Continued Fraction Expansions in Scattering Theory and Statistical Non-Equilibrium Mechanics *

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We consider several main aspects of the practical application of continued fraction expansions in scattering problems and in the field of equilibrium and non-equilibrium statistical mechanics. We present some recursive algorithms needed for an efficient evaluation of continued fraction coefficients. The method is then applied to the summation of badly converging series which occur in scattering theory and to the asymptotic solution of the Schrödinger equation. In addition, the use of the method for the calculation of response functions, correlations and their derivatives in systems whose time-dependence is described by a master equation is discussed. Finally, the construction of error bounds is investigated.

1. Introduction

In recent years there has been considerable interest in the methods for the efficient evaluation of series in quantum mechanics and statistical mechanics. In many cases, the resulting series have an unsatisfactory convergence behaviour or are asymptotic series. Hence, a fundamental strategy consists in constructing analytical continuations, yielding better convergence properties. One possibility consists in converting the, in general, asymptotic series into a continued fraction which leads to an appropriate mathematical representation of the series; the obtained continued fraction is then considered as the value of the function of interest. The continued fraction expansion, which is closely related to the Padé-approximation [1] has been used in solving many problems in applied mathematics. Particularly, the interest in continued fraction methods has been renewed for the computation of analytical functions [2—4]. The continued fraction method has also found application in the solution of linear differential equations [5], integral equations [6] and systems of linear equations recently discussed by Swain [7].

In physics, the continued fraction technique has been used explicitly e.g. in the solution of the Schrödinger equation [8—9], in slow neutron scattering calculations [10—11], in strong interaction theory and in field theory [12]. The more general Padé-approximation has been applied more or less in all fields of physics [1]. In this paper we use continued fraction techniques to study the solution of some general physical problems in the field of scattering theory and statistical mechanics.

In Chapt. 2, we review the most important properties of continued fractions. We then discuss some convergence theorems and the related problem of a possible approximation to the remainder tail of the truncated continued fraction. In Sect. 3, some recursive methods, needed for an efficient evaluation of the continued fraction coefficients, are presented. Of special interest are those algorithms which yield a numerically stable recursion scheme for the continued fraction coefficients. The continued fraction theory is then applied in Chapt. 4 to the calculation of scattering amplitudes and to the summation of slowly convergent or even divergent series arising in quantum mechanical scattering theory and in statistical mechanics. The asymptotic solution of the Schrödinger equation for some special types of potentials is evaluated using continued fraction expansions. The efficient calculation of correlation functions and response functions of stochastic processes describing statistical systems is presented, too.

One of the major problems in the theory of continued fractions is the assessement of the accuracy of the approximation. In Sect. 5 a method for finding the best error bounds for the autocorrelation functions and their time-derivatives of stationary Markov processes is given. The results obtained are briefly discussed in Chapt. 6 with some aspects of further problems in the application of continued fraction functions.

2. Basic Properties of Continued Fractions

In this section we present some of the fundamental properties of the continued fraction expan-

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sions [1, 5, 13—15]. Let the set $\{f_n(z)\}$ denote analytical functions which allow a Taylor series expansion about the origin. If the functions $f_n(z)$ obey the recursion relation

$$f_n(z) = a_n + \frac{b_{n+1} z}{f_{n+1}(z)}, \quad z \in \mathbb{C}, \tag{2.1}$$

where the sets $\{a_n\}$, $\{b_n\}$ denote complex numbers, we obtain the continued fraction

$$f_0(z) = a_0 + \cfrac{b_1 z}{a_1 + \cfrac{b_2 z}{a_3 + \cdots}}$$

$$\equiv a_0 + \frac{b_1 z}{a_1 +} \frac{b_2 z}{a_2 +} \cdots. \tag{2.2}$$

By means of an equivalence transformation [1] we get from Eq. (2.2)

$$f_0(z) = a_0 + \frac{\hat{b}_1 z}{1 +} \frac{\hat{b}_2 z}{1 +} \cdots, \tag{2.3}$$

with

$$\hat{b}_1 = \frac{b_1}{a_1} \quad \text{and} \quad \hat{b}_i = \frac{b_i}{a_i a_{i-1}} \quad \forall i \geqq 2. \tag{2.4}$$

Expansion of Eq. (2.3) yields

$$f_0(z) = a_0 + \hat{b}_1 z - \hat{b}_1 \hat{b}_2 z^2 + O(z^3)$$

$$= \sum_{i=0}^{\infty} \alpha_i z^i, \tag{2.5}$$

showing the relationship of the continued fraction to the corresponding Taylor series of $f_0(z)$.

If the number of terms in Eq. (2.3) is infinite, $f_0(z)$ is called an infinite continued fraction and the terminated fraction

$$f_0^{(n)}(z) = A_n(z)/B_n(z) \tag{2.6}$$

is called the n-th convergent of $f_0(z)$ (i.e. the coefficients $\hat{b}_k$ in Eq. (2.3) are set zero for $k \geqq n+1$). The functions $A_n(z)$, $B_n(z)$ satisfy the recursion relations

$$A_{n+1}(z) = A_n(z) + \hat{b}_{n+1} z A_{n-1}(z) \tag{2.7a}$$

and

$$B_{n+1}(z) = B_n(z) + \hat{b}_{n+1} z B_{n-1}(z). \tag{2.7b}$$

From the theory of Padé-approximants the sequence of convergents of the "corresponding continued fraction" to the Taylor series occupies the stair-step sequence of Padé-approximants [1] [0/0], [1/1], [2/1], ..., where

$$[L/M] = P_L(z)/Q_M(z), \tag{2.8}$$

with $Q_M(0) = 1$.

L, M are the degrees of the polynomials P_L and Q_M, respectively. In general, successive truncations of Eq. (2.3) are seen to yield a useful result. For the convergence properties of continued fraction expansions we refer to the results in the literature [13—15]. Here, we mention the most important convergence theorem, first discussed by van Vleck and Pringsheim [16]: if the coefficients $\hat{b}_n$ in Eq. (2.3) have the property

$$\lim_{n\to\infty} \hat{b}_n = \hat{b} \neq 0, \tag{2.9}$$

then within every simply connected region T in $\mathbb{C}$, containing the origin and no point of the branch

$$g = -\frac{1}{4\hat{b}} + t\left\{\mathrm{Re}\left(-\frac{1}{4\hat{b}}\right), \mathrm{Im}\left(-\frac{1}{4\hat{b}}\right)\right\} \text{ for } \quad t \geqq 0, \tag{2.10}$$

the continued fraction is a regular (except for the poles) analytic function and coincides in the region about the origin with the corresponding series. In the case where the coefficients $\hat{b}_n$ have the property

$$\lim_{n\to\infty} \hat{b}_n = 0, \tag{2.11}$$

the continued fraction is convergent in the whole complex plane except at poles.

The error of the truncated continued fraction can be estimated using the convergence theorem by Blanch [17]. An approximation of the remainder tail in the continued fraction can be obtained in the following way: with $\hat{b}_n z = \alpha_n$ in

$$f_n(z) = \alpha_n/(1 + f_{n+1}(z)), \tag{2.12}$$

and by setting $f_{n+1} = f_n = \bar{f}_n$ an approximation of the tail becomes

$$\bar{f}_n = -\tfrac{1}{2}(1 - \sqrt{1 + 4\alpha_n})$$

$$= \frac{2\alpha_n}{1 + \sqrt{1 + 4\alpha_n}}. \tag{2.13}$$

Continued fraction expansions have found wide application for the numerical evaluation of special analytic functions [3—5]. As an example, let us consider the infinite continued fraction [5] for the function a^x with x real and a complex:

$$a^x = 1 + \frac{(a-1)\,x}{1-}\,\frac{(a-1)(x-1)}{2+}\,\frac{(a-1)(x+1)}{3-}\,\frac{(a-1)(x-2)}{2+}\,\frac{(a-1)(x+2)}{5-}\cdots. \tag{2.14}$$

This continued fraction converges for all $x \in \mathbb{R}$ and all $a \notin (-\infty, 0]$. For $a = 2$ and $x = 1/2$ the successive convergents read 1.5, 1.4, 1.4166, 1.414379, 1.414285, 1.414201, 1.4142157 and the exact value obviously is 1.41421356 ....

