Error bounds of continued fractions for complex transport coefficients and spectral functions

Peter Hänggi

Angaben zur Veröffentlichung / Publication details:

Hänggi, Peter. 1978. “Error bounds of continued fractions for complex transport coefficients and spectral functions.” *Zeitschrift für Naturforschung A* 33 (11): 1380–82. https://doi.org/10.1515/zna-1978-1117.

Error Bounds of Continued Fractions for Complex Transport Coefficients and Spectral Functions

P. Hänggi

Institut für Theoretische Physik,
Universität Stuttgart, Federal Republic of Germany

Z. Naturforsch. **33a**, 1380–1382 (1978);
received July 10, 1978

We study the calculation of complex transport coefficients $\chi(\omega)$ and power spectra in terms of complex continued fractions. In particular, we establish classes of dynamical equilibrium and non-equilibrium systems for which we can obtain a posteriori bounds for the truncation error $|\chi(\omega) - \chi^{(n)}(\omega)| \leqq c(\omega) |\chi^{(n)}(\omega) - \chi^{(n-1)}(\omega)|$ when the transport coefficient is approximated by its n-th continued fraction approximant $\chi^{(n)}(\omega)$.

1. Introduction

An important problem in the field of equilibrium and nonequilibrium statistical mechanics is the calculation of the spectral function (or power spectrum) $S(\omega)$ of time-dependent fluctuations with an autocorrelation function $C(t) = C(-t) \in \mathbb{R}$

$$S(-\omega) = S(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} C(t)\, \mathrm{d}t \geqq 0 \tag{1}$$

$$= \frac{1}{\pi} \operatorname{Re} \lim_{\varepsilon \to 0^+} \int_0^{\infty} e^{-i\omega t - \varepsilon t} C(t)\, \mathrm{d}t . \tag{2}$$

For, due to the fluctuation-dissipation theorem for thermal equilibrium systems [1] this spectral function determines the linear dissipative response, as e.g. the cross-section for scattering of light and neutrons [2]. Further, the electric conductivity, $\chi(\omega)$, depends upon the spectral function of the current fluctuations [1]

$$\chi(\omega) = \lim_{\varepsilon \to 0^+} \int_0^{\infty} C(t)\, e^{-i\omega t - \varepsilon t}\, \mathrm{d}t$$

$$= \lim_{\varepsilon \to 0^+} - i \int_{-\infty}^{\infty} \frac{S(x)\, \mathrm{d}x}{\omega - i\varepsilon + x} . \tag{3}$$

Even in stationary nonequilibrium systems we obtain similar relations for the transport coefficients if a fluctuation theorem holds [3].

In this note we discuss a suitable calculation technique for complex transport quantities via continued fraction expansions and investigate classes of statistical systems for which a posteriori truncation error bounds for these continued fractions can be obtained.

Reprint requests to P. Hänggi, Universität Stuttgart, Institut für Theoretische Physik, Pfaffenwaldring 57/IV, D-7000 Stuttgart-80, F.R.G.

2. Truncation Error Bounds for Complex Susceptibilities

Mori [4] has considered the problem of the calculation of quantities like in eq. (2) and eq. (3): He derived a continued-fraction representation of the Laplace transform of thermal equilibrium autocorrelation functions using the concept of memory functions. The general method of expanding the Laplace transform of an arbitrary autocorrelation function is based upon the (asymptotic) high-frequency expansion of $\chi(\omega)$ [5]

$$\chi(\omega) = \sum_{n=0}^{\infty} (-1)^n \frac{C_n}{(i\omega)^{n+1}} . \tag{4}$$

The moments C_n are defined by

$$C_n = (-1)^n \left. \frac{\mathrm{d}^n C(t)}{\mathrm{d}t^n} \right|_{t=0^+} \tag{5}$$

and are formally related to moments of the function $\chi(\omega)$ *

$$C_n = (-i)^n \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \omega^n \chi(\omega) \tag{6}$$

$$= (i)^n \int_{-\infty}^{\infty} \mathrm{d}\omega\, \omega^n S(\omega) . \tag{7}$$

The asymptotic series in Eq. (4) can be converted into a continued fraction expansion of the form

$$\chi(\omega) = \frac{\lambda_1}{i\omega +} \, \frac{\lambda_2}{1 +} \, \frac{\lambda_3}{i\omega +} \cdots . \tag{8}$$

Here the coefficients $\{\lambda_n\}$ can be constructed from the moments $\{C_n\}$ using determinantal expressions or more efficiently by use of the recursive algorithms presented in Reference [5]. In practice, however, we are forced to terminate the generally infinite continued fraction in Eq. (8) at a finite order. Henceforth, it is important to have realistic estimates of the truncation error $F(z)$

$$F(z) = |\chi(-iz) - \chi^{(n)}(-iz)| , \quad z \in \mathbb{C}, \tag{9}$$

when Eq. (8) is approximated by its n-th approximant $\chi^n(z)$, obtained by setting

$$\lambda_{n+1} = \lambda_{n+2} = \cdots = 0 .$$

* Note that these integral representations for C_n may in general not exist. In practice, the moments are calculated theoretically via Eq. (5) [4, 5] [see also Eq. (21)] or measured experimentally.

