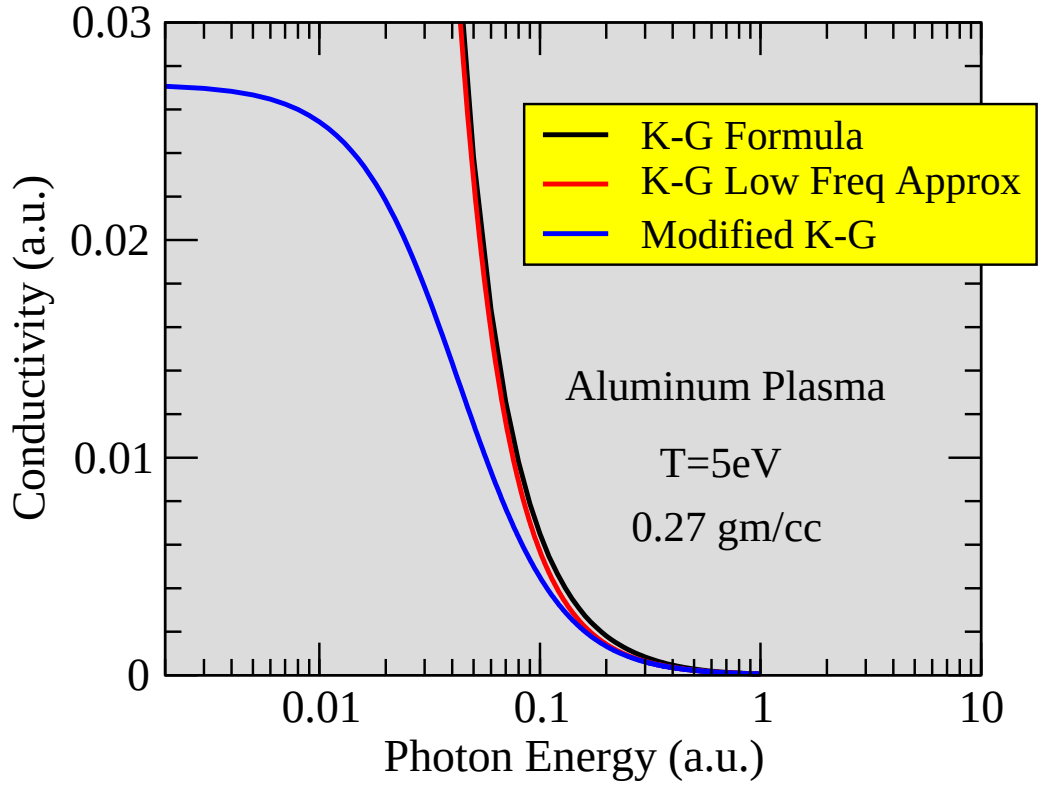
$$\frac{1}{\omega^2} \to \frac{1}{\omega^2 + 1/\tau_p^2} \equiv \frac{\tau_p^2}{\omega^2\tau_p^2 + 1}$$

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

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

[3] M. Yu. Kuchiev and W. R. Johnson, Phys. Rev. E 78, 026401 (2008); *Green's Functions for Solid State Physics*, S. Doniach & E.H. Sondheimer, Imperial College Press (1998), Chap. 5

