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—5]. 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 Chap. 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 Chap. 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 assessment of the accuracy of the approximation. In Sect. 5 a method for finding the best error bounds for the auto-correlation functions and their time-derivatives of stationary Markov processes is given. The results obtained are briefly discussed in Chap. 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 expans-
sions [1, 5, 13–15]. Let the set \( \{a_n\} \) denote analytical functions which allow a Taylor series expansion about the origin. If the functions \( f_n(z) \) obey the recursion relation
\[
f_n(z) = a_0 + \frac{b_{n+1}}{z} + \frac{f_{n+1}(z)}{z}, \quad z \in C, \tag{2.1}
\]
where the sets \( \{a_n\}, \{b_n\} \) denote complex numbers, we obtain the continued fraction
\[
f_n(z) = a_0 + \frac{b_1}{z} a_1 + \frac{b_2}{z^2} a_2 + \cdots \tag{2.2}
\]
By means of an equivalence transformation (1) we get from Eq. (2.2)
\[
f_n(z) = a_0 + \frac{b_1}{z} + \frac{b_2}{z^2} + \cdots \tag{2.3}
\]
with
\[
b_1 = \frac{b_1}{a_1} \quad \text{and} \quad b_i = -\frac{b_i}{a_i a_{i-1}} \quad \forall i \geq 2. \tag{2.4}
\]
Expansion of Eq. (2.3) yields
\[
f_n(z) = a_0 + \frac{b_1 z}{1 - b_2 z^2 + O(z^2)} = \sum_{k=0}^{\infty} a_k z^k, \tag{2.5}
\]
showing the relationship of the continued fraction to the corresponding Taylor series of \( f_n(z) \).

If the number of terms in Eq. (2.3) is infinite, \( f_n(z) \) is called an infinite continued fraction and the terminated fraction
\[
R^n_n(z) = A_n(z)/B_n(z) \tag{2.6}
\]
is called the \( n \)-th convergent of \( f_n(z) \). The coefficients \( \{b_n\} \) in Eq. (2.3) are set zero for \( k \geq n + 1 \). The functions \( A_n(z), B_n(z) \) satisfy the recursion relations
\[
A_0(z) = a_0, \quad B_0(z) = 1 \tag{2.7a}
\]
and
\[
A_{n+1}(z) = A_n(z) + b_{n+1} z A_{n-1}(z) \tag{2.7b}
\]
From the theory of Padé-approximants the sequence of convergents of the "corresponding continued fraction" to the Taylor series occupies the state-space of Padé-approximants [1]
\[
[\text{[01]}, \{11\}, \{21\}, \ldots, \text{where}
L_n(z) = \frac{P_n(z)}{Q_n(z)}, \tag{2.8}
\]
with \( Q_n(0) = 1 \) and \( M \) denote the degree of the polynomials \( P_n \) and \( Q_n \), 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 \( b_n \) in Eq. (2.3) have the property
\[
\lim_{n \to \infty} b_n = b \neq 0, \tag{2.9}
\]
then within every simply connected region \( T \) in \( C \), containing the origin and no point of the branch
\[
g = \frac{1}{4b} + i \left( \text{Re} \left( \frac{1}{4b} \right) \right), \tag{2.10}
\]
the continued fraction is a regular (except for the poles) analytic function and coincides in the region about the origin with the corresponding series. It is the case where the coefficients \( b_n \) have the property
\[
\lim_{n \to \infty} b_n = 0, \tag{2.11}
\]
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 \( b_n z = a_n z \)
\[
f_n(z) = a_0(1 + f_{n+1}(z)), \tag{2.12}
\]
and by setting \( f_{n+1} = f_n = f_0 \) an approximation of the tail becomes
\[
f_n = -\frac{1}{4} \left( 1 - i + 4a_n \right) = \frac{2a_n}{1 + i + 4a_n}. \tag{2.13}
\]
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:
\[
a^x = 1 + \frac{(a-1)x}{1} + \frac{(a-1)x(x-1)}{2} + \frac{(a-1)x(x-1)(x-2)}{3} + \frac{(a-1)x(x-1)(x-2)(x-3)}{4} + \cdots
\]
(2.14)

This continued fraction converges for all \(x \in \mathbb{R}\) and all \(a \neq 1\). For \(a = 2\) and \(x = 1/2\) the successive convergents read 1.5, 1.4, 1.4166, 1.414359, 1.4144285, 1.4144291, 1.4142187 and the exact value obviously is 1.414213562...

