Low-Frequency Conductivity in the Average-Atom Approximation

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Collaborators:
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Related Contributions:
Poster #30 - P. Renaudin et al.   Talk (Friday AM) - R. Piron and T. Blenski

- ☞ Average-Atom & Static Conductivity (Ziman)
- ☞ Kubo-Greenwood Formula (Infrared Catastrophe)
- ☞ "Proper" Static Limit & Conductivity Sum Rule
- ☞ Application to Plasma Optics

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Average-Atom Model of a Plasma

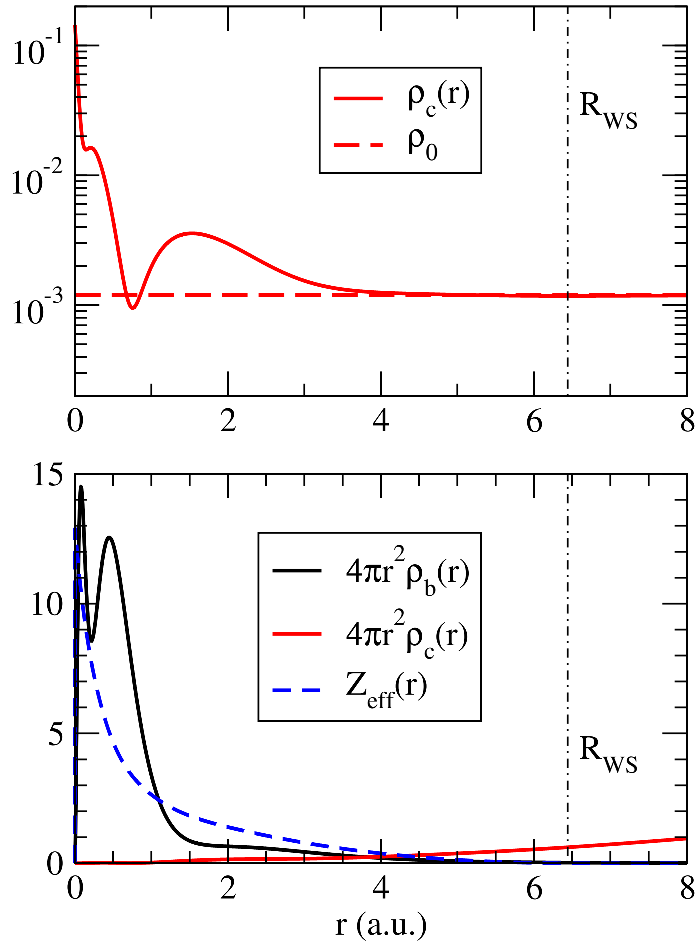
Plasma composed of neutral spheres with Wigner-Seitz radius $R = (3\Omega/4\pi)^{1/3}$ floating in a "jellium" sea.

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

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

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

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



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

Phase-Shifts & Scattering

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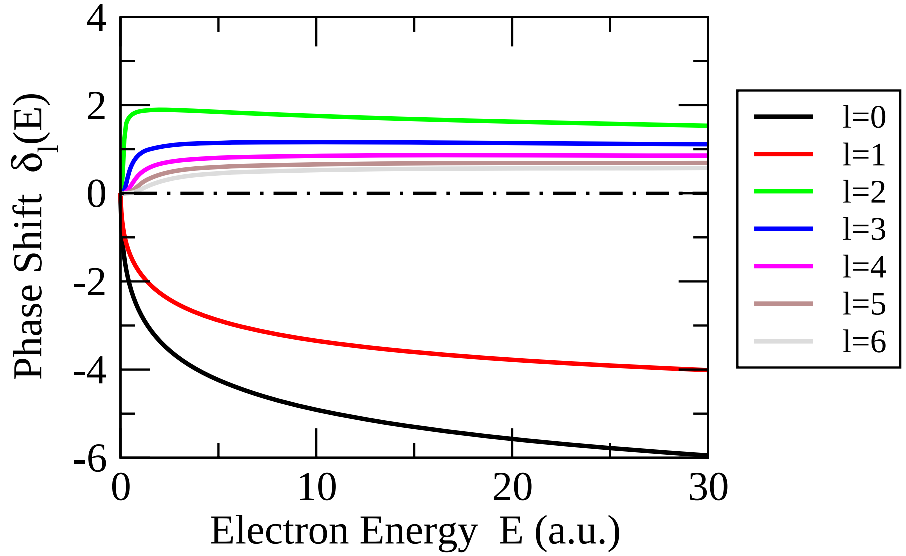


$$f(\theta) = \frac{1}{2ip} \sum_l \left(e^{2i\delta_l} - 1 \right) P_l(\cos\theta) \,, \qquad \sigma_{\text{el}}(\theta) = |f(\theta)|^2$$

