Optical Properties of Plasmas Based on an Average-Atom Model

Walter Johnson, Notre Dame University
Claude Guet, CEA/DAM Ile de France
George Bertsch, University of Washington

Motivation for this work: Joseph Nilsen, LLNL

- Average Atom (NR version of "Inferno")
- Linear Response $\Rightarrow$ Kubo-Greenwood formula for $\sigma(\omega)$
- Kramers-Kronig Dispersion Relation $\Rightarrow$ Dielectric Function $\epsilon(\omega)$
- Index of refraction $n(\omega) + i\kappa(\omega) = \sqrt{\epsilon(\omega)}$

Introduction

Free electron model used in plasma diagnostics:

$$n_{\text{free}}(\omega) = \sqrt{1 - \frac{\omega_0^2}{\omega^2}} \approx 1 - \frac{\omega_0^2}{2\omega^2} < 1 \quad \text{where} \quad \omega_0^2 = 4\pi \frac{e^2}{m} \frac{N_{\text{free}}}{\text{vol}}$$

Recent experiments on Al plasmas find $n > 1$ at few eV temperatures

- LLNL COMET laser facility[1] (14.7 nm Ni-like Pd laser)
- Advanced Photon Research Center JAERI[2] (13.9 nm Ni-like Ag laser)

Reason: Effect of bound electrons on optical properties.

[1] J. Filevich et al. *Proceedings of the 9th International Conference on X-Ray Lasers*, May 23-28 (2004)
[2] H. Tang et al., Appl. Phys. B**78**, 975 (2004)

Average-Atom Model

QM version of generalized Thomas-Fermi model[3]

Inside a neutral (Wigner-Seitz) cell:

$$\left[\frac{p^2}{2m} - \frac{Z}{r} + V\right] u_a(\boldsymbol{r}) = \epsilon u_a(\boldsymbol{r}) \tag{1}$$

$V = V_{\mathsf{dir}}(r) + V_{\mathsf{exc}}(r)$ for $r \leq R$ and $V = 0$ otherwise.

$$\nabla^2 V_{\mathsf{dir}} = -4\pi\rho \tag{2}$$

$V_{\mathsf{exc}}(\rho)$ is given in the local density approximation

[3] R. P. Feynman, N. Metropolis and E. Teller, Phys. Rev. **75** 1561 (1949)

Thermal Average Electron Density

Contributions to the density are

$$\rho_b(r) = \frac{1}{4\pi r^2} \sum_l 2(2l+1) \sum_n f(\epsilon_{nl})\, P_{nl}(r)^2 \tag{3}$$

$$\rho_c(r) = \frac{1}{4\pi r^2} \sum_l 2(2l+1) \int_0^\infty d\epsilon\, f(\epsilon)\, P_{\epsilon l}(r)^2 \tag{4}$$

where

$$f(\epsilon) = \frac{1}{1+\exp[(\epsilon-\mu)/kT]}$$

The chemical potential μ is chosen to insure electric neutrality:

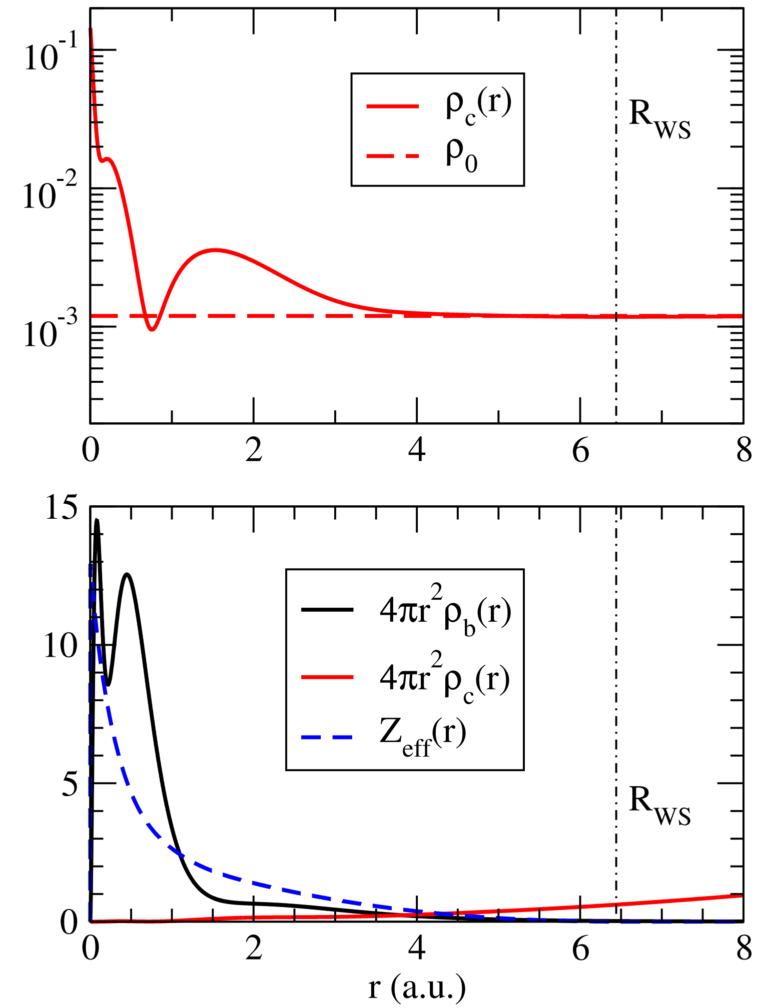
$$Z = \int_{r<R} \rho(r)\, d^3r \equiv \int_0^R 4\pi r^2 \rho(r)\, dr \ . \tag{5}$$

Eqs. (1-5) are solved self-consistently for ρ, V, and μ.

Example

Al: density 0.27 gm/cc, $T = 5$ eV, $R = 6.44$ 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
			9	0.0017	0.0016	0.0001
			10	0.0005	0.0005	0.0000
Nbound		11.5059	Nfree	1.4941	1.3404	0.1537



ρc(r)
ρ0
RWS
10^-1
10^-2
10^-3
0
2
4
6
8
15
10
5
4πr²ρb(r)
4πr²ρc(r)
Zeff(r)
r (a.u.)

Linear Response and the Kubo-Greenwood Formula

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:

$$\sigma(\omega) = \frac{2\pi e^2}{\omega \Omega} \sum_{ij} (f_i - f_j)\ |\langle j | v_z | i \rangle|^2\, \delta(\epsilon_j - \epsilon_i - \omega),$$

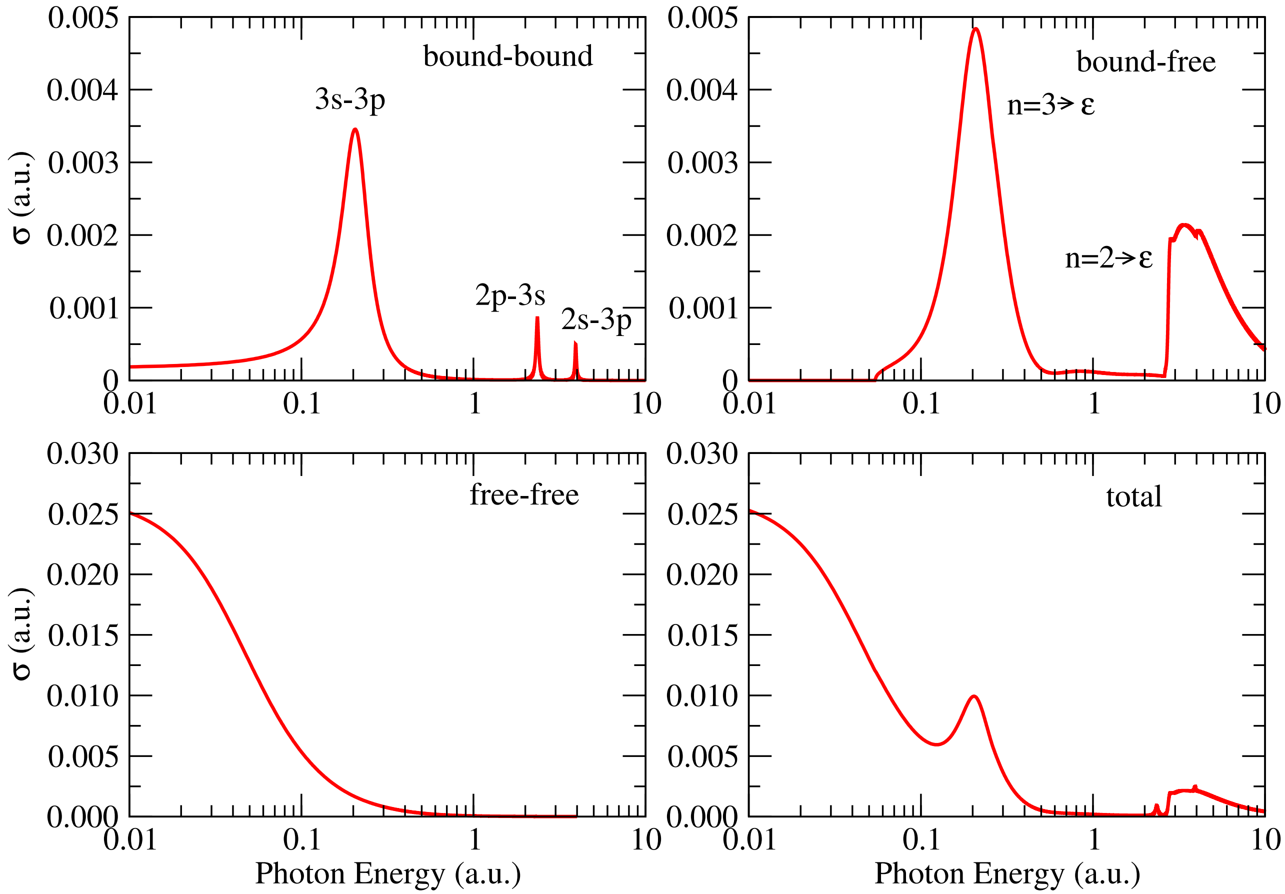
which is an average-atom version of the Kubo[4]-Greenwood[5] formula.