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 continuations of semiconvergent series? If we start from the recursion relation
\[
j_k(x) = b_k(x)[e_{k+1}(x) + j_{k+2}(x)].
\]
(2.15)
we get
\[
j_1(x) = \frac{b_1(x)}{e_1(x)} + j_2(x) + \cdots
\]
(2.16)
The expansion of Eq. (2.16) yields the corresponding series
\[
h_1(x) = \sum_{k=0}^\infty p_k a^{k+1}.
\]
(2.17)
In the following we will restrict the discussion to the so-called \(P, R\) and \(S\) forms:

\[(P)\]
\[
\sum_{k=0}^\infty p_k a^{k+1}.
\]
(2.18a)

\[(R)\]
\[
\sum_{k=0}^\infty (-1)^k r_k a^{2k+1}.
\]
(2.18b)

\[(S)\]
\[
\sum_{k=0}^\infty \frac{a_k}{y^{x+k+1}}.
\]
(2.18c)

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

\[(P)\]
\[
\frac{b_1}{x-a_1} + \frac{b_2}{x-a_2} + \frac{b_3}{x-a_3} + \cdots
\]
(2.19a)

\[(R)\]
\[
\frac{c_1}{x-a_1} + \frac{c_2}{x-a_2} + \frac{c_3}{x-a_3} + \cdots
\]
(2.19b)

\[(S)\]
\[
\frac{d_1}{y} + \frac{d_2}{y} + \frac{d_3}{y} + \cdots
\]
(2.19c)

The \(S\)-form can be obtained by comparing the \(n\)-th convergent of the \(S\)-form with the \((2n-1)\)-th convergent of the \(S\)-form yielding
\[
e_1 = d_1, \quad e_n = d_{n+1} + d_{n3};
\]
\[
f_1 = d_1 y, \quad f_n = -d_{n-3} - d_{n+1}(n > 1).
\]
(2.20)
By setting \(y = 1\) and using Eq. (2.20) we obtain
\[
d_n = c_n \quad \forall n \geq 1.
\]
(2.21)
To obtain a given accuracy, the contracted \(S\)-form requires fewer terms to be evaluated than the usual \(S\)-form.

In the next section we present convenient recursive methods for the calculation of the expansion coefficients in the continued fraction equations (2.18a - 2.18d).

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 \(1/y\) 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)):
\[
b_1 = p_0, \quad b_n = \frac{(p_{n+2} - p_n)}{p_n};
\]
(3.1)
\[
a_1 = \frac{p_1}{p_0}, \quad a_n = \frac{p_{n+2} - p_{n+1} p_n}{p_{n+2}}.
\]

Using a result of Perron [20] for power series we obtain the formulas
\[
b_k = \frac{p_k y_{n-k}}{(y_{n-k+1})!}, \quad a_k = \frac{y_{n-k}}{y_{n-k+1}} - \frac{y_{n-k-1}}{y_{n-k}},
\]
(3.2)
where \(p_k\) and \(y_k\) are given by the determinants
\[
p_0 \cdots p_{n-1} \quad p_0 \cdots p_{n-2} p_n
\]
(3.3a)

\[
y_k = -
\]
(3.3b)

\[
p_{n-1} \cdots p_{n-2} p_{n-1}
\]
(3.3c)
with \( q_0 = 1 \) and \( q_1 = \rho \). \hspace{1cm} (3.3b)

Obviously, Eqs. (3.2) and (3.3) can hardly be used for high order coefficients \( \alpha_n \) and \( \beta_n \) 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 Mort \((21)\) and Schnieder \((24)\) for equilibrium systems the coefficients \( \alpha_n \) and \( \beta_n \) 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 \( P_k \) or \( R_k \) we can construct the \( R \)-matrix defined by

\[
R_{k+1} = R_{k+1}^{-1} = 0, \quad R_{k-1}^{-1} = \begin{pmatrix} 1 & \gamma_{k-1}^2 \gamma_{k-2} \\ \gamma_{k-1}^2 \gamma_{k-2} & \gamma_{k-1}^4 \end{pmatrix} \quad \forall \, n \geq 2, \hspace{1cm} (3.4)
\]

where the further elements are obtained with use of the product-difference (PD) recursion relation of Gordon \((23)\):

\[
R_{k+1} = R_{k+1}^{-1} - R_{k+1}^{-1} R_{k+1} - R_{k+1}^{-1} R_{k+1}^{-1} \hspace{1cm} (3.5)
\]