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:

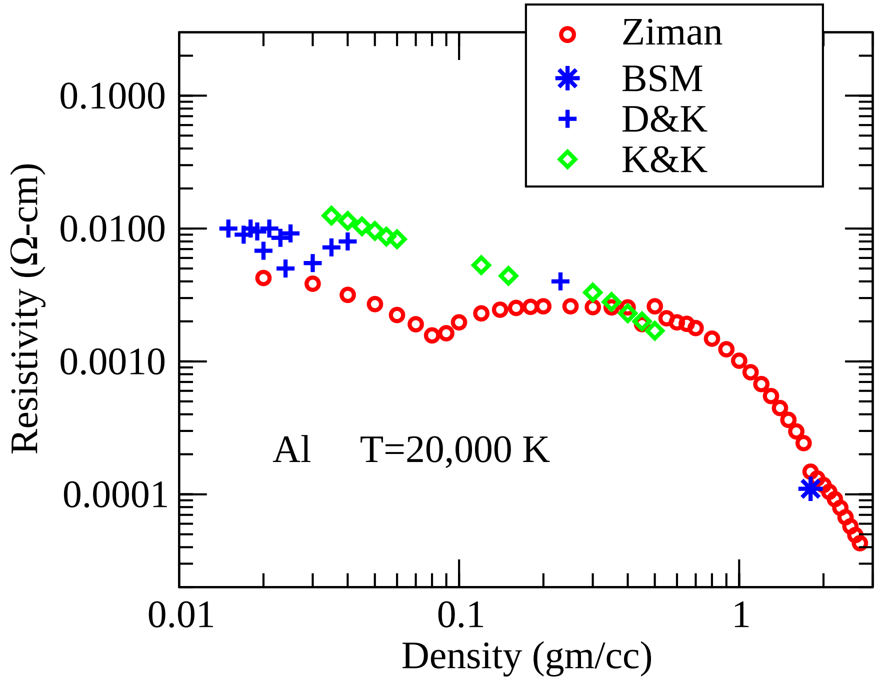
$$\tau_p = \frac{\Lambda_p}{v} \quad \text{(relaxation time)} \qquad \Lambda_p = \frac{\Omega}{\sigma_{\text{tr}}(p)} \quad \text{(mean free path)}$$

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

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)

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[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

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

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

Free-free contribution:

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

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

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]:

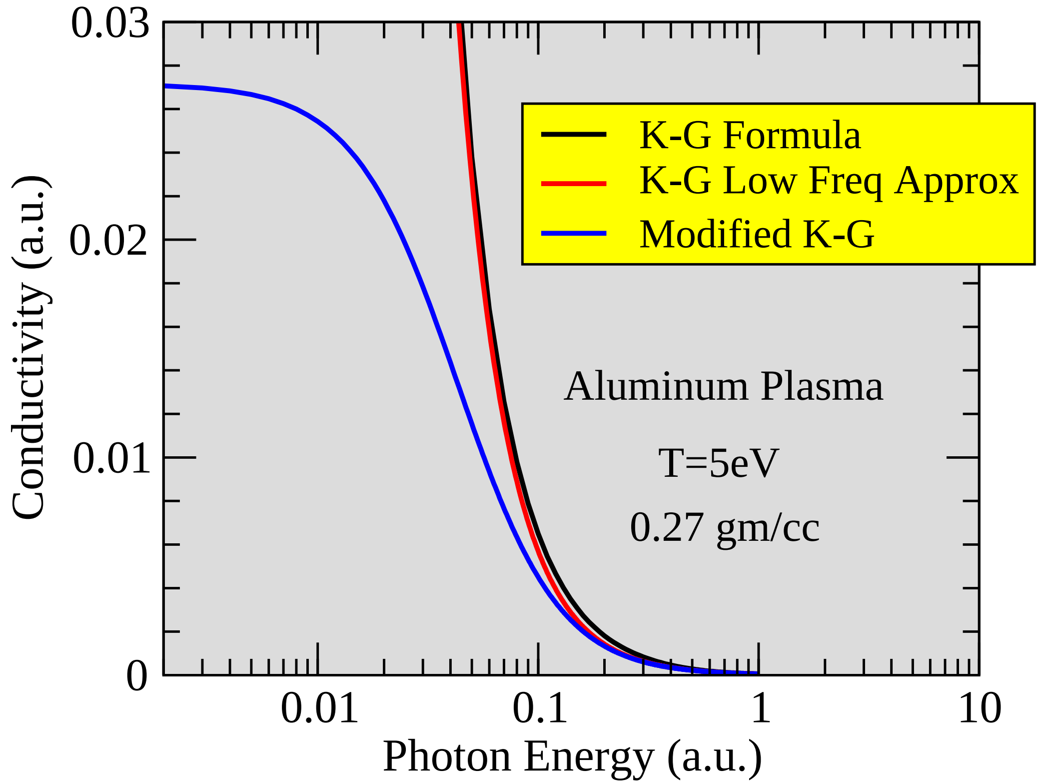
$$\frac{1}{\omega^2} \to \frac{1}{\omega^2 + 1/\tau_p^2} \equiv \frac{\tau_p^2}{\omega^2\tau_p^2 + 1}$$