Comparison of Conductivity Formulas



Conductivity Sum Rule

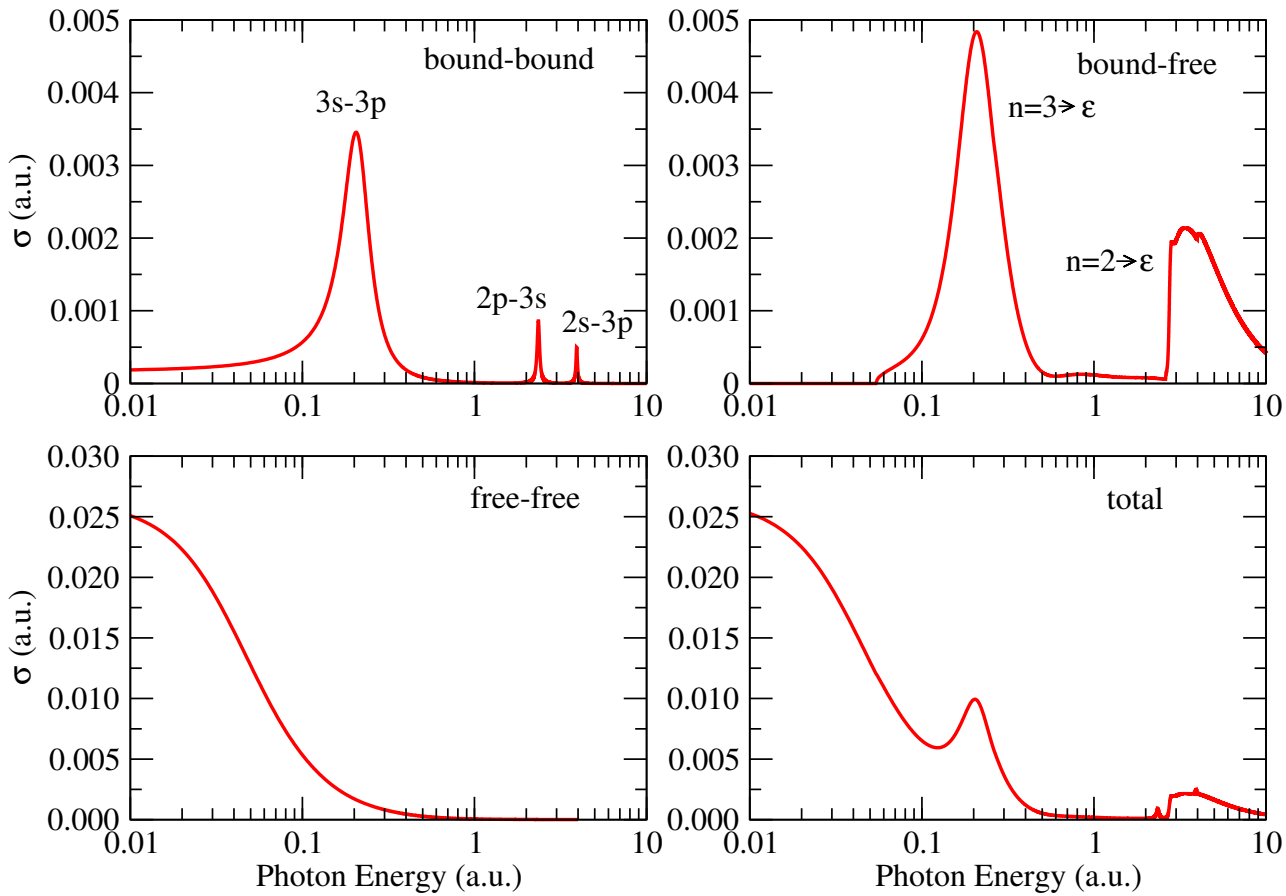
$$\int_0^\infty \sigma(\omega)d\omega = \frac{\pi e^2}{3}\int \frac{d^3p}{(2\pi)^3} v^2 \left(-\frac{\partial f}{\partial E}\right)$$

$$= \frac{e^2\pi}{3}\int \frac{dEd\Omega}{(2\pi)^3}\frac{p^3}{m}\left(-\frac{\partial f}{\partial E}\right)$$

$$= e^2\pi \int \frac{dEd\Omega}{(2\pi)^3}\, pf(E)$$

$$= \frac{e^2\pi}{m}\int \frac{d^3p}{(2\pi)^3}\, f(E) = \frac{e^2\pi}{2m}Z^*$$

Summary of Modified K-G Formula



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 Re$[\sigma(\omega)]$ to find

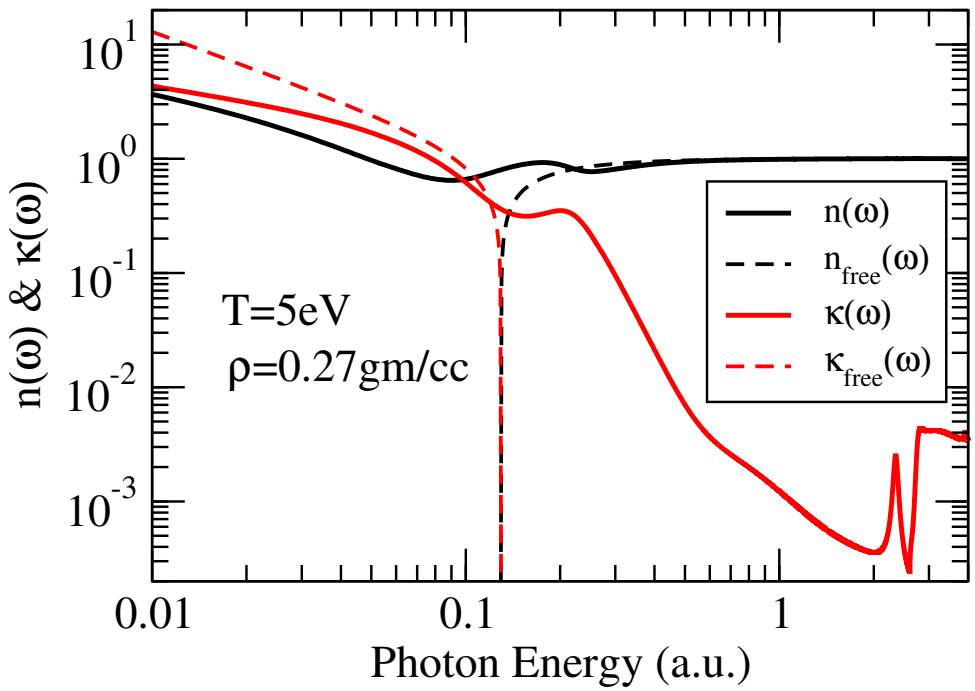
$$\text{Im}[\sigma(\omega)] = \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left(-\frac{\partial f}{\partial E} \right) v^2 \frac{\omega \tau_p^2}{\omega^2 \tau_p^2 + 1}$$