In physics, many problems occur where semiconvergent or asymptotic series are known (for example [18—19]). Therefore, the following problem suggests itself: can we construct continued fractions which serve as adequate analytical continuation of semiconvergent series? If we start from the recursion relation

$$f_n(z) = b_n/(z - a_n + f_{n+1}(z))\,, \tag{2.15}$$

we get

$$f_1(z) = \frac{b_1}{(z-a_1)+}\,\frac{b_2}{(z-a_2)+}\cdots. \tag{2.16}$$

The expansion of Eq. (2.16) yields the corresponding series

$$f_1(z) = \sum_{n=0}^{\infty} p_n/z^{n+1}\,. \tag{2.17}$$

In the following we will restrict the discussion to the so-called P, R and S forms:

$$\text{(P)}\quad \sum_{n=0}^{\infty} \frac{p_n}{z^{n+1}}\,; \tag{2.18a}$$

$$\text{(R)}\quad \sum_{n=0}^{\infty} \frac{(-)^n r_n}{z^{n+1}}\,, \quad r_n = (-)^n p_n\,; \tag{2.18b}$$

$$\text{(S)}\quad \frac{1}{y}\sum_{n=1}^{\infty} \frac{s_n}{y^{2n-1}}\,, \begin{cases} s_n = p_{n-1}\,; \\ y\ = \sqrt{z},\ \arg y \in [0, \pi)\,. \end{cases} \tag{2.18c}$$

The series in Eq. (2.18) have the following "corresponding continued fraction" forms:

$$\text{(P)}\quad \frac{b_1}{(z-a_1)+}\,\frac{b_2}{(z-a_2)+}\,\frac{b_3}{(z-a_3)+}\cdots; \tag{2.19a}$$

$$\text{(R)}\quad \frac{c_1}{z+}\,\frac{c_2}{1+}\,\frac{c_3}{z+}\,\frac{c_4}{1+}\cdots; \tag{2.19b}$$

$$(\text{S}_1)\quad \frac{1}{y}\left(\frac{d_1}{y+}\,\frac{d_2}{y+}\,\frac{d_3}{y+}\cdots\right) = \tag{2.19c}$$

$$(\text{S}_2)\quad \frac{1}{y}\left(\frac{f_1}{(z+e_1)+}\,\frac{f_2}{(z+e_2)+}\,\frac{f_3}{(z+e_3)+}\cdots\right). \tag{2.19d}$$

The S_2-form can be obtained by comparing the n-th convergent of the S_2-form with the $(2n-1)$-th convergent of the S_1-form yielding

$$e_1 = d_2\,, \quad e_n = d_{2n-1} + d_{2n}\,;$$
$$f_1 = d_1 y\,, \quad f_n = -\,d_{2n-2}\,d_{2n-1}\,(n > 1)\,. \tag{2.20}$$

By setting $z = y = 1$ and using Eq. (2.20) we obtain

$$d_n = c_n \quad \forall n \geqq 1\,. \tag{2.21}$$

To obtain a given accuracy, the contracted S_2-form requires fewer terms to be evaluated than the usual S_1-form.

In the next section we present convenient recursive methods for the calculation of the expansion coefficients in the continued fraction equations (2.19a—2.19d).

3. Recursive Methods

A general method for the evaluation of the coefficients in the continued fractions is obtained by using the requirement that a formal expansion in powers of $1/z$ has the same coefficients as those in the series Eqs. (2.18a—2.18c) (matching method). Particularly, we find for the coefficients of the P-form [Eq. (2.19a)]:

$$b_1 = p_0\,, \quad b_2 = -\frac{(p_0\,p_2 - p_1^2)}{p_0^2}\,;$$
$$a_1 = \frac{p_1}{p_0}\,, \quad a_2 = \frac{p_0\,p_3 - p_1\,p_2}{p_0 p_2 - p_1^2} - \frac{p_1}{p_0}\,. \tag{3.1}$$

Using a result of Perron [20] for power series we obtain the formulas

$$b_n = -\frac{\varphi_n\,\varphi_{n-2}}{(\varphi_{n-1})^2}\,, \quad a_n = \frac{\psi_n}{\varphi_n} - \frac{\psi_{n-1}}{\varphi_{n-1}}\,, \tag{3.2}$$

where φ_n and ψ_n are given by the determinants

$$\varphi_n = \begin{vmatrix} p_0 & \cdots & p_{n-1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ p_{n-1} & \cdots & p_{2n-2} \end{vmatrix}, \quad \psi_n = \begin{vmatrix} p_0 & \cdots & p_{n-2}\,p_n \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ p_{n-1} & \cdots & p_{2n-3}\,p_{2n-1} \end{vmatrix} \tag{3.3a}$$

with

$$\varphi_0 = 1 \quad \text{and} \quad \psi_1 = p_1 . \tag{3.3b}$$

Obviously, Eqs. (3.2) and (3.3) can hardly be used for high order coefficients a_n and b_n since the calculation involves the evaluation of large determinants. However, the P-form has found wide application in the theory of statistical mechanics for the calculation of auto-correlation functions [10, 18, 21–24]. In the works of Mori [21] and Schneider [24] for equilibrium systems the coefficients a_n and b_n are obtained in terms of intractable expressions using projector methods.

The most convenient method for the calculation of the coefficients in the continued fractions consists of a recursive calculation scheme. Given the coefficients p_n or r_n we can construct the R-matrix defined by

$$\begin{aligned} &R_{1,1} = 1, \quad R_{n,1} = 0 , \\ &R_{n,2} = p_{n-1} = (-)^{n-1} r_{n-1} \quad \forall n \geqq 2 , \end{aligned} \tag{3.4}$$

where the further elements are obtained with use of the product-difference (PD) recursion relation of Gordon [25]:

$$R_{i,j} = R_{1,j-1} \cdot R_{i+1,j-2} - R_{1,j-2} \cdot R_{i+1,j-1} . \tag{3.5}$$

Within each column one starts at the top and works downwards. When a triangular portion of the R-matrix is filled, the coefficients of the R-form are given by [25]:

$$c_i = R_{1,i+1}/(R_{1,i} \cdot R_{1,i-1}) . \tag{3.6}$$

With the use of the coefficients $\{c_i\} = \{d_i\}$ given by Eq. (3.6) the coefficients $\{a_i\}$ and $\{b_i\}$ in the P-form can be obtained from Eq. (2.20) yielding

$$b_1 = c_1 , \quad a_1 = - c_2 \tag{3.7}$$

and

$$\begin{aligned} b_{n+1} &= - c_{2n} c_{2n+1} , \\ a_{n+1} &= - (c_{2n+1} + c_{2n+2}) . \end{aligned} \tag{3.8}$$

By use of Eq. (3.6) and Eq. (2.21) we obtain another recursive calculation scheme which is in general numerically more stable than the (PD) algorithm. This (P)-algorithm reads:

$$\begin{aligned} d_1 &= D_1 , & D_1 &= s_1 ; \\ d_2 &= - D_2/D_1 , & D_2 &= s_2 ; \\ d_3 &= - D_3/D_2 , & D_3 &= s_3 + s_2 d_2 ; \\ d_4 &= - D_4/D_3 , & D_4 &= s_4 + s_3 (d_2 + d_3) ; \\ d_5 &= - D_5/D_4 , & D_5 &= s_5 + s_4 (d_2 + d_3 + d_4) \\ & & &\quad + s_3 (d_2 d_4) \\ &\vdots & &\vdots \end{aligned} \tag{3.9}$$

The coefficients D_n for $n = 4, 5, \ldots$ can be calculated recursively using the auxiliary vector X of dimension L where

$$L = 2[(n-1)/2] . \tag{3.10}$$

For $n = 4$ we start in the following way (P-algorithm):

$$X(2) = d_2 + d_3 , \quad X(1) = d_2 , \tag{3.11a}$$

and interchange

$$X(2) \to X(1), \quad X(1) \to X(2) . \tag{3.11b}$$

For higher terms ($n \geqq 5$) we work upwards with $X(L-1) = 0$ obtaining

$$X(k) = X(k-1) + d_{n-1} X(k-2) \quad \text{for} \quad k = L, L-2, \ldots, 4 \tag{3.11c}$$

and

$$X(2) = X(1) + d_{n-1} \tag{3.11d}$$

and interchange at each recursion step the odd and the even components, i.e.

$$\begin{aligned} &X(2) \to X(1), \quad X(4) \to X(3); \\ &X(1) \to X(2), \quad X(3) \to X(4) \text{ etc.} \end{aligned} \tag{3.11e}$$

The coefficient d_n is then given by

$$d_n = - D_n/D_{n-1} , \tag{3.11f}$$

where

$$D_n = s_n + \sum_{i=1}^{L/2} s_{n-1} X(2i-1) . \tag{3.11g}$$

Both, the (P) and the (PD) algorithm have many points in common with Rutishauser's [26] quotient-difference (QD) algorithm. According to the sensitivity to round-off errors the logarithms must be calculated on a computer using double precision arithmetic. Here we stress that the coefficients in the continued fraction expansions Eqs. (2.19a–2.19d) remain the same in all finite approximations, i.e. a certain coefficient d_n is not changed when we calculate a higher continued fraction convergent.

4. Application of Continued Fraction Expansions

4.1. *Series with Orthogonal Polynomials*

In the following we apply the method of continued fractions to scattering problems with special emphasis on quantum mechanical problems. In theoretical analysis we have in general a series expansion into a complete set of some kind of orthogonal polynomials. In quantum mechanical scattering, for example, the expansion is the well-known partial-wave decomposition. Similar series occur in the theory of electromagnetic wave propagation or in the solution of the Boltzman equation.