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 \( S \)-form are given by \((23)\):

\[
\alpha_n = R_{n+1} R_{n} R_{n-1} \hspace{1cm} (3.6)
\]

With the use of the coefficients \( \gamma_0 = (d_k) \) given by Eq. (3.6) the coefficients \( \alpha_n \) and \( \beta_n \) in the \( P \)-form are obtained from Eq. (2.20) yielding

\[
\beta_1 = \gamma_1, \quad \alpha_1 = -\gamma_2 \hspace{1cm} (3.7)
\]

and

\[
\beta_{n+1} = -\alpha_n \gamma_n^2 \gamma_{n-1} \hspace{1cm} (3.8)
\]

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:

\[
d_2 = D_2, \quad D_3 = \gamma_1 \hspace{1cm} (3.9)
\]

\[
d_2 = -D_2 D_3, \quad D_4 = \gamma_2 \hspace{1cm} \gamma_2 D_4 = \\gamma_3 D_4 + \gamma_4 D_4 + \gamma_5 D_4 + \gamma_6 D_4 \hspace{1cm} (3.9)
\]

\[
d_4 = -D_2 D_3, \quad D_5 = \gamma_2 D_5 + \gamma_3 D_5 + \gamma_4 D_5 + \gamma_5 D_5 + \gamma_6 D_5 \hspace{1cm} (3.9)
\]

\[
\vdots
\]

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

\[
L = 2(n - 1)/2 \hspace{1cm} (3.10)
\]

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

\[
X(2) = d_1 + D_3, \quad X(1) = d_2 \hspace{1cm} (3.11a)
\]

and interchange

\[
X(2) = X(1), \quad X(1) = X(2) \hspace{1cm} (3.11b)
\]

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

\[
X(k) = X(k - 1) + d_{k-1} X(k - 2) \hspace{1cm} \text{for} \, k = L, L - 2, \ldots, 4 \hspace{1cm} (3.11c)
\]

and

\[
X(k) = X(1) + d_{k-1} \hspace{1cm} (3.11d)
\]

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

\[
X(2) \rightarrow X(1), \quad X(4) \rightarrow X(3); \quad X(1) \rightarrow X(2), \quad X(3) \rightarrow X(4) \hspace{1cm} (3.11e)
\]

The coefficients \( d_k \) is then given by

\[
d_k = -D_k / D_{k+1} \hspace{1cm} (3.11f)
\]

where

\[
D_k = \sum_{i=1}^{k} \gamma_i \gamma_{i+1} X(2i - 1) \hspace{1cm} (3.11g)
\]

Both, the (P) and the (PD) algorithm have many points in common with Rietheuser's \((25)\) 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 \( d_k \) is not changed when we calculate a higher continued fraction convergence.

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 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 Boltzmann equation.

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

$$f(z; \Theta) = \sum_{L=0}^{\infty} c_L(z) Z_L(\cos \Theta), \quad (4.1)$$

depending on the scattering angle \(\Theta\). The coefficients \(c_L(z)\) describe the process and the \(z_L\) 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

$$f(z; \Theta) = \sum_{L=0}^{\infty} a_L(z) \frac{1}{1 + y^{2L+1}} = \sum_{L=0}^{\infty} a_{L+1} \frac{1}{y^{2L+1}}, \quad (4.2a)$$

with

$$a_L(z) = c_L(z) Z_L(\cos \Theta) \quad \text{and} \quad y = \sqrt{z}, \quad (4.2b)$$

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

$$f(z; \Theta) = \frac{d_1}{1 + \frac{d_2}{1 + \frac{d_3}{1 + \ldots}}} \quad (4.3)$$

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 orthonormal polynomials \(Z_L(\cos \Theta)\). We will restrict ourselves in the following to the very important series for the associated Legendre polynomials \(P_L(\cos \Theta)\), which are connected with the Legendre polynomials \(Z_L(\cos \Theta)\) by [2]

$$P_L(\cos \Theta) = (-1)^{L-m} \frac{d^m}{d(\cos \Theta)^m} Z_L(\cos \Theta), \quad l \geq m. \quad (4.4)$$

