Power-spectrum description by complex series expansion

K.-E. Peiponen,* Toshimitsu Asakura, and E. M. Vartiainen†
Research Institute of Applied Electricity, Hokkaido University, Sapporo, Hokkaido 060, Japan
(Received 24 April 1991)

Some of the general properties of the power spectrum are presented, and sum rules for spectrum analysis stated.

PACS number(s): 42.65.Bp, 02.30.+g

I. INTRODUCTION

The description of linear, complex, frequency-dependent optical constants by complex power series was introduced by King in 1977 and 1978 [1,2]. In his method, the upper half of a complex frequency plane, where the optical constant is a holomorphic function, is mapped conformally onto a unit disk. The optical constant is then presented as a Laurent series expansion in the unit disk. The advantage of this method is that, because of some of the symmetry relations of the optical constants, inversion of optical data is possible using only the fast-Fourier-transform technique. Normally, this kind of calculation involves Kramers-Kronig relations [3], but the main benefit of this alternative method is the reduced computation time compared to that involving the Kramers-Kronig relations. Recently the King method has been found applicable in the analysis of the optical data of mixed alkali halide crystals [4].

It has also been observed that the nonlinear susceptibilities of material can be described by a power series [5]. The method is basically the same as King's method, but the nonlinear-optical constant is now holomorphic in a polydisk. The implication of the results in Ref. [5] is that we know through measurement the squared modulus of the nonlinear susceptibility and then calculate the real and imaginary parts. Such a situation occurs, for instance, when nonlinear coherent Raman spectra are under investigation. The technique described above has, therefore, been applied to provide sum rules for the squared modulus of nonlinear Raman susceptibility [6].

In this paper we consider in general terms the description of a power spectrum by complex power series and sum rules. Although the present authors are primarily interested in optical phenomena, they wish to emphasize that the present theory can be applied under quite mild restrictions to describe the power spectrum beyond the optical range. A report on the progress of the theory presented in Refs. [5,6] is also provided.

II. THE POWER SPECTRUM DESCRIBED BY MEANS OF A REAL ANALYTIC FUNCTION

In the case of a band-limited power spectrum, a situation that is usually present with measurements, the band limitation may be caused, for example, because of a finite wavelength region where a signal is scanned or because of the finite-sampling-time interval of a signal. In such cases the power spectrum can be described in terms of a complex power-series description. The normal procedure is to map a semi-infinite strip of the upper half of the complex plane (usually the frequency plane) onto a unit disk. The transform needed for the mapping is supplied by $z=e^{i\Phi}$. This transform maps the finite interval of a real axis onto the boundary of a unit disk $|z|=1$. The phase angle Φ depends on the particular quantity to be measured. As an example, if we have a signal that is time sampled, then $\Phi=2\pi f\Delta t$ where Δt is the sampling time and f is the frequency (limited to the Nyquist range $|f|\le f_c$, $f_c=\frac{1}{2}\Delta t^{-1}$). Because of the present transform, the power spectrum will attain a periodic nature as a function of frequency, caused by a division of the upper half plane into semi-infinite strips of equal width. In practical calculations we limit our consideration to a single semi-infinite strip beyond which the power is believed to be negligible.

The power spectrum can be presented by the squared modulus of the Laurent series [7].

$$P(z)=\left|\sum_{j=-\infty}^{\infty} c_j z^j\right|^2 . \tag{1}$$

The Laurent series is holomorphic in a unit disk $|z|\le 1$ where the point $z=0$ is excluded.

The coefficients c_j are considered to have complex values. The computation of c_j is possible by using the contour integration technique of Ref. [5] or if some symmetry properties have been revealed by the technique applied in the context of coherent Raman spectra analysis

[8]. The series expansion of Eq. (1) is also the basis for maximum entropy estimation where the coefficients are obtained with the aid of autocorrelation values [7].

If we continue the interpretation of Eq. (1) we can write it in the form

$$\begin{aligned} P(z) &= \left[c_0 + \sum_{j=1}^{\infty} (c_j z^j + c_{-j} z^{-j}) \right] \times \left[c_0 + \sum_{j=1}^{\infty} (c_j z^j + c_{-j} z^{-j}) \right]^* \\ &= \left[c_0 + \sum_{j=1}^{\infty} (c_j z^j + c_{-j} \bar{z}^j) \right] \times \left[c_0 + \sum_{j=1}^{\infty} (c_j z^j + c_{-j} \bar{z}^j) \right]^* , \end{aligned} \tag{2}$$

where the asterisks and the overbar denote the complex conjugates and use has been made of the information $z\bar{z}=1$.