---

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

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

Example: Al T=3eV & density= 0.27gm/cc



Optical Properties

For a conducting medium, the dielectric function is related to the *complex* conductivity by

$$\epsilon(\omega) = 1 + 4\pi i \, \frac{\sigma(\omega)}{\omega}$$

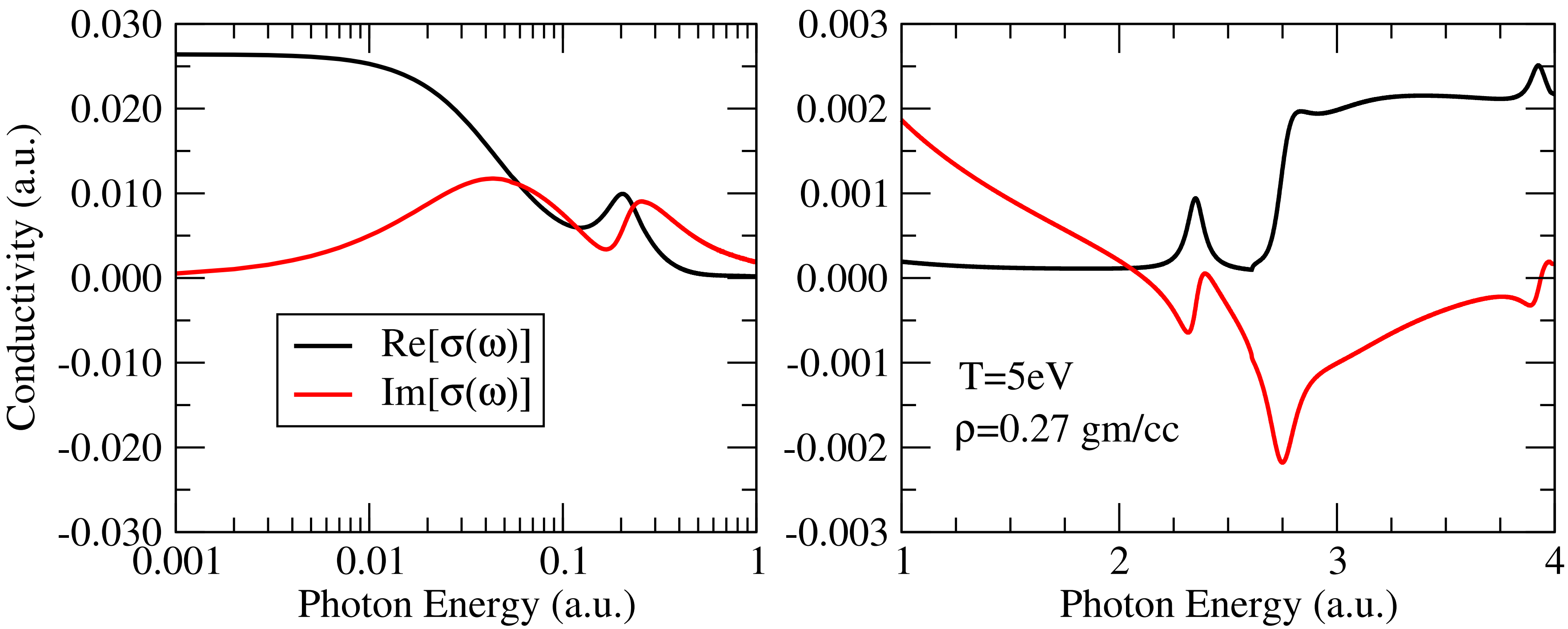
We know $\Re\sigma(\omega)$; we must evaluate $\Im\sigma(\omega)$