For the application of the continued fraction method in these problems we introduce the "scattering amplitude"

$$f(\alpha_i; \Theta) = \sum_{l=0}^{\infty} c_l(\alpha_i) Z_l(\cos\Theta), \tag{4.1}$$

depending on the scattering angle Θ. The coefficients $c_l(\alpha_i)$ describe the process and the α_i are the relevant physical parameters. The functions $Z_l(\cos\Theta)$ denote any complete set of orthogonal polynomials, e.g. Legendre-, Chebyshev-, Jacobi-polynomials etc. The scattering amplitude is now rewritten in the form

$$f(\alpha_i; \Theta) = \sum_{l=0}^{\infty} \frac{a_l(\alpha_i)}{x^{l+1}} = \frac{1}{y} \sum_{l=1}^{\infty} \frac{a_{l-1}(\alpha_i)}{y^{2l-1}}, \tag{4.2a}$$

with

$$a_l(\alpha_i) = c_l(\alpha_i) Z_l(\cos\Theta) \quad \text{and} \quad y = \sqrt{x}, \tag{4.2b}$$

and where, of course, we have to set $x = y = 1$. But before doing so the continued fraction expansion (2.19c) is applied to this series and expanded at $y = 1$, thus obtaining

$$f(\alpha_i; \Theta) = \frac{d_1}{1+} \frac{d_2}{1+} \frac{d_3}{1+} \cdots \tag{4.3}$$

with the d_i's calculated with Equations (3.9—3.11). Of course, this approach is completely independent of the special choice of the orthogonal polynomials $Z_l(\cos\Theta)$. We will restrict ourselves in the following to the very important series for the associated Legendre polynomials $P_l^m(\cos\Theta)$, which are connected with the Legendre polynomials $P_l(\cos\Theta)$ by [2]

$$P_l^m(\cos\Theta) = (-)^m \frac{d^m}{d(\cos\Theta)^m} P_l(\cos\Theta), \quad l \geqq m. \tag{4.4}$$

Our method can be tested for a series in $P_l^m(\cos\Theta)$. From the well-known expansions

$$\sum_{=1}^{\infty} \frac{1}{l} P_l(\cos\Theta) = -\log\left(\sin\frac{\Theta}{2}\left(1 + \sin\frac{\Theta}{2}\right)\right), \tag{4.5a}$$

and

$$\sum_{l=1}^{\infty} \frac{1}{l+1} P_l(\cos\Theta) = \log \frac{1 + \sin\frac{\Theta}{2}}{\sin\frac{\Theta}{2}} - 1, \tag{4.5b}$$

we obtain by formal differentiation, using Eq. (4.4), the result

$$\sum_{l=m}^{\infty} \frac{(2l+1)}{l(l+1)} P_l^m(\cos\Theta) = (m-1)! \left(\frac{1 + \cos\frac{\Theta}{2}}{1 - \cos\frac{\Theta}{2}} \right)^{m/2} \quad \text{for} \quad m \geqq 1. \tag{4.6}$$

For $m = 1$ this series is similar to the partial wave expansion for elastically scattered protons from nuclei in the presence of a spin-orbit interaction [27]. Götz et al. [27] calculated the series using the Padé recursion method, discussed by Alder et al. [28].

The convergence properties of the series (4.6) can be analyzed using the asymptotic expression for large values of l for the polynomials $P_l^m(\cos\Theta)$:

$$P_l^m(\cos\Theta) = (-)^l \left(\frac{2}{\pi l \sin\Theta}\right)^{1/2} \cdot \cos\left(\left(l + \frac{1}{2}\right)\Theta - \frac{\pi}{4} + \frac{m\pi}{2}\right) + O(l^{-3/2})$$
$$\text{for} \quad \varepsilon \leqq \Theta \leqq \pi - \varepsilon, \quad \varepsilon > 0; \quad l \gg m, 1/\varepsilon. \tag{4.7}$$

Thus the terms in the series (4.6) behave asymptotically as $a_l(m) \sim l^{m-3/2}$. For the case $m = 1$ we have $a_l(1) \sim l^{-1/2}$, which leads to a very poor convergence of the series. For a given relative accuracy of 10^{-3} we have to sum up approximately 10^6 terms. Obviously, for the case $m > 1$ the series diverges. In Table 1 we present the values for this series obtained by the continued fraction method of order N (N-th convergent) when $m = 1$. It is seen that the continued fraction converges very rapidly to the exact value [r.h.s. Eq. (4.6)], with increasing N. This convergence behaviour is quite dependent on angle, for large scattering angles ($\Theta \lesssim 180°$) the convergence is much better than for small ones. The results for the formally divergent series ($m \geqq 2$) are shown in Table 2 for the case

Table 1. The N-th convergent of the continued fraction expansion for the series (4.6) with $m = 1$. The scattering angles are $\theta = 40°$, 100° and 160°, respectively.

N \ θ	40°	100°	160°
3	4.6908	0.62747	0.19041
6	3.4011	0.82395	0.17633
9	2.6678	0.83911	0.17633
12	2.7070	0.83910	.
15	2.7584	0.83910	.
18	2.7528	.	.
21	2.7462	.	.
24	2.7469	.	.
27	2.7476	.	.
30	2.7475	.	.
33	2.7475	0.83910	0.17633
exact	2.7475	0.83910	0.17633

Table 2. The N-th convergent of the continued fraction expansion for the series (4.6) with $m = 5$. The scattering angles are $\theta = 40°$, 100° and 160°, respectively.

N \ θ	40°	100°	160°
3	− 340.10	− 404.04	2.6134
6	− 380.80	61.881	− 0.033026
9	2300.2	7.4314	− 0.000136
12	3244.1	9.9607	0.0041035
15	3911.7	9.8559	0.0040911
18	3764.2	9.9834	0.0040908
21	3757.7	9.9834	0.0040908
24	3756.7	.	.
27	3757.5	.	.
30	3757.4	.	.
33	3757.4	9.9834	0.0040908
exact	3757.4	9.9834	0.0040908

$m = 5$. As can be seen, the continued fraction converges nearly as rapidly to the exact result as in the convergent case with $m = 1$. This means that the continued fraction expansion provides the correct analytic continuation of the divergent series in a straightforward way.

As a second example we study a divergent series resulting from the elastic scattering of a particle with charge $Z_1 e$ in the electric field of a nucleus with charge $Z_2 e$ (Rutherford scattering). It is well known (see e.g. Ref. [29]) that this process is described by the scattering amplitude

$$f(\eta; \Theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \cdot \exp\{2i(\sigma_l(\eta) - \sigma_0(\eta))\} P_l(\cos\Theta) \quad (4.8)$$
$$= -\frac{\eta}{2k} \frac{1}{\sin^2 \frac{\Theta}{2}} \exp\{-2i\eta \log(\sin\Theta/2)\},$$

where

$$\eta = Z_1 Z_2 e^2/\hbar v \quad \text{and} \quad k = m^* v/\hbar \quad (4.9)$$

denote the Coulomb parameter and wave number, respectively, of the particle with asymptotic velocity v and reduced mass m^*. The Coulomb phase shifts $\sigma_l(\eta)$ are given by

$$\sigma_l(\eta) = \arg \Gamma(l + 1 + i\eta). \quad (4.10)$$

This series was investigated in Ref. [28] using the Padé-approximation, and it was shown that the correct analytic continuation of the series can be obtained by this method.

In Tables 3 and 4 the results of the continued fraction method for the function $|f(\eta; \Theta)|$ are shown for some typical scattering angles and for $\eta = 10$ and $\eta = 100$, respectively. Again, the continued fraction expansion can be used to sum the divergent series. The order N of the continued fraction (N-th convergent), necessary to obtain a given accuracy, is about the same as the number of terms needed for the construction of the $[L/M]$-Padé-approximation which is $2M + L + 1$. This can be seen by comparing our results with those obtained by Alder et al. [28]. Again, both the continued fraction expansion and the Padé-approximation work best for large scattering angles and small values of η. The reason for this can be understood by physical arguments: in the classical limit the scattering with small Θ and large η corresponds to a large impact parameter and therefore the contributions to the series (4.8) come from higher l-values.

With this divergent series as a background, we now investigate two very slowly convergent series.

Table 3. The N-th convergent of the continued fraction expansion for the modulus of the Rutherford scattering amplitude for $\eta = 10$ and $k = 1$. The scattering angles are $\theta = 60°$, 120° and 180°, reseptively.

N \ θ	180°	120°	60°
6	5.0700	3.2366	0.03457
12	4.9992	7.5257	0.02949
18	5.0000	6.6702	0.05333
24	5.0000	6.6667	0.57953
30	.	6.6667	3.0322
36	.	.	24.395
42	.	.	19.823
48		.	20.000
54	5.0000	6.6667	20.000
exact	5.0000	6.6667	20.000

Table 4. The N-th convergent of the continued fraction expansion for the modulus of the Rutherford scattering amplitude for $\eta = 100$ and $k = 1$. The scattering angles are $\theta = 60°$, 120° and 180°, respectively.

