Low-Frequency Conductivity in the Average-Atom Approximation

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Abstract

The quantum mechanical average-atom model is reviewed and applied to determine scattering phase shifts, mean-free paths, and relaxation times in warm-dense plasmas. Static conductivities $\sigma$ are based on an average-atom version of the Ziman formula. Applying linear response to the average atom model leads to an average-atom version of the Kubo-Greenwood formula for the frequency-dependent conductivity $\sigma(\omega)$. The free-free contribution to $\sigma(\omega)$ is found to diverge as $1/\omega^2$ at low frequencies; however, considering effects of multiple scattering leads to a modified version of $\sigma(\omega)$ that is finite and reduces to the Ziman formula at $\omega = 0$. The resulting average-atom version of the Kubo-Greenwood formula satisfies the conductivity sum rule. The dielectric function $\epsilon(\omega)$ and the complex index of refraction $n(\omega) + i\kappa(\omega)$ are inferred from $\sigma(\omega)$ using dispersion relations. Applications to anomalous dispersion in laser-produced plasmas are discussed.

Key words: plasma, conductivity, dielectric function, index of refraction, dispersion relations, x-ray interferometry
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1 Average-Atom & Static Conductivity

Let us briefly reprise the average atom model, which is a quantum mechanical version of the temperature-dependent Thomas-Fermi theory of a plasma introduced sixty years ago by Feynman, Metropolis, and Teller [1]. In the average-atom model, the plasma is divided into neutral spherical cells, each containing a single nucleus (charge $Z$) and $Z$ electrons. The radius of each cell is the
Wigner-Seitz (WS) radius, determined from the material density $\rho_m$ (gm/cc), the atomic weight $A$ (gm/mol), and Avagadro’s number $A = 6.023 \times 10^{23}$, by $R_{\text{WS}} = (3\Omega/4\pi)^{1/3}$, where $\Omega = A/A \rho_m$ is the cell volume. Individual electrons (bound and continuum) inside a neutral cell are assumed to move in a self-consistent potential. Outside the cell boundaries the potential vanishes. The continuum electrons penetrate the cell boundary and move into the region between atoms where the electron density approaches a constant value $\rho_0$ determined by the temperature $T$ and chemical potential $\mu$. In the quantum-mechanical version of the average-atom model, the density oscillates about $\rho_0$ outside the cell with a small and ever decreasing amplitude [2]. To insure electrical neutrality, it is necessary to assume a uniform positive background charge $\rho_+$ that precisely cancels $\rho_0$. The average atom floats in this positive “jellium” sea. The average ionic charge of sea is $Z^* = \rho_+ \Omega$. The picture that evolves is an average atom of nuclear charge $Z$ with $Z$ bound and continuum electrons moving self-consistently inside a sphere of radius $R_{\text{WS}}$; outside is a neutral plasma consisting of electrons (density $\rho_0$) balanced by positive sea of ions (charge $Z^*$). The electron density is determined using the quantum-mechanical self-consistent field method. The average atom model introduced here is a nonrelativistic version of Liberman’s Inferno model [3] and is very similar to the model described previously by Blenski and Ishikawa [4].

In the quantum-mechanical model, each electron is assumed to satisfy the central-field Schrödinger equation

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

where $a = (n, l)$ for bound states or $(\epsilon, l)$ for continuum states. The wave function $u_a(r)$ is decomposed in a spherical basis as

$$u_a(r) = \frac{1}{r} P_{\epsilon l}(r) Y_{l}^{m}(\hat{r}) \chi_{\sigma a}, \quad (2)$$

where the bound $P_{nl}(r)$ and continuum $P_{\epsilon l}(r)$ radial functions are normalized as

$$\int_0^\infty dr P_{nl}(r) P_{n'l'}(r) = \delta_{nn'}, \quad \int_0^\infty dr P_{\epsilon l}(r) P_{\epsilon'l'}(r) = \delta(\epsilon - \epsilon'). \quad (3)$$

The self-consistent potential consists of two parts: $V(r) = V_{\text{dir}} + V_{\text{xc}}$. The direct part of the potential is obtained from