From analytic properties of $\sigma(\omega)$ one infers the dispersion relation[6]

$$\Im\,\sigma(\omega_0) = \frac{2\omega_0}{\pi} \int_0^\infty \frac{\Re\,\sigma(\omega)}{\omega_0^2 - \omega^2} \, d\omega.$$

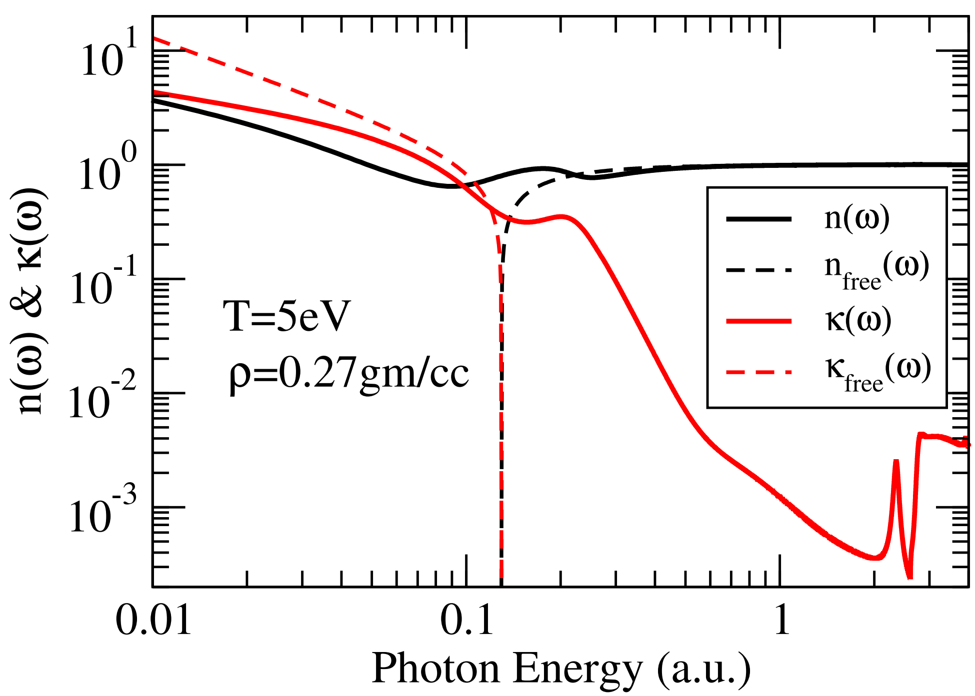
[6] R. de L. Kronig and H. A. Kramers, Atti Congr. Intern. Fisici, **2**, 545 (1927)