N \ θ	180°	120°	60°
9	16.062		
15	50.278		
21	50.028		
27	50.008		
33	50.012		
39	50.000	0.00024	
45	50.000	0.00079	
.	.	.	
.	.	.	
.	.	.	
105		66.126	
111		66.714	
117		66.663	
123		66.667	
129		66.667	
.		.	
.		.	
.		.	
203			237.19
209			198.81
215	.	.	199.92
221	.	.	200.02
227	.	.	200.00
233	50.000	66.667	200.00
exact	50.000	66.667	200.00

First we deal with the scattering of a particle in a repulsive inverse square potential λr^{-2}. This process is described by the scattering amplitude

$$f(\lambda;\Theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\,e^{i\delta_l}\sin\delta_l\,P_l(\cos\Theta)\,, \tag{4.11}$$

where the phase shifts δ_l are given by [30]

$$\delta_l = \frac{\pi}{2}\left\{(l+\tfrac{1}{2}) - \sqrt{(l+\tfrac{1}{2})^2+\lambda}\right\}. \tag{4.12}$$

Since for large values of l the phase shifts behave asymptotically as $\delta_l \sim -\pi\lambda/4l$, the series (4.11) converges very slowly. Inserting this asymptotic expression for δ_l and using Eq. (4.5) we find

This series converges rapidly and the exact value of $f(\lambda;\Theta)$ can be obtained easily. The continued fraction expansion results for the original series (4.11) are shown in Table 5, where for simplicity only the absolute values of $f(\lambda;\Theta)$ are given. Again, a strong convergence improvement is obtained. The direct summation requires up to 10^6 terms for a relative accuracy of 10^{-3}. The series (4.11) was also studied by Corbella et al. [31], using the diagonal Padé-approximation. Table 5 was calculated for the same scattering angles as done by Corbella et al, so the two methods could be compared. It follows again that the continued fraction expansion of order N leads to roughly the same accuracy as a $[L/L]$-Padé-approximation, if $3L+1 \simeq N$. In contrast to the Padé-approximation, however, the calculation using a continued fraction of high order is straightforward and very fast, due to the use of recursive methods. The $[L/M]$-Padé-approximation requires the solution of a system of M linear

Table 5. The N-th convergent of the continued fraction expansion for the modulus of $f(\lambda;\theta)$ for the repulsive inverse square potential. We have chosen $\lambda = 1$ and $k = 1$ and the scattering angles are $\theta = 8°$, 18°, 38° and 58° respectively.

N \ θ	8°	18°	38°	58°
3	17.12	9.788	2.523	1.531
6	16.66	3.113	1.486	0.9397
9	7.116	3.672	1.576	0.8988
12	8.173	4.021	1.555	0.9054
15	11.46	3.825	1.552	0.9046
18	10.07	3.950	1.554	0.9045
21	9.517	3.898	1.554	0.9045
24	9.739	3.905	.	.
27	9.693	3.910	.	.
30	9.998	3.910	.	.
33	10.00	3.908		
36	9.992	3.908		
.		.		
.		.		
.		.		
54	9.906			
57	9.914	.	.	.
60	9.913	.	.	.
63	9.903	.	.	.
66	9.903	3.908	1.554	0.9045
exact	9.903	3.908	1.554	0.9045

$$\begin{aligned} f(\lambda;\Theta) = &-\frac{\pi\lambda}{4k\sin\frac{\Theta}{2}} + \frac{\sin^2\delta_0}{k} - i\,\frac{\pi^2\lambda^2}{8k}\log\left(\sin\frac{\Theta}{2}\left(1+\sin\frac{\Theta}{2}\right)\right) \\ &+\frac{1}{k}\sum_{l=0}^{\infty}\left((2l+1)\sin\delta_l\cos\delta_l + \frac{\pi\lambda}{2} + i\left((2l+1)\sin^2\delta_l - \frac{\pi^2\lambda^2}{8l}\right)\right)P_l(\cos\Theta)\,. \end{aligned} \tag{4.13}$$

equations with M unknown. For large M this may be time-consuming and may become numerically unstable.

We remark that the calculation of the coefficients d_l in a continued fraction expansion of high order may lead to numerical instabilities. This difficulty can be easily circumvented by summing some of the first terms in the original series and then applying the continued fraction expansion to the remainder series. (This method cannot easily be used for the $[L/M]$-Padé-approximation with the orthogonal polynomials!) Numerically, the total number of terms needed for a given accuracy is approximately equal to, or even smaller than the number needed for the complete series.

As a last example we study a series, frequently encountered in nuclear and atomic physics, where reactions in the presence of a Coulomb field [32] are described by

$$f(\varrho, \eta; \Theta) = \sum_{l=m}^{\infty} (2l+1)\, e^{2i\sigma_l(\eta)}\, R_l(\varrho, \eta)\, P_l^m(\cos\Theta). \tag{4.14}$$

The special type of the reaction is determined by the radial integrals $R_l(\eta, \varrho)$. As an example we choose the description of the elastic scattering of positively charged particles in the presence of a Yukawa potential, proportional to $e^{-\mu r}/r$, where $m = 0$. This case was investigated in detail in Ref. [28] using Padé-approximants. The radial integrals for this process are approximately given by

$$R_l(\varrho, \eta) = \tfrac{1}{2}\, e^{-\varrho}\, K_0\left(\varrho \sqrt{\eta^2 + l(l+1)}\right) \quad \text{with} \quad \varrho = \mu(\eta/k)\,, \tag{4.15}$$

where K_0 is the Bessel function of the third kind. The amplitude $f(\varrho, \eta; \Theta)$ for large values of the parameter η can be well approximated by [33]

$$f(\varrho, \eta; \Theta) \cong \frac{2\pi\eta}{\sin^2(\Theta/2)} \cdot \exp\left\{-i\left(2\eta \log\sin\frac{\Theta}{2} + \frac{\pi}{2}\right)\right\} \cdot e^{-\varrho} K_0\left(\frac{\varrho}{\sin(\Theta/2)}\right). \tag{4.16}$$

The convergence behaviour of the series (4.14) becomes immediately evident from the structure of the radial integrals (4.15): They decrease significantly only if $l \gg \eta$. In Fig. 1 we have plotted the number of terms in the continued fraction expansion necessary to obtain a relative accuracy of 10^{-5} and the corresponding number for the direct summation of the series (4.14) as a function of η for several typical values of ϱ. The scattering angle is chosen typically to be $\Theta = 180°$. The same is shown in Fig. 2, but for $\Theta = 150°$. As can be seen, the improvement of the convergence by using the continued fraction expansion is dramatic for large values of η and very dramatic for scattering angles $\Theta \sim 180°$. (Note, that about 20—100 terms in the original series have been summed up directly, as was discussed above.) For small values of η ($\eta \lesssim 10$) the convergence of the original sum is already good enough so that the application of the continued fraction method leads to no significant convergence improvement. Further, we have calculated the $[L/M]$-Padé-approximation to the series (4.14), showing that the corresponding continued fraction of order $N = 2M + L + 1$ leads in general to a much higher accuracy [28].

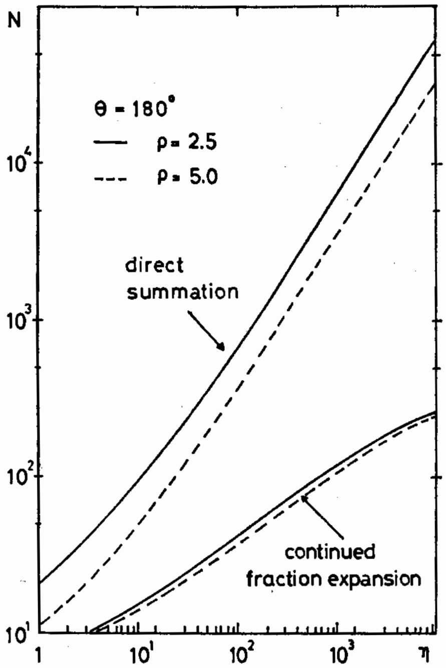

Fig. 1. The number of terms required for a relative accuracy of 10^{-5} for the continued fraction expansion or the direct summation of $|f(\varrho, \eta; \theta)|$ is shown as a function of η. The parameter $\varrho = 2.5$ (solid line) and $\varrho = 5.0$ (dashed line), respectively. The scattering angle is $\theta = 180°$.

Our selected examples for the application of the continued fraction expansion to series with orthogonal polynomials show that this method can be

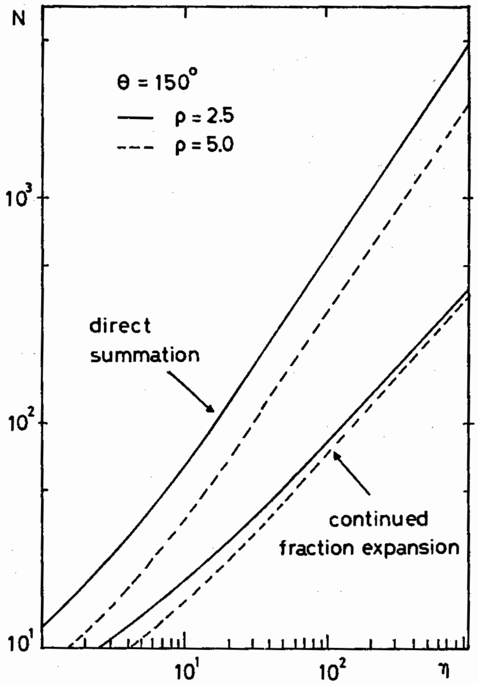

Fig. 2. Same as in Fig. 1, but for $\theta = 150°$.

used advantageously for the summation of all such slowly convergent series. Finally, we note that we have used complex coefficients $a_l(\alpha_l)$ in the calculation of the continued fraction. An alternative approach would be to split the original complex series in its real and imaginary parts and to use the continued fraction expansion separately for both series. Our results show that this approach is somewhat worse than the approach using complex coefficients. (Note that this statement holds also in the case of the Padé-approximation, as we have seen in numerical calculations.)

