Low Frequency Plasma Conductivity in the Average-Atom Approximation

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1. Review of Average-Atom Linear Response Theory
2. Demonstration of a low-frequency divergence in $\sigma(\omega)$
3. Finite relaxation time and resolution of problem

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Average-Atom Model of a Plasma

Plasma composed of neutral spheres with Wigner-Seitz radius $R = (3\Omega_0/4\pi)^{1/3}$ floating in a "jellium" sea.

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

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

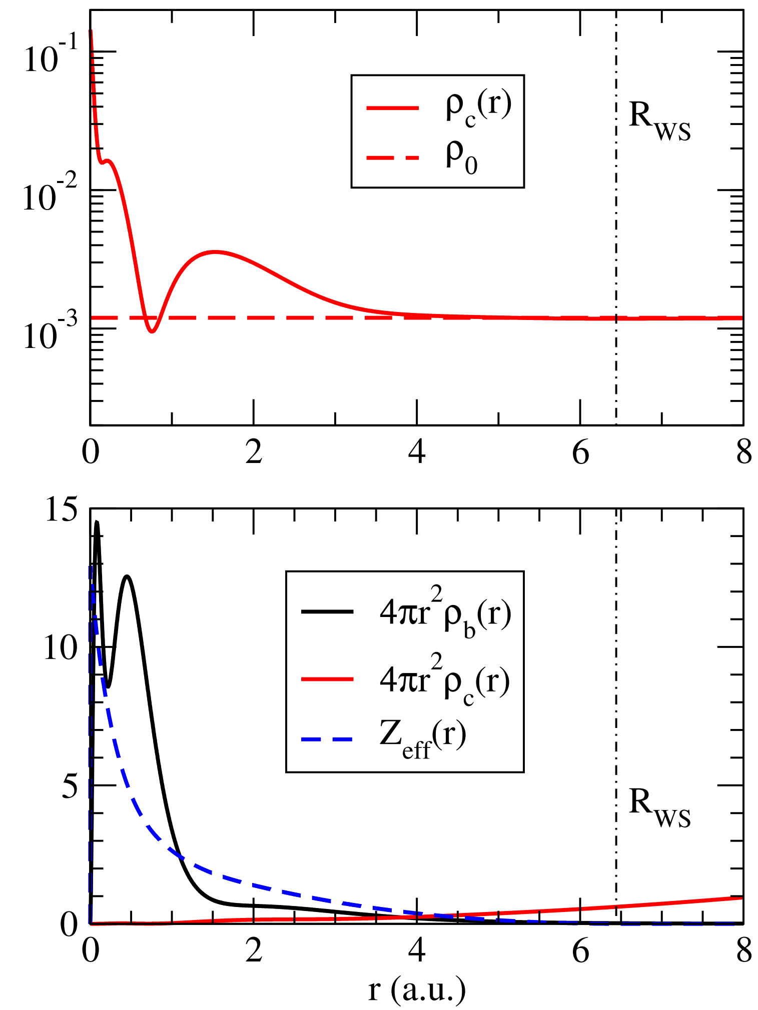
$$4\pi r^2 \rho(r) = \sum_{nl} \frac{2(2l+1)}{1 + \exp[(\epsilon_{nl} - \mu)/kT]} P_{nl}(r)^2$$

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

Example

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



10^{-1}
10^{-2}
10^{-3}
$\rho_c(r)$
ρ_0
R_{WS}
0
2
4
6
8
15
10
5
0
$4\pi r^2 \rho_b(r)$
$4\pi r^2 \rho_c(r)$
$Z_{eff}(r)$
R_{WS}
0
2
4
6
8
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:

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

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

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

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

Infrared "Catastrophe" in Scattering

$$H_1 = V(r) - \frac{e}{mc}\,(\boldsymbol{\epsilon}\cdot\boldsymbol{p})\,e^{-i\omega t}$$

$$T_{21} = 2\pi i\,\delta(E_2 - E_1 - \omega)\,\left(\frac{e}{mc}\right)\left[\langle p_2|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|p_1\rangle - \sum_n \frac{\langle p_2|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|n\rangle\langle n|V|p_1\rangle}{E_n - E_1} - \sum_n \frac{\langle p_2|V|n\rangle\langle n|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|p_1\rangle}{E_n - E_1 - \omega} + \cdots\right]$$