To start with, suppose the susceptibility $\chi(\omega)$ has a Stieltjes integral representation

$$\chi(\omega) = \int_0^\infty \frac{d\psi(x)}{i\,\omega + x} \quad \text{with} \quad d\psi(x) \geqq 0\,. \tag{10}$$

Then, the moments in Eq. (4) form a *Stieltjes sequence* [5, 6]

$$C_n = \int_0^\infty w^n \, d\psi(w) > 0\,, \quad n = 0, 1, \ldots\,. \tag{11}$$

Assuming that the limit $\chi(\omega)$ in Eq. (8) exists and represents the correct analytical continuation, i.e. the limit equals the function defined in Eq. (3)

$$\chi(\omega) = \lim_{n\to\infty} \chi^{(n)}(\omega)\,, \tag{12}$$

we look for error bounds of the form

$$\begin{aligned} &|\chi(-i\,z) - \chi^{(n)}(-i\,z)| \\ &\quad \leqq c(z)\,|\chi^{(n)}(-i\,z) - \chi^{(n-1)}(-i\,z)|\,, \\ &\qquad c(z) > 0 \end{aligned} \tag{13}$$

with $c(z)$ a constant which depends only on $z \in \mathbb{C}$. For the following the theorem of Henrici and Pfluger [7, 8] for Stieltjes continued fractions plays a major role: Let $\chi^{(n)}(-iz)$ denote the n-th approximation of the Stieltjes continued fraction of the form in Eq. (8), where with Eq. (11) $\lambda_n > 0$ for all $n \geqq 1$. Then we have for all $n \geqq 1$ and $z \in \mathbb{C} - [0, -\infty)$

$$|\chi(-i\,z) - \chi^{(n)}(-i\,z)| \leqq \begin{cases} |\chi^{(n)}(-i\,z) - \chi^{(n-1)}(-i\,z)|\,, \\ \quad \text{if} \quad |\arg z| \leqq \pi/2\,, \\ \tan(\tfrac{1}{2}\arg z)\,|\chi^{(n)}(-i\,z) - \chi^{(n-1)}(-i\,z)|\,, \\ \quad \text{if} \quad \pi/2 < |\arg z| < \pi\,. \end{cases} \tag{14}$$

Next we investigate classes of statistical systems for which the expansion of the Laplace transform of complex transport coefficients can be cast in a Stieltjes continued fraction. — Most statistical systems are described in terms of a Markovian dynamics; i.e. the probability function $p(\underline{x}, t)$ over the state variables $\underline{x}$ fulfills a master equation of the form

$$\dot{p}(t) = \Gamma\, p(t)\,, \tag{15}$$

where Γ denotes the generator of the linear transition (conditional probability) $R(\underline{x}t\,|\,\underline{y}t_1)$, $t > t_1$. Let p_{st} denote a stationary probability function

$$\Gamma\, p_{\text{st}} = 0\,. \tag{16}$$

Then, by use of the operator $\overline{\Gamma}$

$$\overline{\Gamma} = p_{\text{st}}^{-1/2}\, \Gamma\, p_{\text{st}}^{1/2} \tag{17}$$

we can formulate a sufficient condition for the moments $\{C_n\}$ being a Stieltjes sequence: Whenever the operator $\overline{\Gamma}$ represents a *hermitian operator* with respect to the usual scalar product

$$(f, \overline{\Gamma} g) = \int f(\underline{x})\, \overline{\Gamma}(\underline{x}, \underline{y})\, g(\underline{y})\, d\underline{x}\, d\underline{y} = (\overline{\Gamma} f, g) \tag{18}$$

the moments $\{C_n\}$ form a Stieltjes sequence! Whence the high-frequency expansion can be recast in a Stieltjes continued fraction, Eq. (8), with all $\lambda_n > 0$.

