Superconvergent Sum Rules for the Optical Constants^{*}

A. Villani[†] and A. H. Zimerman Instituto de Fisica Teórica, São Paulo, Brazil (Received 5 February 1973)

Superconvergent sum rules are written for the optical constants of nonmagnetic materials. First a generalization of some results of Altarelli et aL is attained by means of the Liu and Okubo technique. In particular, we have a set of inequalities. Second, new superconvergent sum rules are obtained by considering suitable powers of the optical constants. They are characterized by strong damping for the high frequencies of the superconvergent sum rules. Sum rules involving higher powers of the electric conductivity are also indicated.

I. INTRODUCTION

Recently, Altarelli ${et}$ $al.$ 1 have discussed some interesting sum rules for the optical constants by procedures similar to those used in the high-energy elementary-particle physics. The purpose of the present work is twofold: first, to generalize the results of Altarelli $et al.$ ¹ by means of a procedur due to Liu and Okubo² used for the π -N scattering amplitude; second, to consider superconvergent sum rules which arise from the consideration of different powers of suitable combinations of the optical constants. Ferrari and Violini³ have recently written dispersion relations for the square of the π -N amplitude (and mentioned also the possibility of writing dispersion relations for powers of the π -N amplitude).

Now, contrary to the π -N amplitude, the optical constants $N(\omega) - 1$, $\epsilon(\omega) - 1$, etc., where $N(\omega)$ is the complex index of refraction and $\epsilon(\omega)$ is the dielectric permeability, for high frequencies $\omega \rightarrow \infty$, go as ω^{-2} and their m th power will go as ω^{-2m} giving us, therefore, the possibility of obtaining very strongly damped superconvergent sum rules.

In Sec. II we write the superconvergent relations and apply the Liu and Okubo 2 technique to the optical problem. Superconvergent sum rules are obtained as well as the corresponding inequalities.

In Sec. III we consider the superconvergent sum rules which follow from the different powers of suitable combinations of the optical constants. In particular, we obtain sum rules which are strongly damped. Suggestions are also made in order to avoid the difficulties which appear in some superconvergent sum rules for the case where the conductivity is different from zero.

Finally, sum rules involving higher powers of the conductivity are indicated.

II. SUPERCONVERGENCE RELATION-APPLICATION OF LIU-OKUBO TECHNIQUE

Let us consider a function $F(\omega)$ which is analytic in the upper-half ω plane (Im ω >0), which does not increase exponentially for $|\omega| \rightarrow \infty$ along any direction in the upper-half plane, and which for ω + ∞ behaves at least as

$$
\omega^{-1-\delta} \quad \text{or} \quad \omega^{-1} \ln^{-\alpha} \omega \,, \tag{1}
$$

with

$$
\delta > 0, \quad \alpha > 1 \,.
$$
 (2)

We shall assume that $F(\omega)$ has a dispersive as well as an absorptive part with definite crossing properties [see for instance Eq. (7) given below]. Therefore, for ω \rightarrow $-\infty$ we will have similar bounds as Eq. (1).

According to the theorem of Phragmen-Lindelöf, $F(\omega)$ will have a bound similar to Eq. (1) for $|\omega|$ $\rightarrow \infty$ in any direction of the upper-half ω plane.⁴

Now let us apply Cauchy's theorem to $F(\omega)$ by taking a contour consisting of the real axis and a semicircle in the upper-half ω plane centered at the origin with the radius $R \rightarrow \infty$. It is very simple to see that for the conditions Eq. (1), the contribution of the semicircle vanishes as long as $R \rightarrow \infty$ and we obtain the superconvergence relation

$$
\int_{-\infty}^{+\infty} F(\omega) \, d\omega = 0 \,. \tag{3}
$$

If $F(\omega)$ contains poles on the real axis in the integral of Eq. (3), we should avoid them by infinitesimal semicircles in the upper-half ω plane.

We will now obtain a whole class of sum rules for the refractive index of an isotropic material. For this purpose in analogy to Liu and Okubo, 2 let us consider the function

$$
S(\omega) = e^{i\pi\beta}/(\omega - a)^{\beta}(\omega + a)^{\beta}, \qquad (4)
$$

a being an arbitrary positive parameter and β a constant in the range

$$
-\frac{1}{2} < \beta < 1. \tag{5}
$$

The function $S(\omega)$ is analytic in the upper-half ω plane with cuts between $(-\infty, -a)$ and $(a, +\infty)$, being real in the interval $(-a, +a)$.

