A Simple Derivation of Some Sum Rules for the Powers of the Optical Constants of Insulators.

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Summary. – In the present paper some of the most widely used sum rules for optical constants of insulators are derived by a simple way compared to earlier versions. Also some new sum rules are presented.

ALTARELLI *et al.* ([1]) (hereafter fererred as to ADNS) have given sum rules for optical constants which are of importance when testing the consistency of theory and experiments. ALTARELLI and SMITH ([2]) (hereafter referred to as AS) have given more general sum rules involving the powers of the optical constants. The derivation of the ADNS and AS rules was based on the super convergence theorem ([1]) which involves profound results of function theory. KING ([3]) has given quite elegantly some sum rules of ADNS and AS as well as those of Villani and Zimerman ([4]) deriving them from the Kramers-Kroning relations ([5]) with the aid of Dirac's delta function. The derivation of King is based on the interchange of the order of integration involved in the Kramers-Kronig relations. The integration domain is the whole spectral range. This interchange of the integration order is not always allowed, however.

In this paper we sketch a simple alternative formulation for most of the ADNS and AS sum rules. This formulation is based on subtracting the Kramers-Kronig relations for the powers of the optical constants.

The complex refractive index $N(\omega) = n(\omega) + ik(\omega)$ is an analytic function in the upper half of complex angular frequency plane. n is the real refractive index and k is the extinction coefficient of the insulator, respectively (sum rules also for metals can

([1]) M. ALTARELLI, D. L. DEXTER, H. M. NUSSENZVEIG and D. Y. SMITH: *Phys. Rev. B*, **6**, 4502 (1972).
([2]) M. ALTARELLI and D. Y. SMITH: *Phys. Rev. B*, **9**, 1290 (1974).
([3]) F. W. KING: *J. Math. Phys.* (*N. Y.*), **17**, 1509 (1976).
([4]) A. VILLANI and A. H. ZIMERMAN: *Phys. Rev. B*, **8**, 3914 (1973).
([5]) L. D. LANDAU and E. M. LIFSHITZ: *Electrodynamics of Continuous Media* (Addison-Wesley, Reading, Mass., 1960).

be easily given). As stated by ALTARELLI and SMITH the Titchmarsh's theorem [6] yields the Kramers-Kronig relations also for the powers $(N(\omega)-1)^m$ and $\omega^m(N(\omega)-1)^m$ as follows:

$$(1)\quad \left\{\begin{aligned} &\mathrm{Re}\,(N(\omega')-1)^m = \frac{2}{\pi}\,P\int_0^\infty \frac{\omega\,\mathrm{Im}\,(N(\omega)-1)^m}{\omega^2-\omega'^2}\,\mathrm{d}\omega\,,\\ &\mathrm{Im}\,(N(\omega)')-1)^m = -\frac{2\omega'}{\pi}\,P\int_0^\infty \frac{\mathrm{Re}\,(N(\omega)-1)^m}{\omega^2-\omega'^2}\,\mathrm{d}\omega \end{aligned}\right.$$

and

$$(2)\quad \omega'^m\,\mathrm{Re}\,(N(\omega')-1)^m = \begin{cases} \dfrac{2\omega'}{\pi}\,P\displaystyle\int_0^\infty \frac{\omega^m\,\mathrm{Im}\,(N(\omega)-1)^m}{\omega^2-\omega'^2}\,\mathrm{d}\omega\,, & m \text{ odd}\,,\\ \dfrac{2}{P}\,P\displaystyle\int_0^\infty \frac{\omega^{m+1}\,\mathrm{Im}\,(N(\omega)-1)^m}{\omega^2-\omega'^2}\,\mathrm{d}\omega\,, & m \text{ even}\,, \end{cases}$$

also

$$(3)\quad \omega'^m\,\mathrm{Im}\,(N(\omega')-1)^m = \begin{cases} -\dfrac{2}{\pi}\,P\displaystyle\int_0^\infty \frac{\omega^{m+1}\,\mathrm{Re}\,(N(\omega)-1)^m}{\omega^2-\omega'^2}\,\mathrm{d}\omega\,, & m \text{ odd}\,,\\ -\dfrac{2\omega'}{\pi}\,P\displaystyle\int_0^\infty \frac{\omega^m\,\mathrm{Re}\,(N(\omega)-1)^m}{\omega^2-\omega'^2}\,\mathrm{d}\omega\,, & m \text{ even} \end{cases}$$

where Re stands for the real part, Im for the imaginary part and P denotes the Cauchy' principal value.