Application of Dispersion Relation



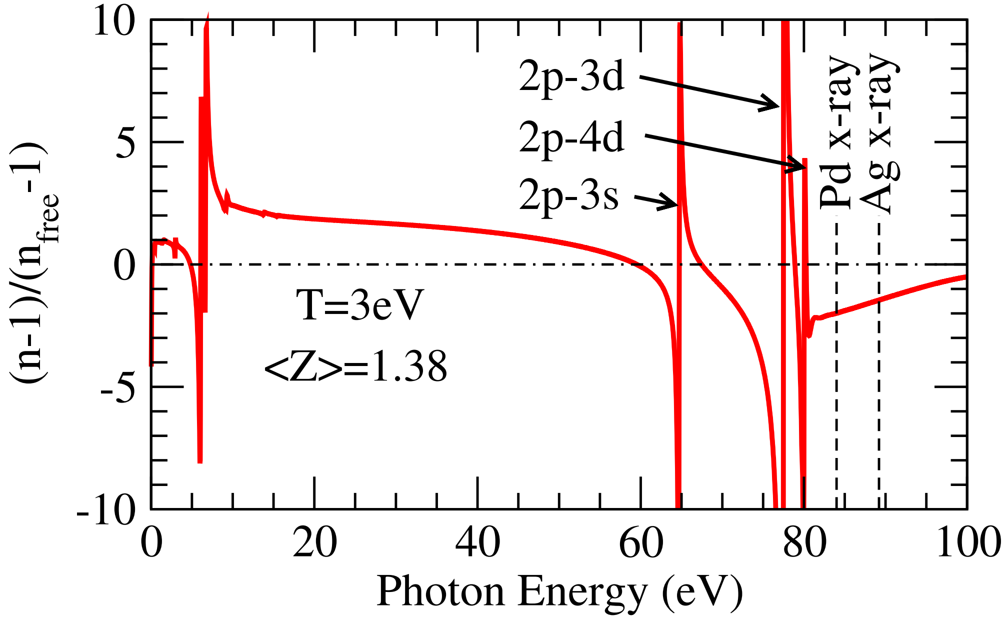
Index of Refraction

$$\Re\epsilon(\omega) = 1 - 4\pi\frac{\Im\sigma(\omega)}{\omega} \qquad \Im\epsilon(\omega) = 4\pi\frac{\Re\sigma(\omega)}{\omega},$$
$$n + i\kappa = \sqrt{\epsilon}.$$



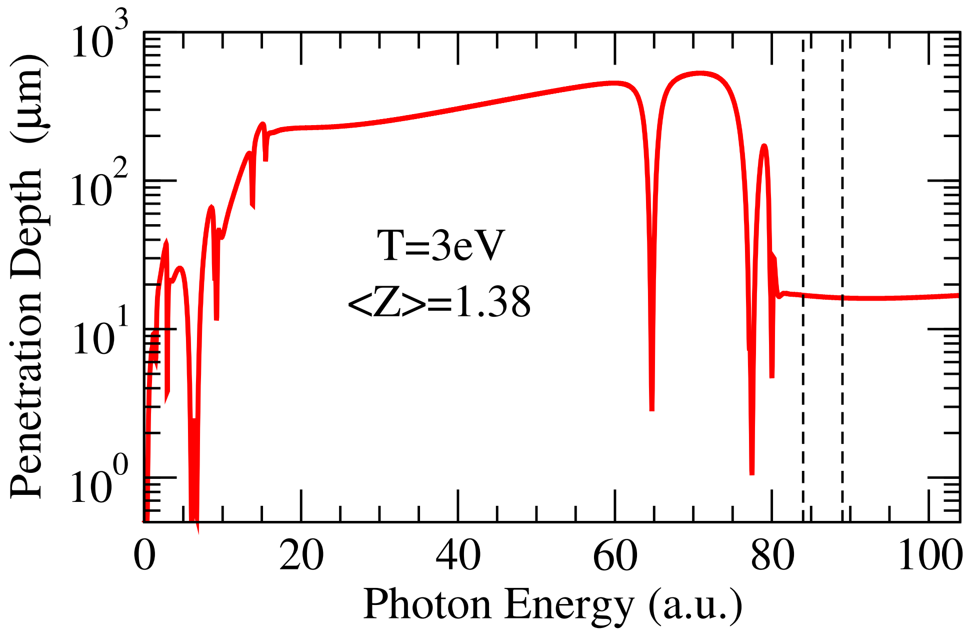
Al: Comparison with Free Electron Model

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



Al: Penetration Depth

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



Conclusions

- Linear response theory applied to average atom model provides a straightforward method for obtaining the frequency-dependent conductivity.
- The dielectric function (and index of refraction) can be reconstructed with the aid of a dispersion relation,
- The model explains observed behavior of low temperature Al plasmas in the 80-90 eV frequency range.
- Even away from bound-bound resonances, the free electron model may be misleading.