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

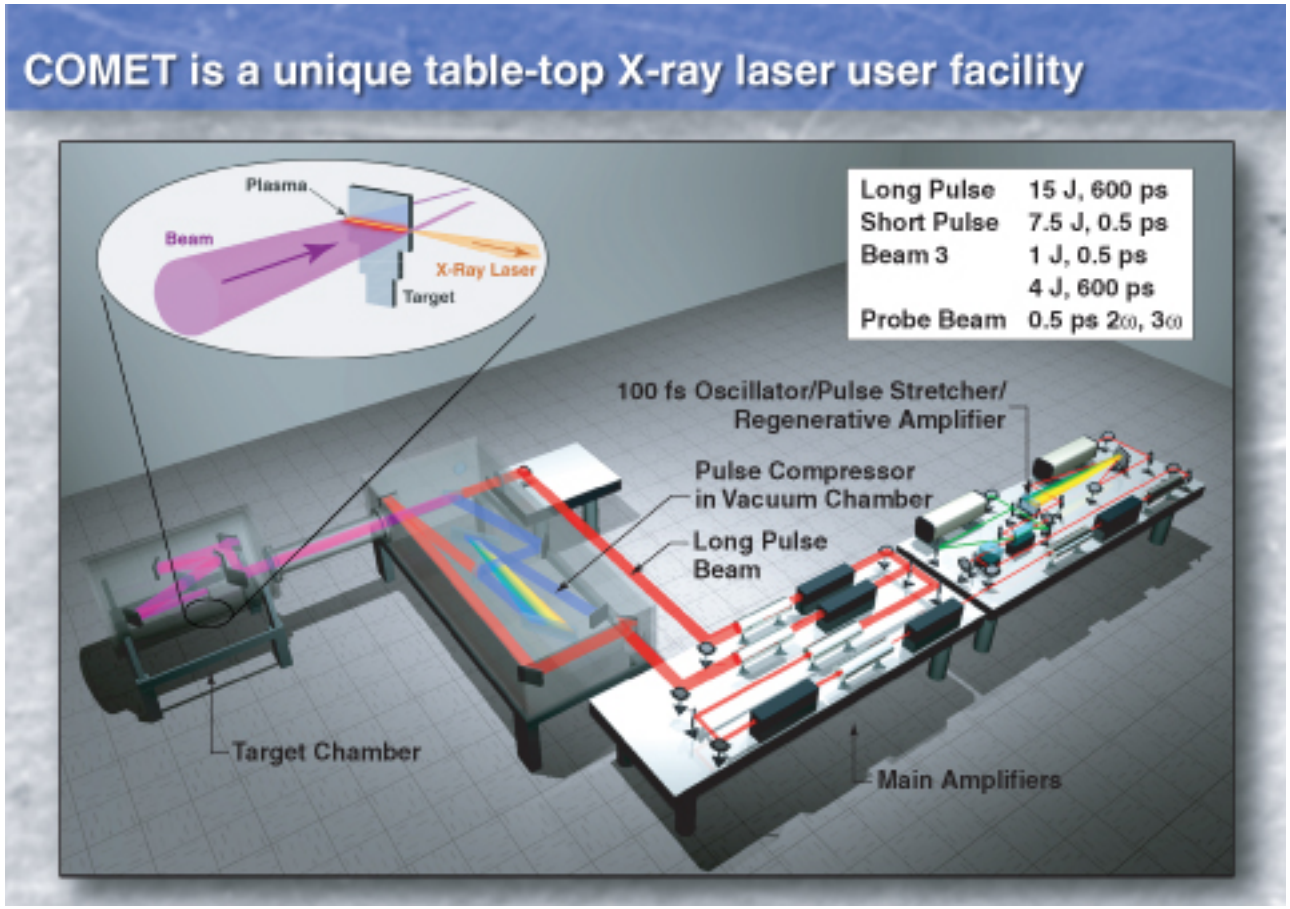
$$\sigma(\omega) = \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left(-\frac{\partial f}{\partial E} \right) v^2 \frac{\tau_p}{1 - i\omega\tau_p}$$