Introducing the complex refractive index $N(\omega)$ $=n(\omega)+ik(\omega)$ which for $\omega \rightarrow \infty$ behaves as $N(\omega) - 1$ $\rightarrow O(\omega^{-2})$, the function $S(\omega)[N(\omega) - 1]$ is analytic in the upper ω plane with the behavior given by Eq.

8

3914

 \mathbf{r}

or

(1) for $\omega \rightarrow \infty$, and, therefore, satisfies the superconvergence relation Eq. (3):

$$
\int_{-\infty}^{+\infty} S(\omega) \left[N(\omega) - 1 \right] d\omega = 0 \,. \tag{6}
$$

Using the crossing relations

$$
n(\omega) = n(-\omega), \quad k(\omega) = -k(-\omega), \tag{7}
$$

we obtain the sum rules

$$
\cos \pi \beta \int_{a}^{\infty} \frac{\left[n(\omega) - 1\right] d\omega}{(\omega - a)^{\beta} (\omega + a)^{\beta}} - \sin \pi \beta \int_{a}^{\infty} \frac{k(\omega) d\omega}{(\omega - a)^{\beta} (\omega + a)^{\beta}} + \int_{0}^{a} \frac{\left[n(\omega) - 1\right] d\omega}{(a - \omega)^{\beta} (\omega + a)^{\beta}} = 0. \quad (8)
$$

The special illustrative cases $\beta = 0$ and $\beta = \frac{1}{2}$ give, respectively

$$
\int_0^\infty \left[n(\omega) - 1 \right] d\omega = 0, \tag{9}
$$

which was already derived by Altarelli et al., 1 and

$$
\int_0^a \frac{\left[n(\omega) - 1\right] d\omega}{(a^2 - \omega^2)^{1/2}} = \int_a^\infty \frac{k(\omega) d\omega}{(\omega^2 - a^2)^{1/2}} \tag{10}
$$

which is a new result.

As $k(\omega) > 0$, from Eq. (10) we obtain the inequality

$$
\int_0^a \frac{\left[n(\omega) - 1\right]d\omega}{(a^2 - \omega^2)^{1/2}} > 0\tag{11}
$$

to be compared with Eq. (9).

More generally, for $0 < \beta < 1$, Eq. (8) gives the inequality

$$
\int_0^a \frac{\left[n(\omega)-1\right]d\omega}{(a-\omega)^{\beta}(\omega+a)^{\beta}} + \cos\pi\beta \int_a^{\infty} \frac{\left[n(\omega)-1\right]d\omega}{(\omega-a)^{\beta}(\omega+a)^{\beta}} > 0,
$$
\n(12)

while for $-\frac{1}{2} < \beta < 0$ the left-hand side of Eq. (12) is negative. Let us note that contrary to Liu and Okubo² which fix the point a at the pion mass, here we take it as an arbitrary positive parameter. We have therefore in Eq. (8) a doubly infinite set of sum rules with a taking positive values along the real axis and β subject to the condition Eq. (5).

III. SUPERCONVERGENT SUM RULES FOR POWERS OF OPTICAL CONSTANTS

Taking the complex index of refraction $N(\omega)$ $= n(\omega) + ik(\omega)$ for an isotropic nonmagnetic material, consider the square of the function $A(\omega) = N(\omega) - 1$.

As for $\omega \to \infty$, $A^2(\omega) \to O(\omega^{-4})$, we have from Eq. (3)

$$
\int_{-\infty}^{+\infty} A^2(\omega) \, d\omega = \int_{-\infty}^{+\infty} \left[(n-1)^2 - k^2 + 2ik(n-1) \right] d\omega = 0 \tag{13}
$$

where the singularity at the origin is avoided by an infinitesimal semicircle in the upper-half ω plane. With $(n+ik)^2 = \epsilon = \epsilon' + i\epsilon''$, it is well known that as $\omega \to 0$, $\epsilon'' \sim 4\pi\sigma(0)\omega^{-1}$, where $\sigma(0)$ is the electric conductivity at zero frequency for the material.