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

where the electron density $\rho = \rho_b + \rho_c$ has contributions from both bound and continuum electrons. In the present work, the exchange-correlation potential
Contributions to the radial electron density in an aluminum plasma, density=0.27 gm/cc, \( T = 5 \) eV. Bound-electron radial density \( 4\pi r^2 \rho_b(r) \) (solid black), continuum radial density \( 4\pi r^2 \rho_c(r) \) (solid red), and effective charge \( Z_{\text{eff}}(r) \) (dashed blue). Inset: continuum density \( \rho_c(r) \) (solid green), background density \( \rho_0(r) \) (dashed black).

is taken to be the Kohn-Sham (exchange-only) potential

\[
V_{\text{xc}} = -\left( \frac{3}{\pi} \rho(r) \right)^{1/3}.
\]

(5)

The bound-state contribution to the density is

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

(6)

where \((n,l)\) ranges over all subshells. Contributions to the density from continuum electrons are given by

\[
4\pi r^2 \rho_c(r) = \sum_l \int d\epsilon \frac{2(2l + 1)}{1 + \exp[(\epsilon - \mu)/kT]} P_{\epsilon l}(r)^2.
\]

(7)

Finally, the chemical potential \( \mu \) is chosen to insure electric neutrality:

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

(8)

The equations (1-8) above are solved self-consistently to give the chemical potential \( \mu \), the self-consistent potential \( V(r) \) and the electron density \( \rho(r) \).

As an illustration of the present average-atom code, consider aluminum at density \( \rho_m = 0.27 \) gm/cc and temperature \( T = 5 \) eV. The WS radius is \( R_{\text{WS}} = 6.44 \) a.u. and the chemical potential is \( \mu = -0.382 \) a.u.. In Fig. 1, we show bound-state and continuum contributions to the radial density along
Fig. 2. Phase shifts for partial waves with $l \leq 6$ in an aluminum plasma with density 0.27 gm/cc, and $T = 5$ eV.

with the effective charge $Z_{\text{eff}}(r)$, related to the self-consistent potential by $V(r) = -Z_{\text{eff}}(r)/r$. In the inset to the figure, the continuum contribution to the electron density $\rho_c(r)$ is compared with the free electron background density $\rho_0$ calculated using the same chemical potential. The density merges smoothly into the background outside the WS sphere.

In Fig. 2, we present phase shifts for partial waves with $l = 0$ to 6 for energies $E \leq 30$ eV, calculated in the average-atom potential illustrated in Fig. 1. From these phase shifts, we can calculate the scattering amplitude

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

(9)

describing elastic scattering of the continuum electrons on the average atom, considered as an impurity in the jellium sea. The corresponding elastic scattering cross section is given by $\sigma_{\text{el}}(\theta) = |f(\theta)|^2$. The transport cross section $\sigma_{\text{tr}}(p)$, which is important in determining the electric conductivity is given by

$$\sigma_{\text{tr}}(p) = \int (1 - \cos \theta) \sigma_{\text{el}}(\theta) d\Omega = \frac{4\pi}{p^2} \sum_{l=0}^{\infty} (l + 1) \sin^2 (\delta_{l+1} - \delta_l).$$

(10)

Classically, the conductivity of a plasma is given by the Drude formula

$$\sigma = \frac{\rho e^2}{m} \tau$$

(Drude Formula)

(11)

where $e$ and $m$ are the electron’s charge and mass. Here, $\rho$ is the electron density and $\tau$ is the relaxation time (mean time between collisions). The relaxation time $\tau_p$, which depends on the electron’s momentum $p$, is evaluated at the Fermi momentum and can be determined from the mean-free-path $\Lambda_p$ by $\tau_p = \Lambda_p/v$, where $v$ is the electron velocity. The mean-free-path is, in turn, related to the transport cross section $\sigma_{\text{tr}}(p)$ by $\Lambda_p = \Omega/\sigma_{\text{tr}}(p)$, where $\Omega$ is the
Fig. 3. Comparison of the static conductivity of an Al plasma at $T = 20,000$ K calculated using the average-atom Ziman formula with experimental results from Benage, Shanahan, and Murillo (BSM) [6], DeSilva and Katsouros (D&K) [7], and Krisch and Kunze (K&K) [8].

the volume per scattering center. The Ziman formula [5],

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

provides a generalization of the Drude formula based on arguments from kinetic theory. Inasmuch as the relaxation time $\tau_p$ for an average atom can be determined directly in terms of average-atom phase shifts, the Ziman formula gives the static conductivity of a plasma within the average-atom framework. In Fig. 3, we compare average-atom calculations of the conductivity of an aluminum plasma at $T = 20,000$ °K and densities ranging from 0.01 to 3 gm/cc with experimental measurements from Refs. [6,7,8]. The theoretical conductivity in qualitative agreement with experiment but differs by as much as an order of magnitude near the center of the plot.