4.2. Asymptotic Solution of the Radial Schrödinger Equation

The continued fraction expansion is also a powerful method for the summation of asymptotic series [19]. Such series result, for example, from the asymptotic solution of the radial Schrödinger equation for Coulomb problems in presence of potentials of type

$$V(r) = V_0/r^\nu\,, \quad \nu \geqq 2\,. \tag{4.17}$$

This type of potential is used e.g. to describe relativistic effects in scattering theory ($\nu = 2$) or nuclear polarization effects ($\nu = 3$). The scattering of two point charges $Z_1 e$ and $Z_2 e$ in this potential leads to a radial Schrödinger equation of the form

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{2\eta\, k}{r} - \frac{l(l+1)}{r^2} - \frac{2m^*}{\hbar^2}\frac{V_0}{r^\nu}\right) g_l(r) = 0\,, \tag{4.18}$$

where l denotes the angular momentum.

The asymptotic form of the wave function is given by

$$g_l(r) = \frac{i}{2}\left(h_l^{(-)}(k\,r) - \alpha_l\, h_l^{(+)}(k\,r)\right), \tag{4.19}$$

where the coefficients α_l determine the cross section. The incoming and outgoing Coulomb waves $h_l{}^{(-)}$ and $h_l{}^{(+)}$ can be expressed in terms of the well-known regular and irregular Coulomb functions F_l and G_l by [2]

$$h_l^{(\pm)}(k\,r) = G_l(k\,r) \pm i\,F_l(k\,r)\,, \tag{4.20}$$

with the asymptotic behaviour

$$h_l^{(\pm)}(k\,r) \sim \cdot \exp\left\{\pm\, i\left(k\,r - \eta\log 2k\,r - l\frac{\pi}{2} + \sigma_l(\eta)\right)\right\}. \tag{4.21}$$

For the solution of Eq. (4.18) we now define a new wave function $H_l(r)$ by

$$H_l(r) = a_l(r) \cdot \exp\left\{i\left(k\,r - \eta\log 2k\,r - l\frac{\pi}{2} + \sigma_l(\eta)\right)\right\} \equiv \mathbb{G}_l(r) + i\,\mathbb{F}_l(r)\,, \tag{4.22}$$

where we impose the following asymptotic behaviour

$$\lim_{r\to\infty} H_l(r) = G_l(k\,r) + i\,F_l(k\,r) = h_l^{(+)}(k\,r)\,. \tag{4.23}$$

Inserting Eq. (4.22) into the differential equation (4.18) we obtain

$$\frac{\mathrm{d}^2 a_l(r)}{\mathrm{d}r^2} + 2i\left(k - \frac{\eta}{r}\right)\frac{\mathrm{d}a_l(r)}{\mathrm{d}r} + (i\,\eta - \eta^2 - l(l+1))\frac{a_l(r)}{r^2} - \frac{2m^*}{\hbar^2}\frac{V_0}{r^\nu}\, a_l(r) = 0\,. \tag{4.24}$$

For sufficiently large r, the function $a_l(r)$ can be expanded in terms of inverse powers of r, i.e.

$$a_l(r) = \sum_{n=0}^{\infty} A_n^l \frac{1}{r^n} = \sum_{n=0}^{\infty} g_n^l \frac{1}{r^n} + i \sum_{n=0}^{\infty} f_n^l \frac{1}{r^n}. \tag{4.25}$$

For the coefficients g_n and f_n we find the following recursion relations:

$$f_{n+1}^l = -\frac{1}{e_n}\left(g_n^l c_n - f_n^l d_n - \frac{2m^*}{\hbar^2} V_0 g_{n-\nu+2}^l\right) \tag{4.26a}$$

and

$$g_{n+1}^l = \frac{1}{e_n}\left(g_n^l d_n + f_n^l c_n + \frac{2m^*}{\hbar^2} V_0 f_{n-\nu+2}^l\right). \tag{4.26b}$$

In Eq. (4.26) we have used the abbreviations

$$\begin{aligned} c_n &= (n(n+1) - \eta^2 - l(l+1)), \\ d_n &= (2n+1)\eta, \\ e_n &= (n+1)2k. \end{aligned} \tag{4.27}$$

From the asymptotic behaviour (4.23) the initial conditions are determined by

$$\begin{aligned} g_0 &= 1, \quad & f_0 &= 0, \\ g_1 &= \frac{\eta}{k}, \quad & f_1 &= \frac{1}{2k}(\eta^2 + l(l+1)). \end{aligned} \tag{4.28}$$

The solution of Eq. (4.18) can now be represented by the functions $\mathbb{G}_l(r)$ and $\mathbb{F}_l(r)$ by

$$g_l(r) = \gamma_l \mathbb{F}_l(r) + \delta_l \mathbb{G}_l(r), \tag{4.29a}$$

and

$$\frac{d}{dr} g_l(r) = \gamma_l \frac{d}{dr}\mathbb{F}_l(r) + \delta_l \frac{d}{dr}\mathbb{G}_l(r). \tag{4.29b}$$

From the knowledge of the numerical solutions of the differential equation at some point r_0, the coefficients γ_l and δ_l are determined. The wave functions $g_l(r)$ are then completely known for all $r \geqq r_0$ by the functions $\mathbb{F}_l$ and $\mathbb{G}_l$ and therefore the coefficients α_l in Eq. (4.19) are determined.

It is seen from the definition of the function $a_l(r)$ and the above recursion relation that the expansion is an asymptotic series, which converges only in an asymptotic sense, i.e. for $r \to \infty$. However, it is often possible to obtain the value of such functions for finite r by terminating the summation of the series after a finite number of terms. This "convergence" behaviour can now be improved significantly by converting the series (4.25) into a continued fraction representation of the form of Equation (2.19c).

This analytic continuation in form of the continued fraction allows the calculation of the functions $\mathbb{F}_l(r)$ and $\mathbb{G}_l(r)$ respectively, at small values of r. The convergence of the truncated continued fraction can be tested by the Wronski-relation which is given by

$$\mathbb{G}_l(r)\frac{d}{dr}\mathbb{F}_l(r) - \mathbb{F}_l(r)\frac{d}{dr}\mathbb{G}_l(r) = k. \tag{4.30}$$

Numerical investigations have shown that for different values of V_0 and ν the functions $\mathbb{F}_l(r)$ and $\mathbb{G}_l(r)$ can be evaluated with the continued fraction expansion for r_0 given by

$$r_0 \geqq \frac{1}{2k}(\eta + \sqrt{\eta^2 + l(l+1)}). \tag{4.31}$$

As a typical example, the number of terms in the evaluation of the continued fraction is shown in Fig. 3 as a function of r, where a relative accuracy of 10^{-6} for α_l was required. Hereby we have used the parameters $\eta = 10$, $k = 1$ fm and angular momentum $l = 0$. The potential parameters are $V_0 = 50$ MeV and $\nu = 3$.

The above discussed method can always be used for potentials which can be expanded into a series in terms of inverse powers of r. Moreover, it is also possible to find an asymptotic expansion around

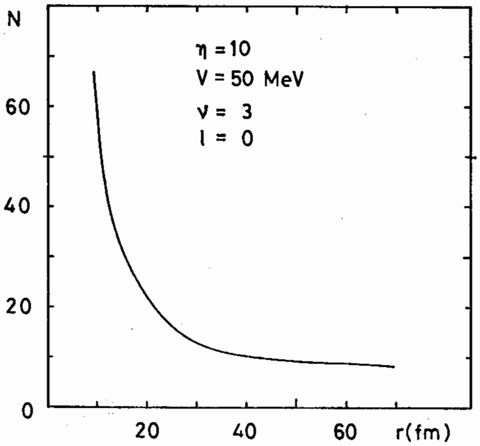

Fig. 3. The number of terms required for a relative accuracy of 10^{-6} for the continued fraction expansion of $\mathbb{F}_l(r)$ and $\mathbb{G}_l(r)$ is shown as a function of r. The parameters used are: $\eta = 10$, $k = 1$fm, $l = 0$, $V_0 = 50$ MeV and $\nu = 3$.

the origin, which can be continued by the continued fraction.