We observe in Eq. (13) that the singularity at $\omega = 0$ gives

$$
2i \int_{-\infty}^{+\infty} k(\omega) n(\omega) d\omega = 4\pi^2 \sigma(0)
$$

and, therefore, one obtains

$$
\int_0^\infty (n^2 - k^2 - 2n + 1) \, d\omega = -\, 2\pi^2 \sigma(0) \tag{14}
$$

$$
\int_0^{\infty} \left[\epsilon' - 1 - 2(n-1) \right] d\omega = -2\pi^2 \sigma(0) \,. \tag{15}
$$

This sum rule is a linear combination of Eq. (9) and

$$
\int_0^\infty (\epsilon'-1) \, d\omega = -2\pi^2 \sigma(0) \,, \tag{16}
$$

which is Eq. (37) of Ref. 1.

Although Eq. (15) is a linear combination of Eqs. (9) and (16), it is important to realize that Eq. (15) is by itself an interesting relation. The reason is that it is more rapidly convergent, since the integrand of its left-hand side goes as ${\omega}^{-4}$ for ${\omega} \rightarrow \infty$, whereas the integrands in Eqs. (9) and (16) go as ω^{-2} .

As $\omega A^2(\omega)$ + ω^{-3} for $\omega \rightarrow \infty$, we have analogous. to Eq. (13)

$$
\int_{-\infty}^{+\infty} \omega[(n-1)^2 - k^2 + 2ik(n-1)]\,d\omega = 0\,;
$$

now using the crossing relations [Eqs. (7)] and the behavior n, $k \sim \omega^{-1/2}$ for $\omega \rightarrow 0$, the following expression is reproduced':

$$
\int_0^\infty \omega [n(\omega) - 1] k(\omega) d\omega = 0.
$$
 (17)

Finally, as $\omega^2 A^2(\omega) \rightarrow O(\omega^{-2})$ for $\omega \rightarrow \infty$, we have $\int_{0}^{\infty} \omega^{2} [(n - 1)^{2} - k^{2}] d\omega = 0$

or

$$
\int_0^\infty \omega^2 [\epsilon'-1-2(n-1)] \, d\omega = 0 \,, \tag{18}
$$

which is a natural consequence of $\epsilon - 1 - \omega_0^2 \omega^{-2}$ and $N-1=-\frac{1}{2}\omega_0^2\omega^{-2}$ for $\omega\rightarrow\infty$.

Consider now $A^3(\omega) \rightarrow O(\omega^{-6})$ for $\omega \rightarrow \infty$. We then have

$$
\int_{-\infty}^{+\infty} \left\{ (n-1) [(n-1)^2 - 3k^2] + ik [3(n-1)^2 - k^2] \right\} d\omega = 0.
$$
\n(19)

If the conductivity of the material at zero frequency is $\sigma(0) = 0$, then we have the highly damped superconvergent sum rule

$$
\int_0^\infty (n-1) \left[(n-1)^2 - 3k^2 \right] d\omega = 0 \ . \tag{20}
$$

If the conductivity $\sigma(0) \neq 0$, then as $n, k \sim \omega^{-1/2}$ near the origin of the ω plane, Eq. (20) does not hold anymore. In this case, let us consider $\omega^m A^3(\omega)$ with $m \ge 1$, which for $\omega \to \infty$ is $O(\omega^{m-6})$. The prewith $m \ge 1$, which for $\omega \to \infty$ is $O(\omega)$. The pre-
vious quantity behaves as $\omega^{-3/2+m}$ near $\omega = 0$. Consequently, one obtains the sum rule

$$
\int_0^\infty \omega^m [3(n-1)^2 - k^2] k \, d\omega = 0 \,, \tag{21}
$$

which is valid only for $m = 1, 3, 5$. Equation (21) is

a generalization of relation (17). Similarly, the expression

$$
\int_0^\infty \omega^m (n-1) [(n-1)^2 - 3k^2] d\omega = 0 \tag{22}
$$

is obtained for $m = 2, 4$.