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

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

[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

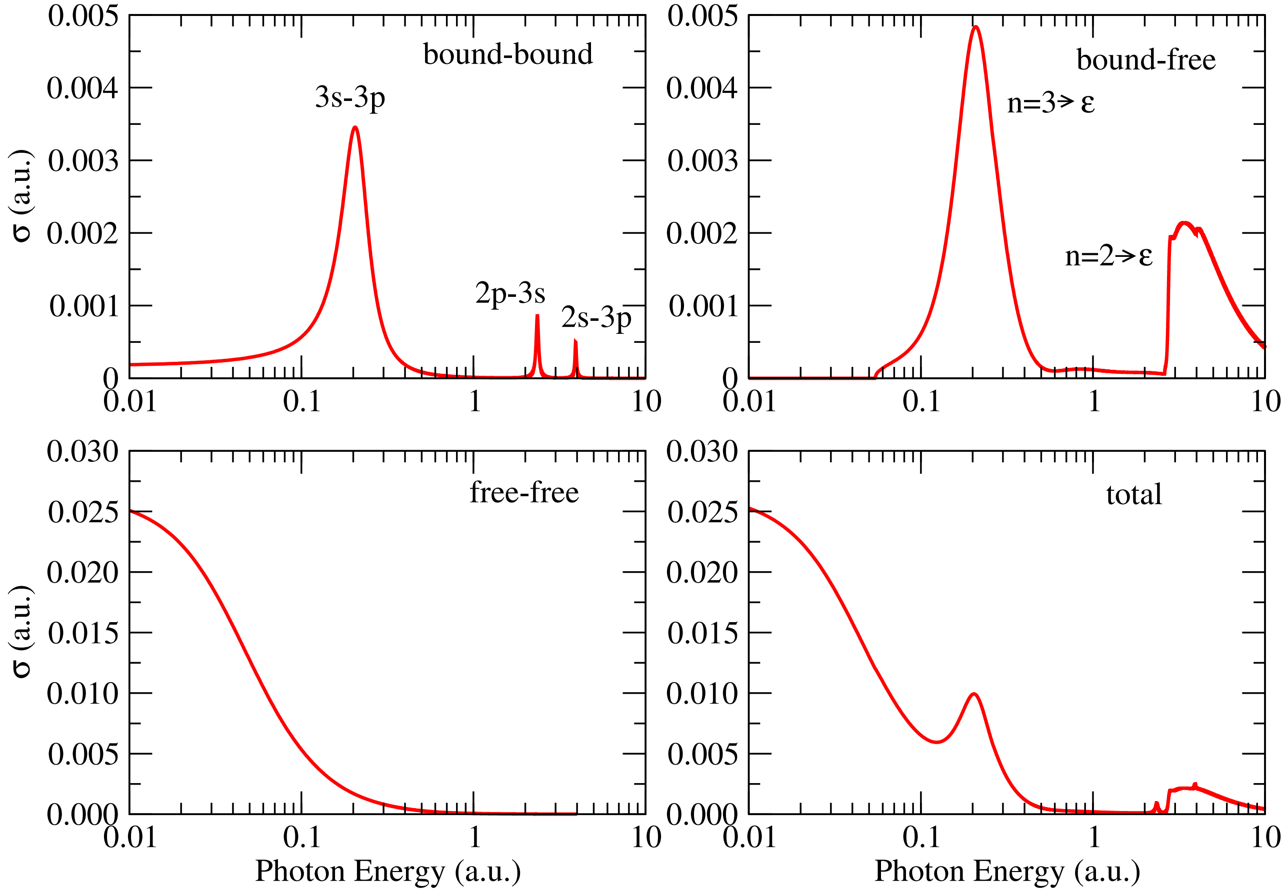
$$\int_0^\infty \sigma(\omega)d\omega = \frac{\pi e^2}{3}\int \frac{d^3p}{(2\pi)^3} v^2 \left(-\frac{\partial f}{\partial E}\right)$$