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

$$\frac{1}{\sin \Theta} P_L(\cos \Theta) = -\log \left(\frac{1 + \sin \Theta}{2 \sin \Theta} \left(1 + \sin \Theta\right)\right), \quad (4.5a)$$

and

$$\sum_{L=0}^{\infty} \frac{1}{L+1} P_L(\cos \Theta) = -\log \frac{1 + \sin \Theta}{\sin \Theta} - 1, \quad (4.5b)$$

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

$$\sum_{L=0}^{\infty} \left(\frac{2L+1}{(l+1)^{1/2}} P_L^m(\cos \Theta) \right) = \frac{m^{1/2}}{\sqrt{2}} \begin{cases} 1 & \text{for } m \geq 1, \\ 0 & \text{for } m = 0. \end{cases} \quad (4.6)$$

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 \(P_L^m(\cos \Theta)\):

$$P_L^m(\cos \Theta) = \left(-1\right)^{l-m} \frac{2^{1/2}}{\sqrt{\pi \sin \Theta}} \cos \left(\frac{l+m+1}{2} \sin \Theta\right) + O\left(l^{-3/2}\right)$$

for \(\varepsilon \leq \Theta \leq \pi - \varepsilon, \quad \varepsilon > 0; \quad l \gg m, 1/\varepsilon. \quad (4.7)$$

Thus the terms in the series (4.6) behave asymptotically as \(a_l(1) \sim l^{-1+2}\). 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 10⁴ 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 \(\Theta \geq 90°\) the convergence is much better than for small ones. The results for the formally divergent series (\(m = 2\)) 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 \( \theta = 40^\circ, 100^\circ \) and \( 160^\circ \), respectively.

<table>
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<th>( N )</th>
<th>40°</th>
<th>100°</th>
<th>160°</th>
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<td>0.1394</td>
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<td>0.1763</td>
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<td>0.1693</td>
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<tr>
<td>27</td>
<td>2.7475</td>
<td>0.3004</td>
<td>0.1703</td>
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<tr>
<td>exact</td>
<td>2.7475</td>
<td>0.3004</td>
<td>0.1703</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
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<tr>
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</table>

\( m = 5 \). 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 \( Z \) in the electric field of a nucleus with charge \( Z \Phi \) (Rutherford scattering). It is well known (see e.g. Ref. [22]) that this process is described by the scattering amplitude

\[
(\gamma; \Theta) = \frac{1}{Z^2 k L} \exp \left( \frac{Z}{2} \frac{\sin^2 \theta}{\sin^2 \Theta} \right) \exp\left( -\frac{Z}{2} \frac{\sin \theta \log (\sin \Theta/2)}{2} \right),
\]

where

\[
\eta = \frac{Z}{Z_1 \gamma} \epsilon + k - m^2 \gamma \epsilon
\]

(4.9)
denote the Coulomb parameter and wave number, respectively, of the particle with asymptotic velocity \( \epsilon \) and reduced mass \( m^2 \). The Coulomb phase shifts \( \sigma(\gamma) \) are given by

\[
\sigma(\gamma) = \arctan \left( \frac{\sqrt{1 + 1 + i \eta}}{\sqrt{1 + 1 - i \eta}} \right).
\]

(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 \( \frac{1}{\gamma(\gamma; \Theta)} \) are shown for some typical scattering angles and for \( \gamma = 10 \) and \( \gamma = 100 \), 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 \( [Z_1; M] \): Padé-approximation which is \( 2M + 1 \).

This can be seen by comparing our results with those obtained by Adler et al. [28]. Again, both the continued fraction expansion and the Padé-approximation work best for large scattering angles and small values of \( \eta \). The reason for this can be understood by physical arguments: in the classical limit the scattering with small \( \Theta \) and large \( \eta \) corresponds to a large impact parameter and therefore the contributions to the series (4.5) come from high \( \gamma \)-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 \( \gamma = 10 \) and \( \gamma = 100 \). The scattering angles are \( \theta = 60^\circ, 120^\circ \) and \( 160^\circ \), respectively.