Infrared "Catastrophe" in Scattering

$$H_1 = V(r) - \frac{e}{mc}\,(\boldsymbol{\epsilon}\cdot\boldsymbol{p})\,e^{-i\omega t}$$

$$\begin{aligned}
T_{21} = 2\pi i\,\delta(E_2 - E_1 - \omega)\,\left(\frac{e}{mc}\right)\Bigg[&\langle p_2|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|p_1\rangle \\
&- \sum_n \frac{\langle p_2|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|n\rangle\langle n|V|p_1\rangle}{E_n - E_1} - \sum_n \frac{\langle p_2|V|n\rangle\langle n|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|p_1\rangle}{E_n - E_1 - \omega} + \cdots\Bigg] \\
= 2\pi i\,\delta(E_2 - E_1 - \omega)\,\left(\frac{e}{mc}\right)\Bigg[&-\frac{1}{\omega}\boldsymbol{\epsilon}\cdot\boldsymbol{q}\ \langle p_2|V|p_1\rangle + \cdots\Bigg]
\end{aligned}$$

Low-Frequency Theorem (QED)

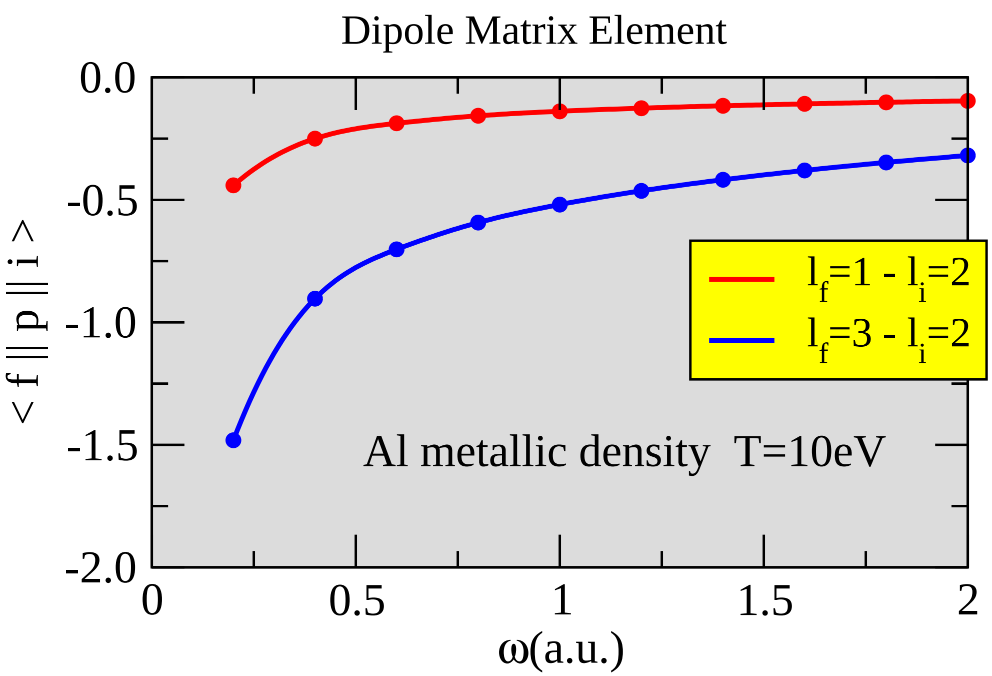
$$\langle p_2|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|p_1\rangle \rightarrow -\frac{1}{\omega}(\boldsymbol{\epsilon}\cdot\boldsymbol{q})\ V(q)$$

Relation between scattering amplitude and potential (Born approximation)

$$f_{\mathsf{el}}(\theta) = -\frac{m}{2\pi}V(q)$$

$$\boxed{\langle p_2|\boldsymbol{\epsilon}\cdot\boldsymbol{p}|p_1\rangle \rightarrow \frac{2\pi}{m\omega}\ (\boldsymbol{\epsilon}\cdot\boldsymbol{q})\ f_{\mathsf{el}}(\theta)}$$

Example of Dipole Matrix Elements



Low-Frequency Kubo-Greenwood

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

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

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

Low-Frequency Kubo-Greenwood

$$\sigma(\omega) \approx \frac{2\pi e^2}{\Omega} \frac{2}{3} \frac{(2\pi)^2}{m^4\omega^2} \iint \frac{d^3p_1}{(2\pi)^3} \frac{d^3p_2}{(2\pi)^3} \left(-\frac{\partial f}{\partial E}\right) \times$$
$$p_1^2(1-\cos\theta)\,\sigma_{\mathsf{el}}(\theta)\delta(E_2 - E_1 - \omega)$$