We first observe that the static value or dc power spectrum in the time sampling case is obtained when $f=0$, i.e., $z=1$. This means that

$$P_{\rm dc}(1) = \left[c_0 + \sum_{j=1}^{\infty} (c_j + c_{-j}) \right] \times \left[c_0 + \sum_{j=1}^{\infty} (c_j + c_{-j}) \right]^* . \tag{3}$$

In practical calculations the summation index is always finite, i.e., the series expansion of Eq. (2) is estimated by means of a polynome. Subsequently, we can apply the Cauchy product with the result that Eq. (2) can be written as follows:

$$P(z) = \sum_k \sum_l C_{kl} z^k \bar{z}^l . \tag{4}$$

This type of function is described as "real analytic" [9,5]. Note that when $l=0$, Eq. (4) presents a holomorphic function whereas for $k=0$ it presents an antiholomorphic function.

Again, when $z\bar{z}=1$, Eq. (4) can restated in the form

$$\begin{aligned} P(z) &= C_0 + \sum_{m=1}^{\infty} C_m z^m + \sum_{m=1}^{\infty} C_m^* \bar{z}^m \\ &= C_0 + 2\,\mathrm{Re}\left[\sum_{m=1} C_m z^m \right] , \end{aligned} \tag{5}$$

where $C_m = C_{kl}$, $m=k-l$ and the coefficients of Eqs. (4) and (5) involve the sum of the products of the coefficients and their complex conjugates that appear in Eq. (2). For instance, we have $C_0 = |c_0|^2 + \sum_{j\neq 0}(|c_j|^2 + |c_{-j}|^2)$, which is a real number.

Note that the estimate of Eq. (5) is valid also for the nonlinear Raman susceptibility of Ref. [6], which was obtained using a different transform from the present one.

III. SUM RULES FOR THE POWER SPECTRUM

It was observed that for a real analytic function we can write a generalized dispersion relation as follows [6]:

$$P(z') = \frac{1}{\pi i} \mathrm{P} \oint_{|z|=1} \frac{P(z)}{z-z'} dz - \frac{1}{\pi} \int\int_{|z|\le 1} \frac{d}{d\bar{z}} P(z) \Big/ (z-z') d(\mathrm{Re} z) d(\mathrm{Im} z) , \tag{6}$$

where P denotes the Cauchy principal value, the derivative in the surface integral is defined as $d/d\bar{z} = \frac{1}{2}[d/d(\mathrm{Re}z) + i\,d/d(\mathrm{Im}z)]$, and z' is a pole on the boundary of the unit disk.

One may now ask why we write such a complicated formula as Eq. (6). The answer lies in our wish to acquire more information about the system by means of sum rules. It was found, however, that extracting information about the system was a laborious task, because of the surface integral. The surface integral involves complex frequencies which cannot be characterized by measurement. Indeed, Eq. (6) is quite general and it allows antiholomorphism different from that in our simple case of real analytic function. It can now, therefore, be shown that the surface integral can be reduced to a contour integral which can be handled more easily.

Starting from Eq. (5), we notice that

$$C_0 = \frac{1}{2\pi i} \oint_{|z|=1} \frac{P(z)}{z} dz . \tag{7}$$

Then,

$$\begin{aligned} \sum_{m(\neq 0)} C_m Z'^m &= \frac{1}{\pi i} \mathrm{P} \oint_{|z|=1} \frac{P(z)}{z-z'} dz - \frac{1}{2\pi i} \oint_{|z|=1} \frac{P(z)}{z} dz \\ &= \left[-\frac{1}{\pi} \int\int_{|z|\le 1} \left[\frac{d}{d\bar{z}} P(z) \Big/ (z-z') \right] \times d(\mathrm{Re} z) d(\mathrm{Im} z) \right]^* \\ &= \left[\sum_{m(\neq 0)} C_m^* \bar{z}'^m \right]^* . \end{aligned} \tag{8}$$

From Eq. (8) it follows that

$$\begin{aligned} P(z') &= \frac{1}{2\pi i} \oint_{|z|=1} \frac{P(z)}{z} dz + 2\,\mathrm{Re}\left[\frac{1}{\pi i} \mathrm{P} \oint_{|z|=1} \frac{P(z)}{z-z'} dz - \frac{1}{2\pi i} \oint_{|z|=1} \frac{P(z)}{z} dz \right] \\ &= \mathrm{Re}\left[\frac{1}{2\pi i} \mathrm{P} \oint_{|z|=1} \frac{3z+z'}{z(z-z')} P(z) dz \right] , \end{aligned} \tag{9}$$

where we have used the fact that, because the integral of

Eq. (7) exists, it must also exist as a Cauchy principal value.