<table>
<thead>
<tr>
<th>( N )</th>
<th>60°</th>
<th>120°</th>
<th>160°</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.0700</td>
<td>3.2398</td>
<td>0.03477</td>
</tr>
<tr>
<td>12</td>
<td>0.0002</td>
<td>7.3037</td>
<td>0.0269</td>
</tr>
<tr>
<td>18</td>
<td>0.0000</td>
<td>0.5072</td>
<td>0.020331</td>
</tr>
<tr>
<td>24</td>
<td>0.0000</td>
<td>0.6667</td>
<td>0.020363</td>
</tr>
<tr>
<td>30</td>
<td>0.0000</td>
<td>0.6667</td>
<td>0.020322</td>
</tr>
<tr>
<td>36</td>
<td>0.0000</td>
<td>0.6667</td>
<td>0.020385</td>
</tr>
<tr>
<td>42</td>
<td>0.0000</td>
<td>0.6667</td>
<td>0.020323</td>
</tr>
<tr>
<td>48</td>
<td>0.0000</td>
<td>0.6667</td>
<td>0.020360</td>
</tr>
<tr>
<td>54</td>
<td>0.0000</td>
<td>0.6667</td>
<td>0.020300</td>
</tr>
<tr>
<td>exact</td>
<td>0.0000</td>
<td>0.6667</td>
<td>0.020000</td>
</tr>
</tbody>
</table>

Table 4. The N-th convergent of the continued fraction expansion for the modulus of the Rutherford scattering amplitude for \( \gamma = 100 \). The scattering angles are \( \theta = 60^\circ, 120^\circ \) and \( 160^\circ \), respectively.

<table>
<thead>
<tr>
<th>( N )</th>
<th>60°</th>
<th>120°</th>
<th>160°</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>12</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>18</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>24</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>30</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>36</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>42</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>48</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>54</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
<tr>
<td>exact</td>
<td>0.0000</td>
<td>6.6667</td>
<td>0.020000</td>
</tr>
</tbody>
</table>
Table 4. The \( N \)-th convergent of the continued fraction expansion for the modulus of the rhombohedral scattering amplitude for \( \eta = 100 \) and \( \delta = 1 \). The scattering angles are \( \theta = 5^\circ, 15^\circ \) and \( 25^\circ \), respectively.

\[
\begin{array}{cccc}
N & 180^\circ & 120^\circ & 60^\circ \\
\hline
9 & 16.069 & 16.069 & 16.069 \\
15 & 50.375 & 50.375 & 50.375 \\
21 & 101.628 & 101.628 & 101.628 \\
27 & 203.255 & 203.255 & 203.255 \\
33 & 406.511 & 406.511 & 406.511 \\
39 & 813.022 & 813.022 & 813.022 \\
45 & 1626.045 & 1626.045 & 1626.045 \\
155 & 66.136 & 66.136 & 66.136 \\
114 & 66.711 & 66.711 & 66.711 \\
115 & 66.988 & 66.988 & 66.988 \\
123 & 66.988 & 66.988 & 66.988 \\
129 & 66.988 & 66.988 & 66.988 \\
203 & 227.19 & 227.19 & 227.19 \\
209 & 227.19 & 227.19 & 227.19 \\
215 & 227.19 & 227.19 & 227.19 \\
221 & 227.19 & 227.19 & 227.19 \\
227 & 227.19 & 227.19 & 227.19 \\
233 & 227.19 & 227.19 & 227.19 \\
exact & 227.19 & 227.19 & 227.19 \\
\end{array}
\]

This series converges rapidly and the exact value of \( f(\delta; \theta) \) 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 \( f(\delta; \theta) \) are given. Again, a strong convergence improvement is obtained. The direct summation requires up to 10\(^6\) terms for a relative accuracy of 10\(^{-4}\). 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 \([L/M]\)-Padé-approximation, if \( 3L + 1 \gg N \). 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 equations.

Table 5. The \( N \)-th convergent of the continued fraction expansion for the modulus of \( f(\delta; \theta) \) for the rhombohedral scattering amplitude for \( \eta = 100 \) and \( \delta = 1 \) and the scattering angles are \( \theta = 5^\circ, 15^\circ, 30^\circ \) and \( 50^\circ \), respectively.