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

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

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

Summary of Modified K-G Formula



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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

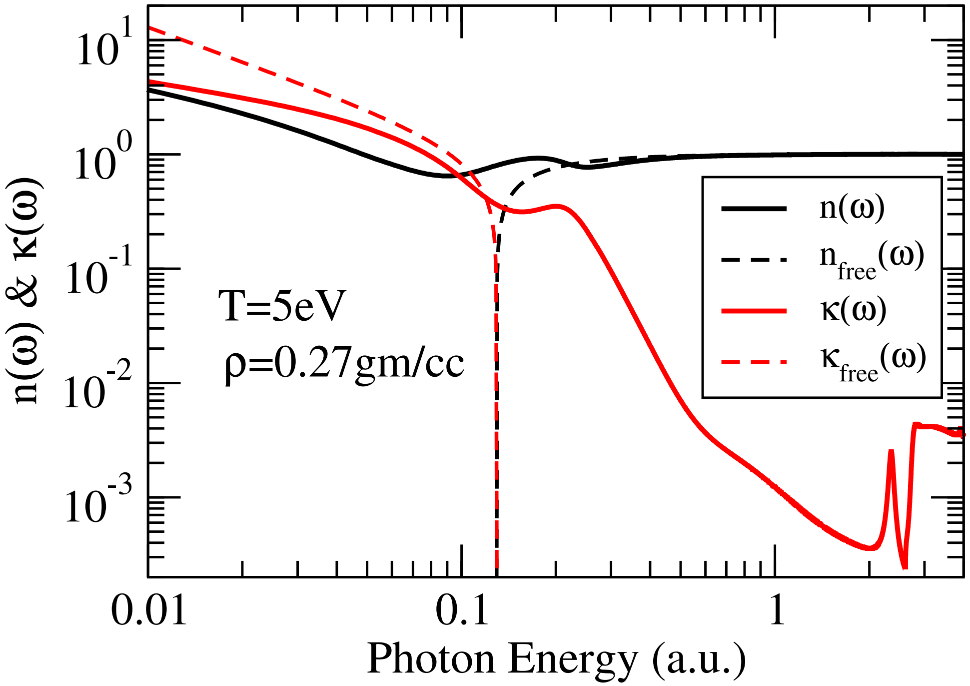
$$\text{Im}[\sigma(\omega)] = \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left(-\frac{\partial f}{\partial E} \right) v^2 \frac{\omega \tau_p^2}{\omega^2 \tau_p^2 + 1}$$

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

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



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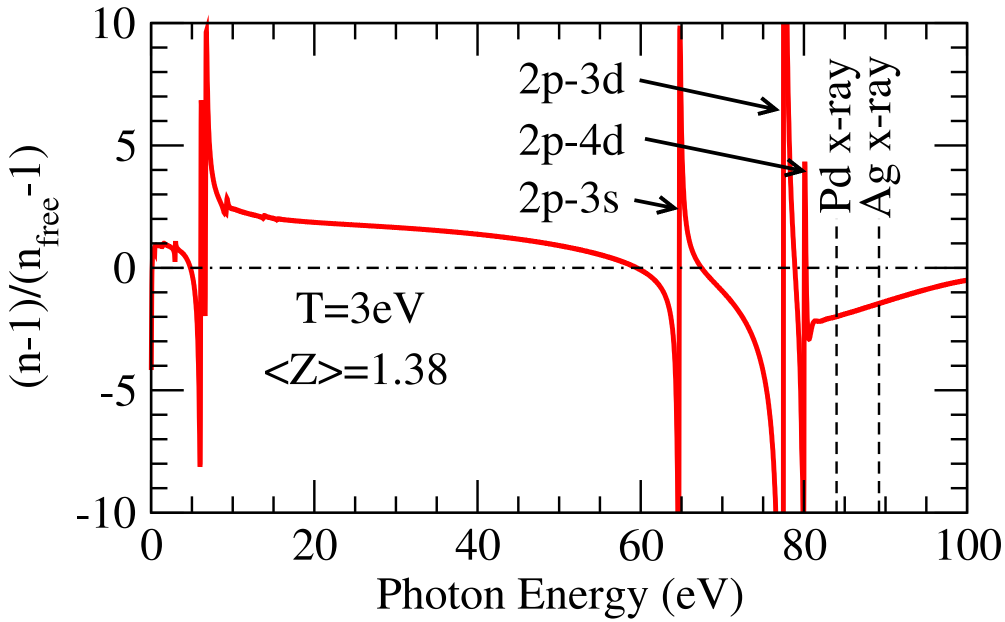
Comparison with Free Electron Model

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



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.