Proof. By use of the spectral representation of the operator $\overline{\Gamma}$

$$\overline{\Gamma} = \sum_\mu\!\!\!\!\int d_\mu\, \varrho_\mu\, |\varphi_\mu\rangle\langle\varphi_\mu| \tag{19}$$

we obtain from Eq. (5) for the static moment C_n of the autocorrelation function $C(t)$

$$\begin{aligned} C(t) &= \langle g[\underline{x}(t)]\, g[\underline{x}(0)]\rangle \\ &= \langle g[\underline{x}(t)]\, [(\exp \Gamma t)\, g\, p_{\text{st}}]_{\underline{x}(t)}\rangle \end{aligned} \tag{20}$$

the expression

$$\begin{aligned} C_n &= (-1)^n \int d\underline{x}\, g(\underline{x})\, [\Gamma^n\, g\, p_{\text{st}}]_{\underline{x}} \\ &= (-1)^n \int d\underline{x}\, g(\underline{x})\, [p_{\text{st}}^{1/2}\, \overline{\Gamma}^n\, p_{\text{st}}^{1/2}\, g]_{\underline{x}} \\ &= \sum_\mu\!\!\!\!\int d_\mu\, |\varrho_\mu|^n\, |(g\, p_{\text{st}}^{1/2}, \varphi_\mu)|^2 \\ &= \int_0^\infty w^n \{\sum_\mu\!\!\!\!\int d_\mu\, \delta(|\varrho_\mu| - w)\, |(g\, p_{\text{st}}^{1/2}, \varphi_\mu)|^2\}\, dw \\ &= \int_0^\infty w^n\, d\psi(w) \quad \text{with} \quad d\psi(w) \geqq 0\,. \end{aligned} \tag{21}$$

Hereby we used the fact that all eigenvalues ϱ_μ of $\overline{\Gamma}$ satisfy the dissipative property $\varrho_\mu \leqq 0$.

The condition in Eq. (18) is satisfied by many systems in thermal equilibrium, e.g. the Brownian motion problems [9] and the stochastic Ising spin models [10]. Generally, all systems obeying a strong detailed balance symmetry [11] fit Eq. (18). Examples are the master equations for nonlinear chemical reactions [12] or for the current fluctuations in an Esaki diode [13]. In particular, all Fokker-Planck systems obeying a usual detailed balance symmetry [11, 14] whose drift vectors are irreversible under time reversal yield a hermitian Fokker-Planck operator [11, 14]. Typical examples are the Fokker-Planck equation for the single-mode Laser and parametric oscillators [14, 15]. For all these systems we obtain for the complex susceptibility in Eq. (3) by use of Eq. (14) the truncation error bound

$$|\chi(\omega) - \chi^{(n)}(\omega)| \leqq |\chi^{(n)}(\omega) - \chi^{(n-1)}(\omega)| \quad (22)$$

and for the power spectrum in Eq. (1) the relation

$$|S(\omega) - S^{(n)}(\omega)| = \frac{1}{\pi} |\mathrm{Re}(\chi(\omega) - \chi^{(n)}(\omega)| \leqq \frac{1}{\pi} |\chi^{(n)}(\omega) - \chi^{(n-1)}(\omega)| . \quad (23)$$

In a similar way we can utilize the results of Eq. (14) to obtain a posteriori bounds for the continued fraction representations of dynamical response functions of the type considered in Reference [16].

Acknowledgement

It is a pleasure to thank Prof. H. Thomas for various useful comments.

[1] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).
[2] L. van Hove, Phys. Rev. **95**, 249 (1954).
[3] P. Hänggi, Helv. Phys. Acta **51**, 202 (1978).
[4] H. Mori, Prog. Theor. Phys. **34**, 399 (1965).
[5] P. Hänggi, F. Rösel, and D. Trautmann, Z. Naturforsch. **33a**, 402 (1978).
[6] J. A. Skohat and J. D. Tamarkin, The Problem of Moments, Math. Surveys 1 American Math. Soc., Providence (1950).
[7] P. Henrici and P. Pfluger, Numer. Math. **9**, 120 (1966).
[8] W. B. Jones, Rocky Mountain J. Math. **4**, 241 (1974).
[9] M. Bixon and R. Zwanzig, J. Stat. Phys. **3**, 245 (1971).
[10] R. J. Glauber, J. Math. Phys. **4**, 294 (1963).
[11] P. Hänggi, Helv. Phys. Acta **51**, 183 (1978).
[12] S. Grossmann and R. Schranner, Z. Physik **B 30**, 325 (1978).
[13] R. Landauer, J. Appl. Phys. **33**, 2209 (1962).
[14] R. Graham, Springer Tracts in Modern Physics **66**, 1 (1973); H. Risken, Z. Physik **251**, 231 (1972).
[15] H. Risken, Fortschritte der Physik **16**, 261 (1968).
[16] R. Gordon, J. Math. Phys. **7**, 1087 (1968).