\[
\begin{array}{cccc}
N & 5^\circ & 15^\circ & 30^\circ \\
\hline
3 & 17.12 & 9.788 & 2.926 & 1.531 \\
9 & 16.44 & 3.179 & 1.489 & 0.9879 \ 
15 & 7.118 & 3.672 & 1.576 & 0.988 \\
21 & 8.173 & 4.091 & 1.255 & 0.9604 \\
27 & 11.46 & 0.255 & 1.552 & 0.9046 \ 
33 & 10.07 & 1.385 & 1.395 & 0.938 \\
39 & 9.217 & 3.698 & 1.554 & 0.9045 \ 
45 & 8.738 & 3.905 & & \\
51 & 9.695 & 3.910 & & \\
63 & 8.906 & 3.193 & & \\
75 & 8.906 & 3.193 & & \\
81 & 8.906 & 3.193 & & \\
90 & 8.906 & 3.193 & & \\
exact & 8.906 & 3.193 & & \\
\end{array}
\]

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

\[
f(\lambda; \theta) = \sum_{k=0}^{N} \frac{1}{(2k+1)!} \frac{\lambda}{\sin \theta} P_k(\cos \theta),
\]

where the phase shifts \( \delta_k \) are given by [30]

\[
\delta_k = \pi \left( \frac{k}{2} \right) \left( \frac{k}{2} - \frac{k}{\lambda} + \frac{k}{\lambda} \right).
\]

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

\[
f(\lambda; \theta) = -\frac{\pi \lambda}{8} \frac{\theta}{\sin \theta} \log \left( \frac{\sin \theta}{2} \left( 1 + \sin ^2 \theta \right) \right)
\]

\[
+ \sum_{k=0}^{N} \frac{1}{(2k+1)!} \sin \delta_k \cos \delta_k + \frac{\pi \lambda}{8} \frac{\theta}{\sin \theta} \log \left( \frac{\sin \theta}{2} \left( 1 + \sin ^2 \theta \right) \right).
\]

(4.13)

\[
\text{exact}
\]

4.906 3.193 1.554 0.9415

\[
\text{exact}
\]

4.906 3.193 1.554 0.9415

\[
\text{exact}
\]

4.906 3.193 1.554 0.9415
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 \( d_k \) 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 can be 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

\[
f(q; \eta; \Theta) = \sum_{n=0}^{\infty} (H + 1) e^{2\pi i n \Theta} E_{n}(q; \eta) P_{n}(\cos \Theta).
\]

(1.14)

The special type of the reaction is determined by the radial integrals \( E_{n}(q; \eta) \). As an example we choose the description of the elastic scattering of positively charged particles in the presence of a Yukawa potential, proportional to \( e^{-r/\eta} \), where \( \eta = 6 \). This case was investigated in detail in Ref. [25] using Padé-approximants. The radial integrals for this process are approximately given by

\[
E_{n}(q; \eta) = \frac{4}{3} K_{0}(q^2) \left[ q^2 + (H + 1) \right],
\]

with \( q = \mu(\eta) \),

(4.15)

where \( K_{0} \) is the Bessel function of the third kind.

The amplitude \( f(q; \eta; \Theta) \) for large values of the parameter \( \eta \) can be well approximated by [33]

\[
l(q; \eta; \Theta) \approx \frac{2q\eta}{\sin(\Theta/2)} \cdot e^{-\frac{q}{2} \left( \frac{\pi}{2} \cos \left( \frac{\theta}{2} + \frac{\eta}{2} \right) \right)}.
\]

(4.16)

The convergence behavior of the series (4.14) becomes immediately evident from the structure of the radial integrals (4.15). They decrease significantly only if \( \eta \gg q \). In Fig. 1 we have plotted the

![Fig. 1. The number of terms required for a relative accuracy of 10^{-3} for the continued fraction expansion of the direct summation of \( f(q; \eta; \Theta) \) is shown as a function of \( \eta \). The parameter \( q = 2.0 \) (solid line) and \( q = 5.0 \) (dotted line), respectively. The scattering angle is \( \Theta = 180^\circ \).](image)

number of terms in the continued fraction expansion necessary to obtain a relative accuracy of 10^{-3} and the corresponding number for the direct summation of the series (4.14) as a function of \( \eta \) for several typical values of \( q \). The scattering angle is chosen typically to be \( \Theta = 180^\circ \). The curve is shown in Fig. 2, but for \( \Theta = 150^\circ \). As can be seen, the improvement of the convergence by using the continued fraction expansion is dramatic for large values of \( \eta \) and very dramatic for scattering angles \( \Theta < 150^\circ \). (Note, that about 20-100 terms in the original series have been summed up directly, as was discussed above.) For small values of \( \eta \) (\( \eta \ll 10 \)) 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 [38].