It is no lack of generality to choose $\omega'=\omega_0$, where ω_0 is the zero of $n(\omega)-1$, *i.e.* $n(\omega_0)-1=0$. This choice gives among the others (ANDS rules) as far as the author knows also some new sum rules. Now we can write the relations

$$(4)\quad -\frac{2\omega_0}{\pi}\,P\int_0^\infty \frac{\mathrm{Re}\,(N(\omega)-1)^m}{\omega^2-\omega_0^2}\,\mathrm{d}\omega = \begin{cases} 0\,, & m \text{ even}\,,\\ -k^m(\omega_0)\,, & m=3,7,\ldots,\\ -k^m(\omega_0)\,, & m=1,5,\ldots. \end{cases}$$

When $m=1$ one obtains the familiar triviality of Kramers-Kronig relations. As $m=2$ there holds the sum rule

$$(5)\quad P\int_0^\infty \frac{(n(\omega)-1)^2}{\omega^2-\omega_0^2}\,\mathrm{d}\omega = P\int_0^\infty \frac{k^2(\omega)}{\omega^2-\omega_0^2}\,\mathrm{d}\omega\,.$$

[6] H. M. NUSSENZVEIG: *Causality and Dispersion Relations* (Academic Press, New York, N. Y., 1972).

Further, we can write

$$\frac{2}{\pi}\,\mathrm{P}\!\int_0^\infty \frac{\omega\,\mathrm{Im}\,(N(\omega)-1)^m}{\omega^2-\omega_0^2}\,\mathrm{d}\omega = \begin{cases} 0\,, & m \text{ odd}\,,\\ -k^m(\omega_0)\,, & m=2,6,\ldots,\\ k^m(\omega_0)\,, & m=4,8\ldots \end{cases} \tag{6}$$

and

$$\begin{cases} \dfrac{-2\omega_0}{\pi}\,\mathrm{P}\!\displaystyle\int_0^\infty \frac{\omega^m\,\mathrm{Re}\,(N(\omega)-1)^m}{\omega^2-\omega_0^2} = 0\,, & m \text{ even}\,,\\ -\dfrac{2}{\pi}\,\mathrm{P}\!\displaystyle\int_0^\infty \frac{\omega^{m+1}\,\mathrm{Re}\,(N(\omega)-1)^m}{\omega^2-\omega_0^2} = \begin{cases} \omega_0^m k^m(\omega_0)\,, \\ -\omega_0^m k^m(\omega_0)\,, \end{cases} & \begin{matrix} m=1,5,\ldots,\\ m=3,7,\ldots. \end{matrix} \end{cases} \tag{7}$$

Also

$$\begin{cases} \dfrac{2\omega_0}{\pi}\,\mathrm{P}\!\displaystyle\int_0^\infty \frac{\omega^m\,\mathrm{Im}\,(N(\omega)-1)^m}{\omega^2-\omega_0^2}\,\mathrm{d}\omega = 0\,, & m \text{ odd}\,,\\ \dfrac{2}{\pi}\,\mathrm{P}\!\displaystyle\int_0^\infty \frac{\omega^{m+1}\,\mathrm{Im}\,(N(\omega)-1)^m}{\omega^2-\omega_0^2}\,\mathrm{d}\omega = \begin{cases} -\omega_0^m k^m(\omega_0)\,, \\ \omega_0^m k^m(\omega_0)\,, \end{cases} & \begin{matrix} m=2,6,\ldots,\\ m=4,8,\ldots. \end{matrix} \end{cases} \tag{8}$$