2  Kubo-Greenwood Formula (Infrared Catastrophe)

The linear response of an average atom to an applied time-dependent electric field $\mathbf{E}(t) = F \hat{z} \sin \omega t$ leads to an average-atom version of the Kubo-Greenwood formula [9,10,11] for the frequency-dependent conductivity $\sigma(\omega)$. 
We describe the field by the vector potential

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

leading to the following time-dependent Schrödinger equation for electron orbitals:

\[ \left[ T_0 + V(r) - \frac{eF}{\omega} v_z \cos \omega t \right] \psi_i(r, t) = i \frac{\partial}{\partial t} \psi_i(r, t). \]  \hspace{1cm} (13)

We seek a solution to Eq. (13) in the form

\[ \psi_i(r, t) = u_i(r) e^{-i \epsilon_i t} + w^+_i(r) e^{-i(\epsilon_i + \omega)t} + w^-_i(r) e^{-i(\epsilon_i - \omega)t}, \]

where \( u_i(r) \) is a solution to the time-independent average-atom equation (1) and where \( w^\pm_i(r) \) are small perturbations. We find

\[ [T_0 + V(r)] u_i(r) = \epsilon_i u_i(r) \]  \hspace{1cm} (14)

\[ [T_0 + V(r) - (\epsilon_i \pm \omega)] w^\pm_i(r) = \frac{eF}{2\omega} v_z u_i(r). \]  \hspace{1cm} (15)

In writing these equations, we ignore the modification of the potential \( V(r) \) induced by the field. Next, we expand the perturbed orbital as in terms of unperturbed eigenfunctions as:

\[ w^+_i(r) = \sum_j X^j_i u_j(r), \quad w^-_i(r) = \sum_j Y^j_i u_j(r). \]  \hspace{1cm} (16)

From (15), we find

\[ X^j_i = \frac{eF}{2\omega} \frac{\langle j | v_z | i \rangle}{\epsilon_j - i \eta - \epsilon_i - \omega}, \quad Y^j_i = \frac{eF}{2\omega} \frac{\langle j | v_z | i \rangle}{\epsilon_j - i \eta - \epsilon_i + \omega}. \]  \hspace{1cm} (17)

The current associated with the perturbed atom is

\[ J_z(t) = 2e \sum_i f_i \langle \psi_i(t) | v_z | \psi_i(t) \rangle \]

\[ = 2e \sum_i f_i \left[ \left( \langle u_i | v_z | w^+_i \rangle + \langle w^-_i | v_z | u_i \rangle \right) e^{-i\omega t} + \text{c.c.} \right]. \]  \hspace{1cm} (18)

In the above equation \( \Omega \) is the volume/atom. The function \( f_i \) is the Fermi distribution function for state \( i \) which accounts for the initial state occupation in the average atom. The response current may be rewritten in terms of the expansion coefficients as

\[ J_z(t) = 4e \sum_{ij} f_i \left[ \mathcal{R} \left( \langle i | v_z | j \rangle X^j_i + \langle j | v_z | i \rangle Y^j_i \right) \cos \omega t \right. \]

\[ + \mathcal{I} \left( \langle i | v_z | j \rangle X^j_i + \langle j | v_z | i \rangle Y^j_i \right) \sin \omega t \]. \]  \hspace{1cm} (19)
The conductivity is determined by that part of the current $J_{in}$ that is in phase with the driving field, which is given by

$$J_{in}(t) = \frac{4e}{\Omega} \sum_{ij} f_i \Im \left( \langle i|v_z|j \rangle X_i^j + \langle j|v_z|i \rangle Y_i^j \right) \sin \omega t, \quad (20)$$