4.3. *Correlations and Response Functions for Stochastic Processes*

The stochastic behaviour of coarse-grained variables of a system can be described in most cases as a stochastic time-homogeneous Markov process $\boldsymbol{x}(t) = \{x_1(t), \ldots\}$ with a time-independent dissipative forward generator Γ [34—36]. If we study the linear response of the system to external dynamic forces $\boldsymbol{F}(t)$, the perturbed system can be described by a time-dependent generator $\hat{\Gamma}(t)$ of a non-stationary Markov process [35—36]:

$$\hat{\Gamma}(t) = \Gamma + \boldsymbol{F}(t)\,\boldsymbol{\Omega}^{\text{ext}}, \tag{4.32a}$$

yielding the master equation for the perturbed probability $\hat{p}(\boldsymbol{x}\,t)$:

$$\mathrm{d}\hat{p}(t)/\mathrm{d}t = \hat{\Gamma}(t)\,\hat{p}(t). \tag{4.32b}$$

The stochastic operators Γ and Ω_i are in general dissipative linear integro-differential operators acting on probability functions. Using functional derivatives the linear response tensor $\overset{\leftrightarrow}{\chi}(t-\tau)$ is then defined by the relation of the response of the state variables $\boldsymbol{x}(t)$*:

$$\begin{aligned}\overset{\leftrightarrow}{\chi}(t-\tau) &= \left.\frac{\delta\langle \boldsymbol{x}(t)\rangle^{\text{perturbed}}}{\delta \boldsymbol{F}(t)}\right|_{\boldsymbol{F}=\boldsymbol{0}} \\ &= \int \boldsymbol{x}\,\{\delta\hat{p}(\boldsymbol{x}(t))/\delta\boldsymbol{F}(\tau)\}_{\boldsymbol{F}=\boldsymbol{0}}\,\mathrm{d}\boldsymbol{x}. \end{aligned}\tag{4.33}$$

Here we have assumed that the perturbation is applied after the system has been prepared at time t_0 in a given stationary state described by the stationary probability function $p_{\text{st}}(\boldsymbol{x})$ of the unperturbed Markov system

$$\Gamma p_{\text{st}} = 0. \tag{4.34}$$

The response tensor $\overset{\leftrightarrow}{\chi}(t)$ can be expressed in the form of a generalized fluctuation theorem, first discussed by Hänggi and Thomas [36]. The theorem can be written as a correlation over the unperturbed stationary system

$$\overset{\leftrightarrow}{\chi}(\tau) = \Theta(\tau)\,\langle(\boldsymbol{x}(\tau) - \langle\boldsymbol{x}\rangle^{\text{unperturbed}})\,\boldsymbol{\Phi}(\boldsymbol{x}(0))\rangle \tag{4.35a}$$

$$= \Theta(\tau)\int(\boldsymbol{x} - \langle\boldsymbol{x}\rangle^{\text{unperturbed}})\,[e^{\Gamma\cdot\tau}\boldsymbol{\Phi}\,p_{\text{st}}]_{\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x}, \tag{4.35b}$$

* Here we use the notation $\boldsymbol{x}(t)$ to denote the stochastic process as well as for the random variables $\boldsymbol{x}(t)$ at time t. The specific meaning will be understood from the context

where $\boldsymbol{\Phi}(\boldsymbol{x})$ is in general a non-linear fluctuation:

$$\boldsymbol{\Phi}(\boldsymbol{x}) = [\boldsymbol{\Omega}\,p_{\text{st}}]_{\boldsymbol{x}}/p_{\text{st}}(\boldsymbol{x}), \tag{4.36a}$$

with

$$\langle\boldsymbol{\Phi}(\boldsymbol{x})\rangle = \int\boldsymbol{\Phi}(\boldsymbol{x})\,p_{\text{st}}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = 0. \tag{4.36b}$$

In Eq. (4.35) $\Theta(\tau)$ denotes the step function. In practice, the calculation of a correlation function, $c(\tau)$, of two state functions $g(\boldsymbol{x})$ and $f(\boldsymbol{x})$,

$$c(\tau) = \langle g(\boldsymbol{x}(\tau))\,f(\boldsymbol{x}(0))\rangle, \tag{4.37}$$

and response functions $\chi_{ij}(\tau)$ in terms of the exact stationary joint probability $p^{(2)}(\boldsymbol{x}(\tau);\boldsymbol{x}(0))$ of the unperturbed stationary Markov process $\boldsymbol{x}(t)$ is intractable. Usually the calculations require a great deal of numerical analysis to determine the eigenvalues and left and right eigenvectors of the, in general, non-symmetric generator Γ. Therefore, approximation methods requiring the minimum of computer time and human effort are very important.

By using the Taylor series expansion of Eq. (4.35), the component $\chi_{ij}(\tau)$ becomes

$$\chi_{ij}(\tau) \equiv \chi(\tau) = \Theta(\tau)\sum_{n=0}^{\infty}\frac{p_n}{n!}\tau^n, \quad \tau \geqq 0. \tag{4.38}$$

The static moments p_n are given by

$$\begin{aligned} p_n &= \left.\frac{d^n\chi(\tau)}{\mathrm{d}\tau^n}\right|_{\tau=0^+} \\ &= \int(x_i - \langle x_i\rangle^{\text{unperturbed}})\,[\Gamma^n\,\Phi_j\,p_{\text{st}}]_{\boldsymbol{x}}\,\mathrm{d}\boldsymbol{x} \end{aligned}\tag{4.39a}$$

$$= \langle\langle(x_i - \langle x_i\rangle^{\text{unperturbed}})\,\Gamma^n\,\Phi_j\rangle\rangle. \tag{4.39b}$$

Equation (4.35) can be rewritten in terms of conditional averages

$$\begin{aligned}\chi_{ij}(\tau) = \Theta(\tau)\,\langle\Phi_j(\boldsymbol{x}(0))& \\ \cdot\langle(x_i(\tau) - \langle x_i\rangle^{\text{unperturbed}})\,|\,\boldsymbol{x}(0)\rangle\rangle&, \end{aligned}\tag{4.40}$$

where the time evolution of the conditional average is governed by the backward generator Γ^+

$$(\Gamma^+(\boldsymbol{x},\boldsymbol{y}) = \Gamma(\boldsymbol{y},\boldsymbol{x})).$$

Hence the moments p_n can often be written more simply in terms of the backward generator Γ^+:

$$\begin{aligned} p_n &= \int[(\Gamma^+)^n_{y_i}]_{\boldsymbol{x}}\,\Phi_j(\boldsymbol{x})\,p_{\text{st}}(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \\ &= \langle[(\Gamma^+)^n_{y_i}]_{\boldsymbol{x}}\,\Phi_j(\boldsymbol{x})\rangle. \end{aligned}\tag{4.41}$$

The Fourier transform $\chi(\omega)$ of $\chi(\tau)$,

$$\chi(\omega) = \lim_{\varepsilon \downarrow 0} \int_0^\infty \exp(\tau(i\,\omega - \varepsilon))\,\chi(\tau)\,d\tau\,, \quad (4.42)$$

can be written with Eq. (4.38) in terms of the sum rule expansion as

$$\chi(\omega) = \sum_{n=0}^{\infty} \frac{p_n}{z^{n+1}}\,, \quad \text{where} \quad z = -\,i\,\omega\,. \quad (4.43)$$

The powerful methods described in Sects. 2 and 3 can now be used to calculate the Fourier transform $\chi(\omega)$ of the response function $\chi(\tau)$ or to calculate the Laplace transform $c(\omega)$ of a general stationary correlation function $c(\tau)$. By applying the continued fraction method to Eq. (4.43) we obtain

$$\begin{aligned}\chi(\omega) &\equiv \chi'(\omega) + i\,\chi''(\omega)\\ &= \frac{b_1}{(z-a_1)+}\,\frac{b_2}{(z-a_2)+}\cdots \quad (4.44)\\ &= \frac{c_1}{z+}\,\frac{c_2}{1+}\,\frac{c_3}{z+}\cdots.\end{aligned}$$

The continued fraction expansions are completely determined by the static moments p_n.

The imaginary part of $\chi(\omega)$, $\chi''(\omega)$, describes the dissipation in conservative systems. $\chi''(\omega)$ has the S-form

$$\begin{aligned}\chi''(\omega) &= \sum_{n=1}^{\infty} \frac{s_n}{\omega^{2n-1}}\\ &= \frac{d_1}{\omega+}\,\frac{d_2}{\omega+}\cdots, \; s_n = (-)^{n+1}\,p_{2n-2}\,.\end{aligned} \quad (4.45)$$

For a one-dimensional Gauss-Markov process with a gradient type perturbation,

$$\Omega^{ext} = -\,\nabla\,, \quad (4.46)$$

the response function $\chi(\tau)$ can be written in terms of the relaxation rate γ as [35—36]

$$\chi(\tau) = \Theta(\tau)\exp(-\,\gamma\,\tau), \quad \gamma > 0\,. \quad (4.47)$$

Using the moments

$$p_0 = 1, \quad p_n = (-)^n\,\gamma^n, \quad n \geqq 1\,, \quad (4.48)$$

we have

$$c_1 = 1, \quad c_2 = \gamma, \quad c_i = 0, \quad i \geqq 3\,, \quad (4.49)$$

which gives the exact result for Eq. (4.42)

$$\chi(\omega) = 1/(-\,i\,\omega + \gamma)\,. \quad (4.50)$$

More generally, for a response function $\chi(\tau)$ consisting of a finite number of exponential terms,

$$\chi(\tau) = \sum_{n=0}^{N} a_n\,e^{-\lambda_n \tau}$$

the continued fraction in Eq. (4.44) terminates and yields the exact result.

For all problems with a finite discrete state space of N different states, the generator Γ is an ordinary stochastic matrix $\overleftrightarrow{\Gamma}$. A general correlation function will then be given by a finite sum of exponentials whose inverse relaxation times $\{\lambda_n\}$ are identical with the eigenvalues of $-\overleftrightarrow{\Gamma}$. Hence the straightforward application of the continued fraction technique in the P-form Eq. (4.44) yields an exact result after N-steps. This eliminates the numerical analysis needed to determine the eigenvalues and all the eigenvectors of $\overleftrightarrow{\Gamma}$! The continued fraction method only requires the specific form of the generator and the right eigenvector for eigenvalue $\lambda_n = 0$, the stationary probability.