We wish to emphasize that the result of Eq. (9) is generally valid for all kinds of transformation where the upper half of the complex plane, as in Ref. [5], or a semi-infinite strip, as in the present case, is mapped onto a unit disk. If we write the result of Eq. (9) using frequency f as a variable, then the corresponding expressions for the integrals, appearing in Eq. (9), depend on the particular chosen transform used in mapping the frequency domain onto the unit disk. Furthermore, if we wish to write sum rules using the result of Eq. (9) and, e.g., the technique of Altarelli and Smith [10], which involves dispersion relations for the powers of an analytic function, also in that case the sum-rule integrals, involving f as a variable, depend on the chosen transform. In every case, sum rules involve the coefficients of the series expansion of Eq. (5), for which we may try to provide physical interpretations.

To illustrate this we will study the physical interpretation of the integral of Eq. (7), which also appears in Eq. (9). If we convert the result of Eq. (7) back to the frequency description, a sum rule for a time-sampled signal for which $z=e^{2\pi i f \Delta t}$ can be written as

$$\frac{1}{2\pi i}\int_{|z|=1}\frac{P(z)}{z}dz \rightarrow \frac{1}{f_c}\int_{-\infty}^{\infty}P(f)df=C_0 \ . \tag{10}$$

From this we can deduce that the coefficient C_0 expresses average power. If f_c is known, the integral will give the integrated power.

IV. DISCUSSION

We have shown that a power spectrum can be described by means of a real analytic function in a unit disk. To illustrate this we considered a power spectrum sampled as a function of time. Use was made of a certain type of transform applicable for band-limited data, which was valid also in the case where the frequency f is known [8]. Further, we have shown that a complicated dispersion formula from a previous study can be modified in the case of a real analytic function to supply a more applicable form. This form can also be used for computer calculations, since it is similar in nature, formally, to the Kramers-Kronig formula of dispersion theory. The explicit form of sum rules as a function of the frequency, obtained using Eq. (9), depends on the chosen transforms.

The present theory is valid for the nonlinear susceptibilities described by a complex power series as presented in Refs. [5,6]. It is hoped that the present theory, which employs complex power series and sum rules, will provide information, for example, on the surface roughness of materials via optical detection as proposed in Ref. [11], where sum rules were presented for a Gaussian surface roughness distribution.

---

*Permanent address: Väisälä Laboratory, Department of Physics, University of Joensuu, SF-80100 Finland.

†Permanent address: Department of Information Technology, Lappeenranta University of Technology, SF-55851, Finland.

[1] F. W. King, J. Phys. C **10**, 3199 (1977).

[2] F. W. King, J. Opt. Soc. Am **68**, 994 (1978).

[3] L. D. Landau and E. M. Liftshitz, *Electrodynamics of Continuous Media* (Addison-Wesley, Reading, MA, 1960).

[4] P. Ketolainen, K.-E. Peiponen, and K. Karttunen, Phys. Rev. B **43**, 4492 (1991).

[5] K.-E. Peiponen, Phys. Rev. B **37**, 6463 (1988).

[6] K.-E. Peiponen, E. M. Vartiainen, and T. Tsuboi, Phys. Rev. A **41**, 527 (1990).

[7] W. H. Press, B. P. Flannery, S. A. Tenkolsky, and W. T. Vetterling, *Numerical Receipes* (Cambridge University Press, New York, 1986).

[8] E. M. Vartiainen, E.-E. Peiponen, and T. Tsuboi, J. Opt. Soc. Am B **7**, 722 (1990).

[9] O. Lehto and K. I. Virtanen, *Quasiconformal Mappings in the Plane* (Springer-Verlag, Berlin, 1973).

[10] M. Altarelli and D. Y. Smith, Phys. Rev. B **9**, 1290 (1973).

[11] K.-E. Peiponen and T. Tsuboi, Opt. Laser Technol. **22**, 127 (1990).