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

where

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

Low-Frequency KG Formula

$$\frac{1}{\Lambda_p} = \frac{\sigma_{\text{tr}}(p)}{\Omega} \qquad \tau_p = \frac{\Lambda_p}{v} = \frac{\Omega}{v\sigma_{\text{tr}}(p)}$$

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

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

Rule: K-G formula reduces to Ziman formula under replacement $1/(\omega^2\tau_p) \longrightarrow \tau_p$

Influence of Collisions

$$\psi(\boldsymbol{p}, t) \to \exp\left[i\left(\boldsymbol{p}\cdot\boldsymbol{r} - Et\right) - \frac{\Gamma_p}{2}t\right]$$

where

$$\frac{\Gamma_p}{2} = \frac{1}{\tau_p}$$

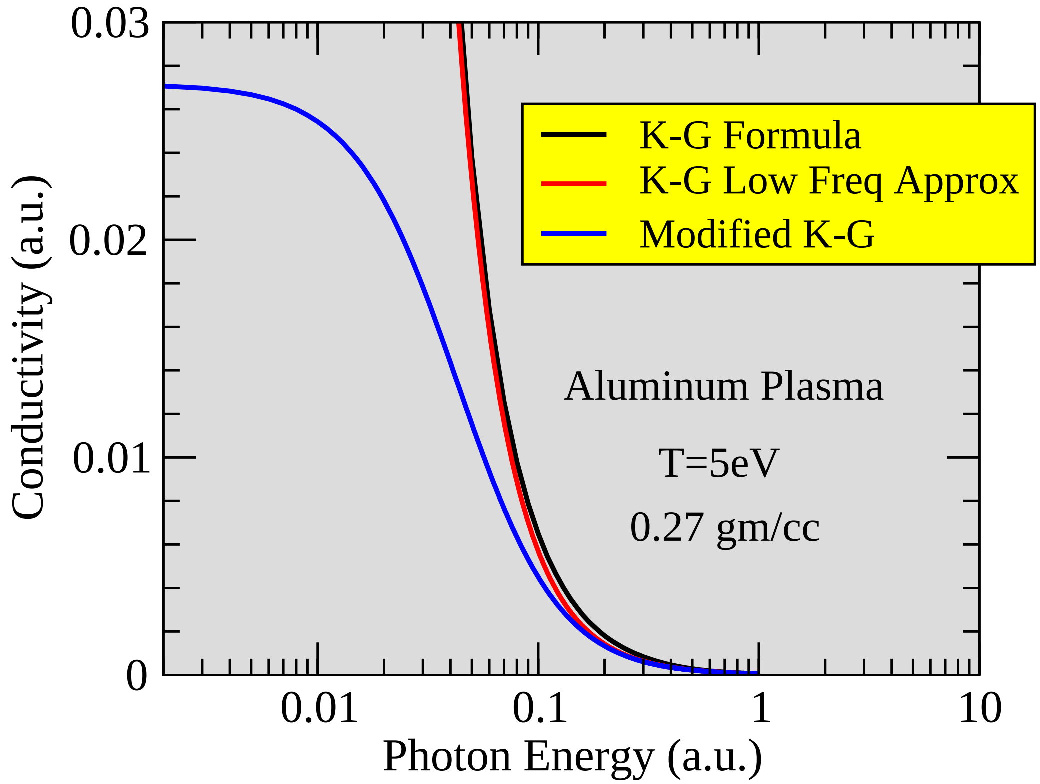
Effect:

$$\frac{1}{(\Delta E)^2} \to \frac{1}{(\Delta E)^2 + \Gamma_p^2/4} = \frac{1}{\omega^2 + 1/\tau_p^2}$$