This procedure can be extended for arbitrary powers of $A(\omega)$. Quantities of the form A^3 , A^4 , A^5 , ωA^5 , etc., give rise to highly damped superconvergent sum rules. It is easy to write them with the help of the crossing relations Eq. (4), if the conductivity is zero. If the conductivity $\sigma(0)$ $\neq 0$, we should consider $\omega^r A^s(\omega)$, where for a given value of integer $s > 2$, the minimum value of r is to be chosen in a way such that the singularity at the origin gives for $\omega^r A^s$, at most, the behavior ω^{-1} . The maximum value of r is dictated by the behavior of A^s for high frequencies. We assume that¹ at least $k(\omega) \sim \omega^{-2} \ln^{-\alpha} \omega$ for $\omega \to \infty$, with $\alpha > 1$. The corresponding superconvergent sum rules are for a fixed r and increasing s more and more damped. The reason for this is that $A(\omega)$ decrease vamped. The reason for this is that $A(\omega)$ declines that ω^{-2} for $\omega \rightarrow \infty$ and has a singularity which is rather weak at the origin, ω^{-1}

If the conductivity is zero we can also write superconvergent sum rules for different powers of $\epsilon(\omega)$ – 1 which are strongly damped. On the contrary, if $\sigma(0) \neq 0$, we will have the corresponding sum rules for $\omega^r(\epsilon - 1)^s$, where r for a given s is chosen in a way similar to that one discussed for $\omega^r A^s$.

We can also consider different powers of $\epsilon^{-1}(\omega)$ —¹ which give rise to superconvergent sum rules. This problem is presently under investigation.

The derivation of superconvergent sum rules for the powers A^3 , A^4 , etc., as well as for $(\epsilon - 1)^2$, $(\epsilon - 1)^3$, etc., in the case $\sigma(0) \neq 0$ as we have seen presents difficulties because of the bad singular behavior at the origin, $\omega = 0$. This complication could be avoided if, for instance, we consider the function

~Supported by B.N.D.E. (Contract No. FUNTEC-125). ~Presently at the Instituto de Fisica da Universidade de Sao Paulo.

$$
E(\omega) = \epsilon_1(\omega) / \sigma_1(0) - \epsilon_2(\omega) / \sigma_2(0), \qquad (23)
$$

where $\epsilon_1(\omega)$ and $\sigma_1(0)$ are the complex dielectric function and conductivity for the material 1 and $\epsilon_2(\omega)$, $\sigma_2(0)$ are the corresponding quantities for material 2. Now as $E(\omega)$ has no singularity at ω = 0 and is of $O(\omega^{-2})$ for $\omega \to \infty$, we could write superconvergent sum rules for powers of $E(\omega)$ which are highly damped.

The problem of the sensitivity of these superconvergent sum rules against experimental errors is under investigation.

Finally, let us consider the function

$$
\omega^{m-1}[\epsilon(\omega)-1]^m, \qquad (24)
$$

with *m* an integer ≥ 1 . It behaves for $\omega \rightarrow \infty$ as $O(\omega^{m-1})$ and therefore it satisfies the superconvergence relation Eq. (3). It has, for a conducting material, a simple pole given by

$$
(4\pi i\sigma)^m/\omega\ .\tag{25}
$$

Therefore Eq. (3) gives

$$
\int_{-\infty}^{+\infty} \omega^{m-1} [\epsilon(\omega) - 1]^m d\omega = i\pi [4\pi i\sigma(0)]^m, \qquad (26)
$$

where, in the integral on the left-hand side, we have already separated the contribution of $\omega = 0$.

For $m = 1$ we obtain Eq. (16). For $m = 2$, Eq. (26) gives

$$
\int_0^\infty \omega \epsilon^{\prime\prime} (\epsilon^{\prime} - 1) d\omega = -4\pi^2 \sigma^2(0) \,. \tag{27}
$$

In this way Eq. (26) gives a whole class of sum rules involving arbitrary powers of the conductivity of the material.

By a similar procedure it is possible to derive also generalized f sum rules.⁵

ACKNOWLEDGMENTS

We thank Professor P. R. de Paula e Silva and Professor H. M. Nussenzveig (at PUC-E. da Guanabara) for their critical remarks.

- 'See, for instance, N. N. Meiman, Zh. Eksp. Teor. Fiz.
- 43, 2277 (1962) [Sov. Phys. -JETP 16, 1609 (1963)]
- 5 A. Villani and A. H. Zimerman, Phys. Lett. A 44, 295 (1973).

^{&#}x27;M. Altarelli, D. L. Dexter, H. M. Nussenzveig, and D. Y. Smith, Phys. Rev. B 6, 4502 (1972).

^{&#}x27;Y. C. Liu and S. Okubo, Phys. Rev. Lett. 19, 190 (1967).

³E. Ferrari and G. Violini, Nuovo Cimento Lett. 5, 1027 (1972).