Dielectric Function, Index of Refraction

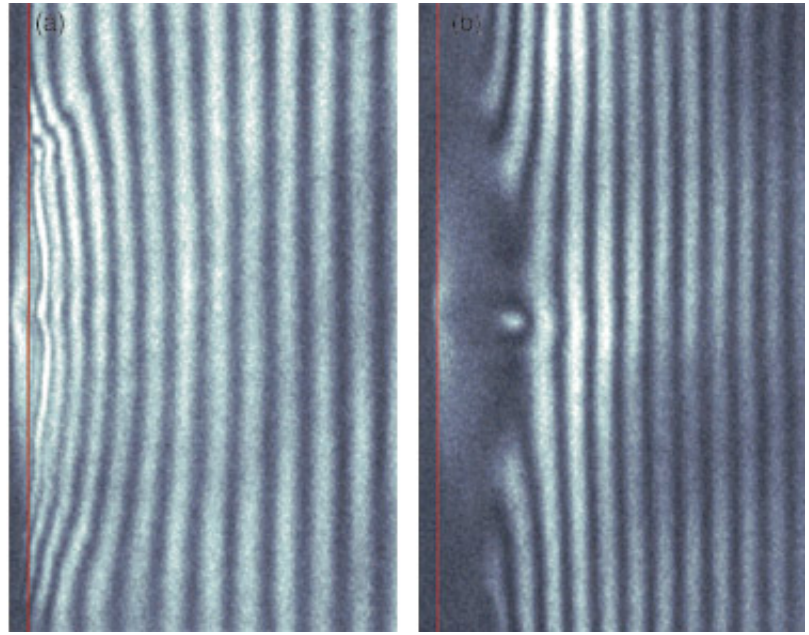
$$\epsilon_r(\omega) = 1 + 4\pi i \frac{\sigma(\omega)}{\omega}, \quad n(\omega) + i\kappa(\omega) = \sqrt{\epsilon_r(\omega)}.$$



Laser Interferometry



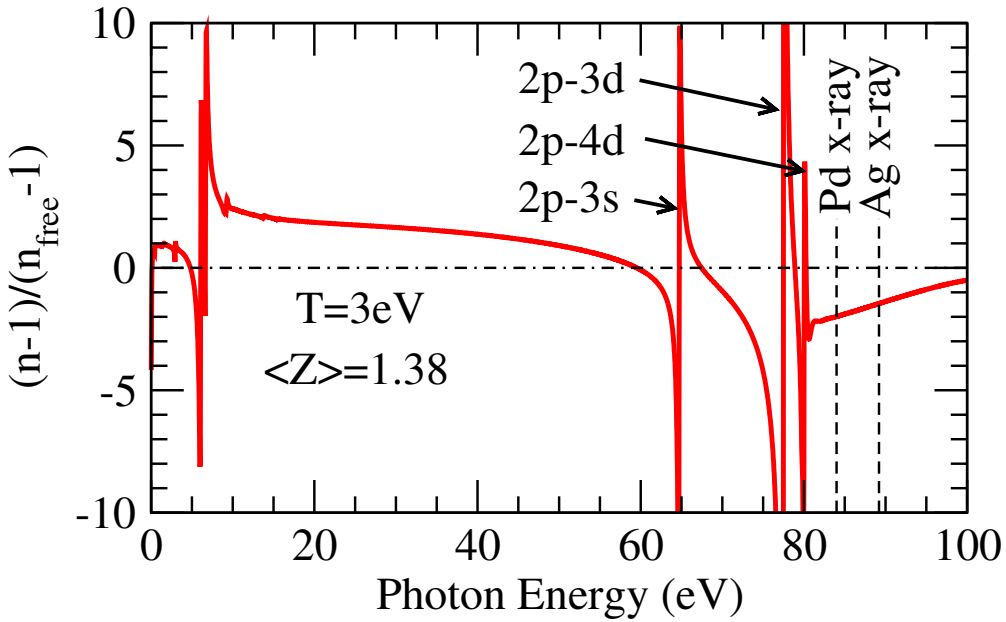
Negative Plasma Densities Raise Questions