The out-of-phase part of the current corresponds to a “reactive” response that does not dissipate energy. One finds that

$$\Im \left( \langle i|v_z|j \rangle X_i^j + \langle j|v_z|i \rangle \right) = e^F \frac{2}{\omega} \sum_j \left( \pi \delta(\epsilon_j - \epsilon_i - \omega) \langle i|v_z|j \rangle^2 - \pi \delta(\epsilon_j - \epsilon_i + \omega) \langle j|v_z|i \rangle^2 \right). \quad (21)$$

Interchanging indices $i \leftrightarrow j$ in second term leads to $J_{in}(t) = \sigma(\omega) E_z(t)$ with

$$\sigma(\omega) = \frac{2\pi e^2}{\omega \Omega} \sum_{ij} (f_i - f_j) \left| \langle j|v_z|i \rangle \right|^2 \delta(\epsilon_j - \epsilon_i - \omega). \quad (22)$$

Eq.(22) is an average-atom version of the Kubo-Greenwood (KG) formula. Contributions to the KG formula arise from bound-bound, bound-free, and free-free transitions from initial states $i$ to final states $j$. The bound-bound and bound-free transitions are regular for all values of $\omega$; however, the free-free contributions, which are dominant at low frequencies, diverge as $1/\omega^2$, as will be shown in the following paragraph.

The matrix element appearing in Eq.(22) when taken between free-particle states vanishes unless the initial-state and final-state momenta are identical:

$$\langle p_2|v_z|p_1 \rangle = \delta(p_2 - p_1) v_z. \quad (23)$$

By contrast, the matrix element of $v_z$ between continuum states in a potential $V(r)$ is inversely proportional to the energy difference $E_2 - E_1 = \omega$. Thus, considering $V(r)$ in lowest-order perturbation theory, one easily shows that

$$\langle p_2|v_z|p_1 \rangle \rightarrow -\frac{1}{m\omega} q_z V(q), \quad (24)$$

where $q = p_2 - p_1$ is the momentum transfer between initial and final states. With the aid of the relation between scattering amplitude and potential in lowest-order perturbation theory (Born approximation),

$$f(\theta) = -\frac{m}{2\pi} V(q), \quad (25)$$

one can rewrite the dipole matrix element between continuum states in a potential in terms of the scattering amplitude as

$$\langle p_2|v_z|p_1 \rangle = \frac{2\pi}{m^2 \omega} q_z f(\theta). \quad (26)$$
3 "Proper" Static Limit & Conductivity Sum Rule

Squaring the dipole matrix element in Eq. (26), and averaging over directions, we obtain

$$\langle \langle p_2 \mid v_z \mid p_1 \rangle \rangle^2 = \frac{2 (2\pi)^2}{3 m^3 \omega^2} p^2 (1 - \cos \theta) \sigma_{el}(\theta).$$  \hspace{1cm} (27)

where

$$f_1 - f_2 \approx -\omega \frac{\partial f}{\partial E}.$$  \hspace{1cm} (28)

This leads to the following approximation for the free-free contribution to the conductivity

$$\sigma(\omega) \approx \frac{2 e^2}{3 \omega^2 \Omega} \int \frac{d^3 p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^3 \sigma_{tr}(p)$$

$$= \frac{2 e^2}{3} \int \frac{d^3 p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^3 \frac{1}{\omega^2 \tau_p},$$  \hspace{1cm} \text{(Low-Freq K-G formula)} \hspace{1cm} (29)

which diverges as $1/\omega^2$. In Fig. 5, this low-frequency approximation (shown in the red line) is seen to be in excellent agreement with numerical calculations based on Eq. (22) (shown in the black line) over the entire range of frequencies where either contributes. It is interesting to note the similarities between the
Fig. 5. The free-free contribution to the KG equation (black line) is compared with its low-frequency approximation (red line). The modified expression for the free-free part of the KG equation is shown in the blue line.

The low-frequency approximation (29) and the Ziman formula (12): The factor $\tau_p$ in the Ziman formula is replaced by $1/(\omega^2 \tau_p)$ in the low-frequency KG formula.