The initial relaxation functions $\langle g(\boldsymbol{x}(t))\rangle$ for a system prepared in a non-stationary state at time t_0 with the initial probability $p_0(\boldsymbol{x}\,t_0)$, can also be determined using the same techniques. Using the propagator $R(\tau) = \exp(\Gamma\,\tau)$ of the unperturbed master equation, the non-stationary probability at time t, $p(\boldsymbol{x}\,t)$, becomes

$$p(t) = R(t-t_0)\,p_0 = \exp\{\Gamma(t-t_0)\}\,p_0\,. \quad (4.51)$$

Hence, the moments $\{g_n\}$ of the Taylor series for the relaxation function $\langle g(\boldsymbol{x}(t))\rangle$ are

$$g_n = \int g(\boldsymbol{x})\,[\Gamma^n\,p_0]_{\boldsymbol{x}}\,d\boldsymbol{x}, \quad n = 0, 1, \ldots. \quad (4.52)$$

5. Lower and Upper Bounds

In practice we must terminate the infinite continued fraction at a finite order. So far, in this paper, the quality and consequence of such finite approximations have not been discussed. In recent works on Padé-approximations, correction terms have been derived which give upper and lower bounds for the exact result [1, 25, 37]. This is even possible in cases in which the actual exact result is not known. Here we study some applications to the theory of stationary stochastic processes by using theory of Stieltjes series [38]. For a vectorial stochastic Markov process $\boldsymbol{x}(t) = \{x_1(t), \ldots\}$ which fulfills the strong detailed balance condition [35] the real stochastic dissipative operator Γ can be symmetrized by

$$\bar{\Gamma} = \bar{\Gamma}^{+} = p_{\rm st}^{-1/2}\,\Gamma\, p_{\rm st}^{1/2}\,, \tag{5.1}$$

where $p_{\rm st}$ again denotes the unique stationary probability function. The symmetric dissipative operator $\bar{\Gamma}$ may have eigenfunctions $\psi_\nu(\boldsymbol{x})$ and eigenvalues $\lambda_\nu \leqq 0$. Assuming that the set of eigenfunctions form a complete set (i.e. $\bar{\Gamma}$ is even self-adjoint)

$$\delta(\boldsymbol{x}-\boldsymbol{y}) = \widehat{\sum_\nu\!\!\int} \mathrm{d}\nu\, \psi_\nu(\boldsymbol{x})\, \psi_\nu(\boldsymbol{y})\,, \tag{5.2}$$

we have for $\bar{\Gamma}$ the spectral representation

$$\bar{\Gamma} = \widehat{\sum_\nu\!\!\int} \mathrm{d}\nu\, \lambda_\nu\, |\psi_\nu\rangle\langle\psi_\nu|\,. \tag{5.3}$$

The stationary two-time joint-probability $p^{(2)}$ then is

$$p^{(2)}(\boldsymbol{x},\boldsymbol{y};\tau) = (p_{\rm st}(\boldsymbol{x})\, p_{\rm st}(\boldsymbol{y}))^{1/2} \cdot \sum_\nu\!\int \mathrm{d}\nu\, \psi_\nu(\boldsymbol{x})\, \psi_\nu(\boldsymbol{y})\, e^{\lambda_\nu|\tau|}\,. \tag{5.4}$$

For an auto-correlation function $S(\tau)$ of any state function $g(\boldsymbol{x})$,

$$S(\tau) = \langle g(\boldsymbol{x}(\tau))\, g(\boldsymbol{x}(0))\rangle = \sum_{n=0}^{\infty} (-)^n \frac{r^n}{n!}\, \tau^n\,, \tag{5.5}$$

the static moments,

$$\begin{aligned} r_n &= (-)^n \left.\frac{\mathrm{d}^n S(\tau)}{\mathrm{d}\tau^n}\right|_{\tau=0^+} \\ &= (-)^n \int \mathrm{d}\boldsymbol{x}\, g(\boldsymbol{x})\, [\Gamma^n g\, p_{\rm st}]_{\boldsymbol{x}} \\ &\quad \text{for} \quad n = 0, 1, \ldots, \end{aligned} \tag{5.6}$$

can be expressed in terms of a Stieltjes integral by using Eq. (5.4):

$$r_n = \int_0^\infty u^n\, \mathrm{d}p(u)\,, \tag{5.7}$$

where

$$\mathrm{d}p(u)/\mathrm{d}u = \widehat{\sum_\nu\!\!\int} \mathrm{d}\nu\, \delta(|\lambda_\nu| - u)\, |\langle p_{\rm st}^{1/2}\, g\,|\,\psi_\nu\rangle|^2 \geqq 0. \tag{5.8}$$

In particular, r_0 is given by

$$S(O^+) = r_0 = \widehat{\sum_\nu\!\!\int} \mathrm{d}\nu\, |\langle p_{\rm st}^{1/2}\, g\,|\,\psi_\nu\rangle|^2 < +\infty\,, \tag{5.9}$$

so that with Eq. (5.8) $p(u)$ is a bounded monotonic non-decreasing function. Therefore, the Laplace transform $S(\omega)$ for real ω,

$$S(\omega) = \int_0^\infty \mathrm{d}\tau\, S(\tau)\, e^{-\omega\tau} \quad \text{with} \quad \omega > 0, \tag{5.10a}$$

can be written with Eq. (5.5) as a Stieltjes series of the form

$$S(\omega) = \sum_{n=0}^{\infty} (-)^n\, r^n/\omega^{n+1}\,. \tag{5.10b}$$

The powerful methods developed for Stieltjes series [38] can then be used directly. The function $S(\omega)$* has then a Stieltjes integral representation

$$S(\omega) = \int_0^\infty \frac{\mathrm{d}p(u)}{\omega+u} \quad \text{with} \quad \omega > 0\,. \tag{5.11}$$

The Laplace transform $S^{(n)}(\omega)$ of the n-th time-derivative of the auto-correlation $S(\tau)$ becomes

$$S^{(n)}(\omega) = \omega^n\, S(\omega) - \sum_{i=1}^{n} \omega^{n-i}\, (-)^{i-1}\, r_{i-1}\,; \quad n = 1, 2, \ldots\,. \tag{5.12}$$

The functions $S^{(n)}(\omega)$ are for even n a Stieltjes series with $\mathrm{d}p^{(n)}(u) = u^n \mathrm{d}p(u)$ and for odd n a negative Stieltjes series. The Stieltjes series can be replaced by its "correrponding continued fractions" $c^{(n)}(\omega)$ of the R-form. If we consider a sequence of approximants $c_k{}^{(n)}(\omega)$, obtained by setting

$$c_{k+1}^{(n)} = c_{k+2}^{(n)} = \cdots = 0$$

the best upper and lower bounds are obtained. [This follows from Eq. (5.11) and Eqs. (5.17) to (5.18)]:

$$c_{2k+1}^{(n)}(\omega) \geqq (-)^n\, S^{(n)}(\omega) \geqq c_{2k}^{(n)}(\omega) \quad \text{for} \quad n, k = 0, 1, \ldots\,. \tag{5.13}$$

Note also that for a general continued fraction with only positive elements the odd and even approximants always yield monotonically decreasing upper bounds and monotonically increasing lower bounds [20]. The Stieltjes continued fraction

$$c^{(n)}(z) = \frac{c_1{}^{(n)}}{z+}\,\frac{c_2{}^{(n)}}{1+}\,\frac{c_3{}^{(n)}}{z+}\cdots \tag{5.14}$$

converges for all complex $z \notin (-\infty, 0]$ uniformly to a regular analytic function

$$S(z) = \int_0^\infty \frac{\mathrm{d}p^{(n)}(u)}{z+u} \quad \text{if [39]} \sum_{\nu=1}^{\infty} b_\nu \quad \text{diverges,} \tag{5.15}$$

* Note that the function in Eq. (5.10b) is in general not identical with the function in (5.11), but represents an asymptotic series of the functions in (5.10a) and (5.11).

where

$$b_1 = \frac{1}{c_1^{(n)}}, \quad b_{2\nu+1} = \frac{c_2^{(n)} c_4^{(n)} \dots c_{2\nu}^{(n)}}{c_1^{(n)} c_3^{(n)} \dots c_{2\nu+1}^{(n)}},$$
$$b_{2\nu} = \frac{c_1^{(n)} c_3^{(n)} \dots c_{2\nu-1}^{(n)}}{c_2^{(n)} c_4^{(n)} \dots c_{2\nu}^{(n)}}. \quad (5.16)$$

The asymptotic expansion of $S(z)$ is then given by a series like that of Equation (5.10b). If the sum in Eq. (5.15) converges, the continued fraction is divergent for all $z \in \mathbb{C}$.