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

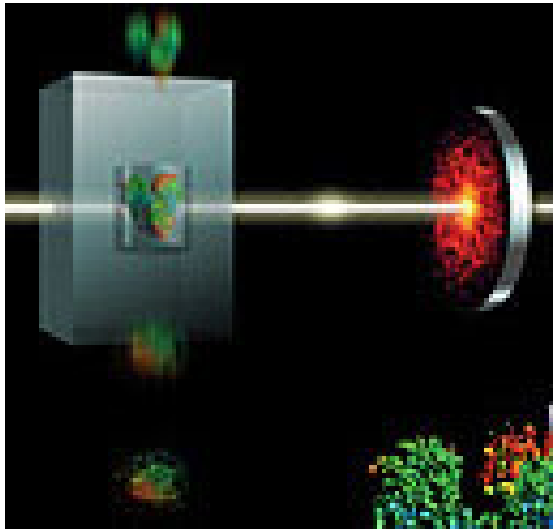
Comparison with Average-Atom Model

Aluminum plasma with ion density $n_{\text{ion}} = 10^{20}/\text{cc}$ (With Joe Nilsen)



Compton Scattering & LCLS

LCLS (linac coherent light source) at SLAC in Menlo Park, California. is a free-electron laser that generates xray 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.

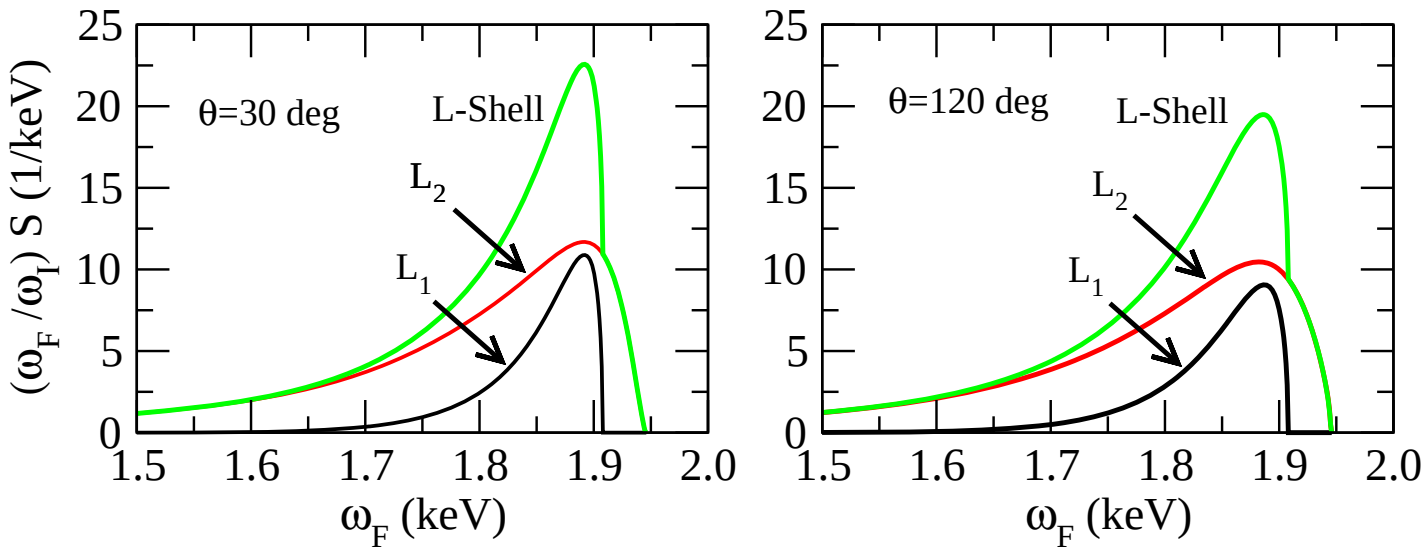
$$\frac{d\sigma}{d\Omega} = r_0^2 \left(\epsilon_1^* \cdot \epsilon_2\right)^2$$

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

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

  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 $0 \leq \omega_2 \leq E_{\text{b}}$.

Average-Atom Bound-Free Scattering



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 = 5eV) obtained using the average-atom code to describe the bound electron.

Conclusions

- 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!!