The resolution of the differences between the low-frequency approximation to the KG formula and the Ziman formula was discussed in detail in [13] so an heuristic discussion should suffice here. First, we note that the asymptotic behavior of the average atom scattering wave function is modified from a plane wave $\exp[i(\mathbf{p} \cdot \mathbf{r} - Et)]$ to a damped plane wave $\psi(\mathbf{p}, t) \rightarrow \exp[i(\mathbf{p} \cdot \mathbf{r} - Et) - t/\tau_p]$ when multiple scattering is considered. The effect of this modification is that the factor $1/\omega$ in the free-free dipole matrix element Eq. (24) is replaced by

$$\frac{1}{\omega} \rightarrow \frac{1}{\omega - i\tau_p}. \quad (30)$$

With this in mind, the low-frequency KG formula becomes

$$\sigma(\omega) \rightarrow \frac{2e^2}{3} \int \frac{d^3p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) \frac{\psi^2}{\omega^2 \tau_p^2 + 1}. \quad (\text{Modified KG Formula}) \quad (31)$$

This modified KG formula reduces to the Ziman formula for $\omega \ll 1/\tau_p$ and to the low-frequency KG formula when $\omega \gg 1/\tau_p$. Thus, for “super-low” frequencies, those much smaller than the inverse relaxation time, the modified KG formula reduces to the expected Ziman limit. Fig. 5 compares the modified KG formula (blue line) with the KG formula (black line) and its low-frequency limit (red line).

The modified KG formula for the free-free contribution to the conductivity
Fig. 6. Contributions to the frequency-dependent conductivity of an Al plasma $(T = 5 \text{ eV}, \text{density } 0.27 \text{ gm/cc})$. Lower left: free-free contribution; upper left: bound-bound contribution; upper right: bound-free contribution; lower right: resultant conductivity $\sigma(\omega)$.

satisfies the conductivity sum rule

$$\int_{0}^{\infty} \sigma(\omega) d\omega = \frac{\pi e^2}{3} \int \frac{d^3p}{(2\pi)^3} v^2 \left( -\frac{\partial f}{\partial E} \right) = \frac{e^2 \pi}{m} \int \frac{d^3p}{(2\pi)^3} f(E) = \frac{e^2 \pi}{2m} Z^*, \quad (32)$$

where $Z^*$ is the background ionic charge. In Fig. 6, we show the three contributions to the frequency-dependent conductivity $\sigma(\omega)$, from free-free transitions, bound-bound transitions and bound-free transitions for aluminum at $T = 5 \text{ eV}$, and density $0.27 \text{ gm/cc}$.

4 Application to Plasma Optics

On general grounds of causality, one may infer the imaginary part of the dielectric function from its real part using a Kramers-Kronig (KK) dispersion relation $[14,15,16,17]$. Owing to the close connection between the frequency-dependent conductivity and the dielectric function, the real and imaginary parts of the complex conductivity also satisfy a KK dispersion relation. This is particularly useful here since it permits us to obtain the imaginary part
of the conductivity by a rather simple calculation. Moreover, because of the close connection between the conductivity and the dielectric function, we can obtain the later directly. Once we have the dielectric function in hand, the optical properties of plasmas are completely characterized.

Given that \( \sigma(\omega) \) is an even function of \( \omega \) that is analytic in the upper half plane and falls faster than \( 1/\omega \) for large \( \omega \), we may write

\[
\Im \sigma(\omega_0) = -\frac{2\omega_0}{\pi} \int_0^\infty \frac{\Re \sigma(\omega)}{\omega^2 - \omega_0^2} d\omega. \tag{33}
\]

Applying this equation to the modified K-G formula for \( \Re \sigma(\omega) \), we find

\[
\Im \sigma(\omega) = 2e^2 \frac{2}{3} \int \frac{d^3p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^2 \frac{\omega \tau_p}{\omega^2 \tau_p^2 + 1}. \tag{34}
\]

This leads to the following expression for free-free contribution to the complex conductivity \( \sigma(\omega) \) as an analytic function of \( \omega \),

\[
\sigma(\omega) = 2e^2 \frac{2}{3} \int \frac{d^3p}{(2\pi)^3} \left( -\frac{\partial f}{\partial E} \right) v^2 \frac{\tau_p}{1 - i\omega \tau_p}. \tag{35}
\]

Contributions to \( \Im \sigma(\omega) \) from bound-bound and bound-free contributions are obtained from Eq.(33) by numerical integration. In Fig. 7, we plot real and imaginary parts of \( \sigma(\omega) \) for an Al plasma \( T = 5 \) eV and density 0.27 gm/cc.