Of most practical use are the approximate quadrature formulas due to Skohat and Tomarkin [38] and Gordon [25]. Given only a finite number of static moments r_n for $n = 0, 1, \dots, 2M-1$ one can derive the following approximative quadrature formulas for an arbitrary Stieltjes-integrable state function f:

$$\int_0^\infty f(u)\, \mathrm{d}p^{(n)}(u) = \sum_{i=1}^{M} \varrho_{iM}^{(n),e} f(y_{iM}^{(n),e}) + \frac{c_{2M}^{(n)} c_{2M+1}^{(n)} f^{(2M)}(\xi)}{(2M)!}, \quad (5.17)$$

or

$$\int_0^\infty f(u)\, \mathrm{d}p^{(n)}(u) = \sum_{i=1}^{M} \varrho_{iM}^{(n),0} f(y_{iM}^{(n),0}) + \frac{\tilde{c}_{2M-1}^{(n)} \tilde{c}_{2M-2}^{(n)} f^{(2M-1)}(\xi)}{(2M-1)!}, \quad (5.18)$$

where $\xi \in (0, \infty)$ and the coefficients $\{c\}$ and $\{\tilde{c}\}$ are all positive for a monotonic non-decreasing bounded function $p^{(n)}(u)$. The parameters in Eqs. (5.17) and (5.18) can be found from the finite approximants

$$c_{2M}^{(n)}(\omega) = \sum_{i=1}^{M} \frac{\varrho_{iM}^{(n),e}}{\omega + y_{iM}^{(n),e}}, \quad \text{e: even}, \quad (5.19)$$

and

$$c_{2M-1}^{(n)}(\omega) = \sum_{i=1}^{M} \frac{\varrho_{iM}^{(n),0}}{\omega + y_{iM}^{(n),0}}, \quad \text{o: odd}, \quad (5.20)$$

with

$$y_{1M}^{(n),0} = 0. \quad (5.21)$$

Following Gordon [25] a direct calculation of the parameters in Eqs. (5.17) and (5.18) consists in a diagonalisation procedure for the symmetric tridiagonal matrix $\overleftrightarrow{M}$:

$$\overleftrightarrow{M} = \begin{pmatrix} c_2^{(n)} & -(c_2^{(n)} c_3^{(n)})^{1/2} & & & 0 \\ -(c_2^{(n)} c_3^{(n)})^{1/2} & (c_3^{(n)} + c_4^{(n)}) & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ 0 & & & -(c_{2M-2}^{(n)} c_{2M-1}^{(n)})^{1/2} & (c_{2M-1}^{(n)} + c_{2M}^{(n)}) \end{pmatrix}. \quad (5.22)$$

Using the orthogonal transformation matrix $\overleftrightarrow{U}$ the parameters $y_{iM}^{(n),e}$ are then given by the eigenvalues

$$y_{iM}^{(n),e} = (\overleftrightarrow{U}^{-1} \overleftrightarrow{M} \overleftrightarrow{U})_{ii} \quad (5.23)$$

and the weight factors by

$$\varrho_{iM}^{(n),e} = c_1^{(n)} U_{1i}^{(2)}; \quad c_1^{(n)} = r_0^{(n)}. \quad (5.24)$$

The odd parameters are obtained by setting the $c_{2M}^{(n)}$ in the original matrix $\overleftrightarrow{M}$ equal to zero.

By using the Taylor series for the auto-correlation function

$$S(\tau) = \sum_{n=0}^{\infty} (-)^n \frac{r_n}{n!} \tau^n, \quad \tau \geqq 0, \quad (5.25)$$

we find together with Eq. (5.7) for the n-th time derivative of $S(\tau)$

$$\frac{\mathrm{d}^n S(\tau)}{\mathrm{d}\tau^n} = (-)^n \int_0^\infty e^{-u\tau} \mathrm{d}p^{(n)}(u), \quad n = 0, 1, 2, \dots. \quad (5.26)$$

Using the quadrature formulas with $f(u) = e^{-u\tau}$ the best upper and lower bounds become

$$\sum_{i=1}^{M} \varrho_{iM}^{(n),0} \exp(-y_{iM}^{(n),0} \tau) \geqq (-)^n \frac{\mathrm{d}^n S(\tau)}{\mathrm{d}\tau^n} \geqq \sum_{i=1}^{M} \varrho_{iM}^{(n),e} \exp(-y_{iM}^{(n),e} \tau), \quad n \notin \mathbb{N} \cup \{0\}. \quad (5.27)$$

The relations in Eqs. (5.27) and (5.13) also have wide application in equilibrium statistical thermodynamics, where the following fluctuation-dissipation-theorem holds [18, 35,36]

$$\chi(\tau) = -\Theta(\tau)\,\beta\frac{\mathrm{d}}{\mathrm{d}\tau}S(\tau)\,. \tag{5.28}$$

Here, β denotes the Boltzmann factor. In addition, the Fourier transform $\chi(i\omega) = -\beta\cdot S^{(1)}(\omega)$ fulfills as a consequence of the Kramers-Kronig-relation the sum rule

$$-\beta\int_0^\infty S^{(1)}(\omega)\,\mathrm{d}\omega = \int_0^\infty \chi''(\omega)\,\mathrm{d}\omega\,, \tag{5.29}$$

where the left hand side can be approximated by the error bounds from Equation (5.13).

As a physical example for the theory, we consider the dynamical behaviour of a bi-stable tunnel diode undergoing a non-equilibrium phase transition [34], [40]. If $p(Nt)$ is the probability that there are N electrons on the diode capacitance at time t, the master equation for the rate of change of the probability $p(Nt)$ is given by the Fokker-Planck equation

$$\frac{\partial p(Nt)}{\partial t} = [\Gamma p(t)]_N \tag{5.30}$$

$$= -\frac{\partial}{\partial N}\left(A(N)\,p(Nt) - \frac{\partial}{\partial N}(D(N)\,p(Nt))\right).$$

This system obeys a strong detailed balance condition yielding for the probability current $I(N)$:

$$I(N) = A(N)\,p_{\mathrm{st}}(N) - \frac{\partial}{\partial N}(D(N)\,p_{\mathrm{st}}(N)) = 0\,. \tag{5.31}$$

The symmetric operator $\bar{\Gamma}$ becomes in this case

$$\bar{\Gamma} = \frac{\mathrm{d}}{\mathrm{d}N}D(N)\frac{\mathrm{d}}{\mathrm{d}N} - \frac{1}{4}\left(\frac{\bar{A}(N)^2}{D(N)} + 2\frac{\partial}{\partial N}\bar{A}(N)\right), \tag{5.32}$$

with

$$\bar{A}(N) = A(N) - \mathrm{d}D(N)/\mathrm{d}N\,. \tag{5.33}$$

Hence, if an imaginary time is introduced, the physical system can be described by the Schrödinger equation for a particle with a "space"-dependent mass in a potential. For the diode, the drift $A(N)$ and diffusion $D(N)$ are given by [40]

$$A(N) = \lambda + |i_Z(N)| - i_E(N) - i_T(N)\,, \tag{5.34}$$

$$D(N) = \tfrac{1}{2}(\lambda + |i_Z(N)| + i_E(N) + i_T(N))\,. \tag{5.35}$$

The Esaki current i_E and the thermal current i_T tend to discharge the diode capacitance, whereas the Zener current i_Z and the supply current λ (pump parameter) tend to charge the diode capacitance. The auto-correlation function $S(\tau)$ of the fluctuations of the charge number N on the diode capacitance is then

$$S(\tau) = \langle \delta N(\tau)\,\delta N(0)\rangle\,, \tag{5.36}$$

with

$$\delta N(\tau) = N(\tau) - \langle N\rangle_{\mathrm{st}}\,. \tag{5.37}$$

The results in Eq. (5.27) can now be applied directly using the moments

$$r_n = (-)^n\langle\langle \delta N(0)\,\Gamma^n\,\delta N(0)\rangle\rangle \tag{5.38}$$

and can be compared with the exact results for the physical system. Using $M = 1$ and Eq. (5.27) the upper and lower bounds $S(\tau)$ are given by

$$r_0 = S(O^+) \geqq S(\tau) \tag{5.39}$$

$$\geqq S(O^+)\exp\left(-\frac{r_1}{r_0}\tau\right),\quad \tau \geqq 0\,.$$

Using the first four moments r_0, r_1, r_2, r_3 we find

$$\frac{r_2 r_0 - r_1^2}{r_2} + \frac{r_1^2}{r_2}\exp\left(-\frac{r_2}{r_1}\tau\right) \geqq S(\tau) \geqq r_0\,(1-a)\cdot\exp(-y_1\tau) + r_0\,a\cdot\exp(-y_2\tau)\,, \tag{5.40}$$

with a, y_1, y_2 given by Eqs. (5.23)–(5.24). An equivalent result for the auto-correlation of the intensity fluctuations in a single mode Laser has been given by Smith [41] using the Risken-Fokker-Planck equation [42]. Further, the results developed here can be used to test the accuracy of the auto-correlation functions obtained in a recent work on non-linear brownian motion [23] and on diffusion inperiodic potentials in superionic conductors [43].

6. Conclusions

In the present paper we have considered some of the main aspects of the practical application of continued fraction expansions in scattering theory and in the calculation of response and correlation functions in statistical problems.

The different problems considered could not be represented directly in a continued fraction form, but by using the efficient recursive algorithms developed in Sect. 3 they can be recast in the correct form. The most convenient method would allow the direct construction of the continued fraction coefficients since this by passes the possible numerical instability in the usual method of moments. Recently, this has been possible for calculations of oscillator strength distributions in atoms [44] and for the calculation of wave vector dependent diffusion coefficients derived from the Boltzmann equation [45].

In this paper we have also found suitable correction terms and bounds for a finite approximation of a continued fraction. The generalization to more complicated situations than those discussed in Sect. 5 with rigorous bounds on the physical functions is very desirable. Moreover, it would be interesting if continued fraction expansions could be established on more physical grounds. Further, the results derived in this paper challenge to establish the mathematical and physical conditions under which the continued fractions or Padé-approximants provide the correct analytic continuation.

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