We now make use of eqs. (4) and (7). If $m=2$ one can write

$$\frac{2\omega_0}{\pi}\,\mathrm{P}\!\int_0^\infty \frac{\omega^2\,\mathrm{Re}\,(N(\omega)-1)^2}{\omega^2-\omega_0^2}\,\mathrm{d}\omega - \frac{2\omega_0^3}{\pi}\,\mathrm{P}\!\int_0^\infty \frac{\mathrm{Re}\,(N(\omega)-1)^2}{\omega^2-\omega_0^2}\,\mathrm{d}\omega = 0\,, \tag{9}$$

which reduces to

$$\int_0^\infty (n(\omega)-1)^2\,\mathrm{d}\omega = \int_0^\infty k^2(\omega)\,\mathrm{d}\omega \tag{10}$$

as given by ADNS. We can proceed by multiplying the relation of eq. (4) by the appropriate even power of ω_0 and subtracting the relation given by eq. (7) from the new relation obtained by multiplying.

A recurrence formula can be also given, but it is more instructive to proceed step by step. For odd m we can write with the aid of eqs. (4) and (7) when $m=1$

$$\frac{2}{\pi}\,\mathrm{P}\!\int_0^\infty \frac{\omega^2\,\mathrm{Re}\,(N(\omega)-1)}{\omega^2-\omega_0^2}\,\mathrm{d}\omega - \frac{2}{\pi}\,\mathrm{P}\!\int_0^\infty \frac{\omega_0^2\,\mathrm{Re}\,(N(\omega)-1)}{\omega^2-\omega_0^2}\,\mathrm{d}\omega = 0\,. \tag{11}$$

This leads to the glorious sum rule of Altarelli *et al.*

$$\int_0^\infty (n(\omega)-1)\,\mathrm{d}\omega = 0\,. \tag{12}$$

When $m = 3$ one obtains

$$\int_0^\infty (\omega^2 + \omega_0^2)\,\mathrm{Re}\,(N(\omega) - 1)^3\,\mathrm{d}\omega = 0\,.$$

This gives the AS sum rules

$$\left\{\begin{aligned}&\int_0^\infty \omega^2\,\mathrm{Re}\,(N(\omega) - 1)^3\,\mathrm{d}\omega = 0\,,\\&\int_0^\infty \mathrm{Re}\,(N(\omega) - 1)^3\,\mathrm{d}\omega = 0\,.\end{aligned}\right. \tag{13}$$

The procedure can be continued as is obvious.

Next we will make use of eqs. (6) and (8). Let us choose $m = 5$ whence

$$\frac{2\omega_0}{\pi}\,P\!\int_0^\infty \frac{\omega^5\,\mathrm{Im}\,(N(\omega) - 1)^5}{\omega^2 - \omega_0^2}\,\mathrm{d}\omega - \frac{2}{\pi}\,P\!\int_0^\infty \frac{\omega\omega_0^5\,\mathrm{Im}\,(N(\omega) - 1)^5}{\omega^2 - \omega_0^2}\,\mathrm{d}\omega = 0\,. \tag{14}$$

This leads to the AS sum rule

$$\int_0^\infty \omega^3\,\mathrm{Im}\,(N(\omega) - 1)^5\,\mathrm{d}\omega = 0\,, \tag{15}$$

but also to a new sum rule

$$\int_0^\infty \omega\,\mathrm{Im}\,(N(\omega) - 1)^5\,\mathrm{d}\omega = 0\,. \tag{16}$$

Next set $m = 4$ and obtain the AS sum rule

$$\int_0^\infty \omega^3\,\mathrm{Im}\,(N(\omega) - 1)^4\,\mathrm{d}\omega = 0\,, \tag{17}$$

but also the new sum rule

$$\int_0^\infty \omega\,\mathrm{Im}\,(N(\omega) - 1)^4\,\mathrm{d}\omega = 0\,. \tag{18}$$

Sum rules for the powers of the optical constants are of importance because the integral of the sum rule converges the stronger the higher the power. In practical calculations this means that a narrow integration domain is enough for testing. Experimentally it is usually possible to measure the dispersion or absorption only for a limited frequency range, as is well known.