The (complex) plasma dielectric function is given in terms of the conductivity by

\[
\epsilon_\infty(\omega) = 1 + 4\pi i \frac{\sigma(\omega)}{\omega}. \tag{36}
\]
Fig. 8. Real and imaginary parts of the complex index of refraction \( n(\omega) \) and \( \kappa(\omega) \) for Al at 10 eV and metallic density compared with their free-particle counterparts \( n_{\text{free}}(\omega) \) and \( \kappa_{\text{free}}(\omega) \).

We introduce the complex index of refraction \( n + i\kappa \) through the equation
\[
n(\omega) + i\kappa(\omega) = \sqrt{\epsilon_r(\omega)}.
\]  
(37)

It follows that
\[
n(\omega) = \sqrt{\frac{\sqrt{[\Re \epsilon(\omega)]^2 + [\Im \epsilon(\omega)]^2} + \Re \epsilon(\omega)}{2}}
\]  
(38)
\[
\kappa(\omega) = \sqrt{\frac{\sqrt{[\Re \epsilon(\omega)]^2 + [\Im \epsilon(\omega)]^2} - \Re \epsilon(\omega)}{2}}.
\]  
(39)

The two functions \( n(\omega) \) and \( \kappa(\omega) \) are illustrated in Fig. 8, where they are plotted for the case of Al at \( T = 5 \) eV and density 0.27 gm/cc.

The classical free-electron expression for \( \epsilon_r(\omega) \) is
\[
\epsilon_r(\omega) = 1 - \frac{\omega_0^2}{\omega^2}
\]
where \( \omega_0 \) is the plasma frequency \( \omega_0^2 = 4\pi e^2 \rho_0/m \). It follows that at low frequencies \( \omega < \omega_0 \), \( n_{\text{free}} = 0 \), while for \( \omega > \omega_0 \), \( \kappa_{\text{free}} = 0 \). In Fig. 8, we compare the average-atom results for \( n(\omega) \) and \( \kappa(\omega) \) with the free-electron approximation for aluminum at \( T = 5 \) eV and density 0.27 eV.

Instances where \( n > 1 \), which are forbidden in the free-electron model, have been observed in interferograms of an Al plasma produced by a 14.7 nm Ni-like Pd soft x-ray laser at the Lawrence Livermore National Laboratory comet laser facility [18]. Similar anomalies were observed in interference patterns of an Al plasma produced by a 13.9 nm Ni-like Ag laser at the Advanced
Fig. 9. The ratio of \(n(\omega) - 1\) to \(n_{\text{free}} - 1\) for Al at ion density \(10^2 0/\text{cc}\). The ratio is negative at the frequencies of Ni and Ag lasers explaining the effects of anomalous dispersion observed in experiments \([18]\) and \([19]\).

The free-electron model leads to the conclusion that the square of the plasma frequency \(\omega^2\) is negative! In Ref. \([19]\) this behavior was correctly attributed to the \(2p - 3d\) transition in Al\(^{+2}\). To examine such anomalous dispersion in terms of the average-atom model, we compare \(n(\omega) - 1\) predicted by the average-atom model with its free electron counterpart \(n_{\text{free}} - 1\) in Fig. 9. The number of free electrons per ion from the average-atom model is \(Z^* = 1.38\) for the density and temperature illustrated. As can be seen in the figure, the ratio is near \(-2\) in a band of photon energies that includes those of the Pd and Ag lasers, which are indicated by the dashed lines at 84 and 89 eV. This explains the behavior seen experimentally. The primary effect on the dispersion integral in this region comes from \(2p - 2s\) and \(2p - 3d\) transitions and from photoionization of the \(2p\) subshell (threshold at 80.2 eV).

5 Conclusion

In conclusion, the Kubo-Greenwood formula for \(\sigma(\omega)\) applied to the average-atom model diverges as \(1/\omega^2\) at low frequencies. Including multiple scattering (finite relaxation time) leads to a modified version of the KG formula for the free-free contribution to \(\sigma(\omega)\) that is finite and reduces to the static Ziman formula at \(\omega = 0\). The Kubo-Greenwood formula modified at low frequencies provides a useful approximation for studies of the optical properties of plasmas.
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References