With this in mind, the Modified KG Formula becomes

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

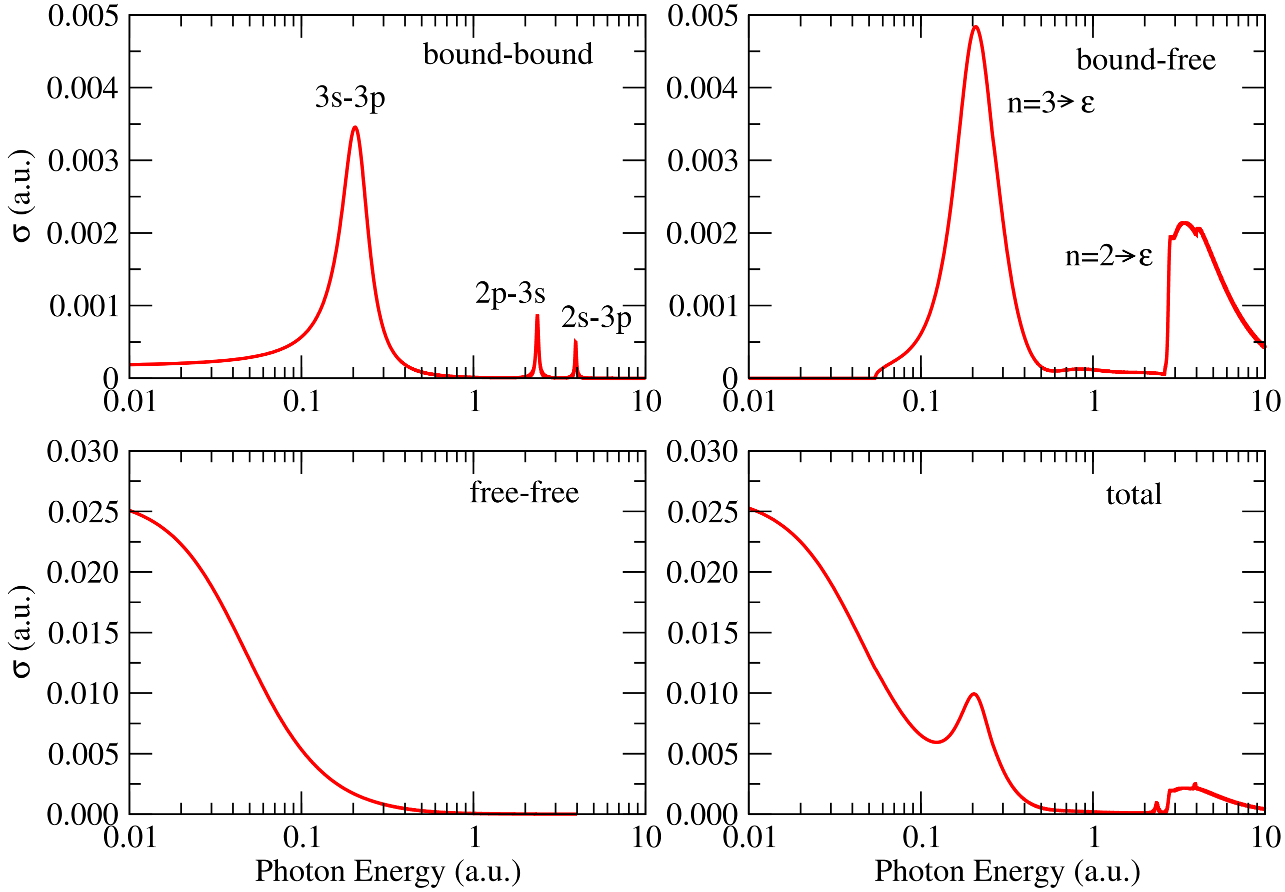
Comparison of Conductivity Formulas



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 KG 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 $\text{Re}[\sigma(\omega)]$ 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

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

Alternatively,

$$\text{Re}[\epsilon_r(\omega)] = 1 - 4\pi \frac{\text{Im}[\sigma(\omega)]}{\omega} \qquad \text{Im}[\epsilon_r(\omega)] = 4\pi \frac{\text{Re}[\sigma(\omega)]}{\omega}$$

Index of Refraction:

$$n(\omega) + i\kappa(\omega) = \sqrt{\epsilon_r(\omega)}$$

Reflection Coefficient:

$$R(\omega) = \left| \frac{1 - n(\omega) - i\kappa(\omega)}{1 + n(\omega) + i\kappa(\omega)} \right|^2$$

Applications

With Joe Nilsen

Conclusions

- Linear response theory applied to the average-atom model of a plasma leads to a version of the Kubo-Grenwood formula for conductivity.

- The resulting formula has a second-order pole at $\omega = 0$.

- Including finite relaxation time in the time dependence of scattering wave function replaces pole by "Drude" type energy denominator.

- Evaluating the relaxation time using phase shifts from the AA model lead to the Ziman formula at $\omega = 0$.