Our selected examples for the application of the continued fraction expansion to series with orthogonal polynomials show that this method can be
used advantageously for the summation of all such slowly convergent series. Finally, we note that we have used complex coefficients \(a_{n}(kr)\) in the calculation of the continued fraction. An alternative approach would be to split the original complex series into 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 \(16\). Such series result, for example, from the asymptotic solution of the radial Schrödinger equation for Coulomb problems in presence of potentials of type

\[
V(r) = \frac{\alpha}{r^2}, \quad r \geq 2. \tag{4.17}
\]

This type of potential is used e.g. to describe relativistic effects in scattering theory \(r=2\) or nuclear polarization effects \(r=3.3\). 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

\[
\frac{d^2}{dr^2} + \frac{\alpha}{r^2} \frac{d}{dr} = \frac{\alpha n}{r^2} - \frac{(l + \frac{1}{2})}{r^2} - \frac{2m^* V_0}{h^2}
\]

where \(\alpha\) denotes the angular momentum.

The asymptotic form of the wave function is given by

\[
g(r) = \frac{i}{2} \left( H_{l+\frac{1}{2}}^{(-)}(kr) - \alpha H_{l+\frac{1}{2}}^{(+)}(kr) \right), \tag{4.19}
\]

where the coefficients \(\alpha\) determine the cross section.

The incoming and outgoing Coulomb waves \(H_{l+\frac{1}{2}}^{(+)}\) and \(H_{l+\frac{1}{2}}^{(-)}\) can be expressed in terms of the well-known regular and irregular Coulomb functions \(F_1\) and \(G_1\) [2]\n
\[
H_{l+\frac{1}{2}}^{(\pm)}(kr) = G_1(kr) \pm i F_1(kr), \tag{4.20}
\]

with the asymptotic behaviour

\[
H_{l+\frac{1}{2}}^{(+)}(kr) \sim -\exp \left\{ \pm i \left( kr - \alpha \log 2kr - \frac{l + \frac{1}{2}}{2} + \alpha \eta \right) \right\}. \tag{4.21}
\]

For the solution of Eq. (4.18) we now define a new wave function \(F_1(r)\) by

\[
H_1(r) = a_1(r)
\]

\[
\cdot \exp \left\{ \pm i \left( kr - \alpha \log 2kr - \frac{l + \frac{1}{2}}{2} + \alpha \eta \right) \right\}
\]

\[
= G_1(r) + i F_1(r), \tag{4.22}
\]

where we impose the following asymptotic behaviour

\[
H_1(r) \sim G_1(kr) + i F_1(kr) \sim N^{(+)}(kr). \tag{4.23}
\]

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

\[
\frac{d^2}{dr^2} \left[ -\frac{\alpha}{r^2} \frac{d}{dr} \right] a_1(r) + \left( \frac{\alpha}{r^2} - \frac{l(f + 1)}{r^2} \right) a_1(r)
\]

\[
= \frac{2m^* V_0}{h^2} a_1(r) = 0. \tag{4.24}
\]
For sufficiently large \( r \), the function \( a_l(r) \) can be expanded in terms of inverse powers of \( r \), i.e.

\[
a_l(r) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{1}{r^n} + \sum_{n=0}^{\infty} \frac{\gamma_n}{k^2} \frac{1}{r^n} + \sum_{n=0}^{\infty} \frac{\Delta_n}{r^n}.
\]

(4.25)

For the coefficients \( \gamma_n \) and \( \Delta_n \) we find the following recursion relations:

\[
\gamma_{l+1} = -\frac{1}{\epsilon_0} \left( \frac{d}{dr} \delta_{l+1} \right) + \frac{1}{k^2} \frac{m^*}{V} \int_0^{\infty} \psi_0 \psi_{l+1} dr
\]

(4.26a)

and

\[
\Delta_{l+1} = \frac{1}{\epsilon_0} \left( \frac{d}{dr} \delta_{l+1} \right) + \frac{1}{k^2} \frac{m^*}{V} \int_0^{\infty} \psi_0 \psi_{l+1} dr
\]

(4.26b)

In Eq. (4.26) we have used the abbreviations

\[
\epsilon_0 = (n(n+1)) - l(l+1),
\]

(4.27)

\[
\delta_{l+1} = (2n+1) \eta,
\]

\[
\eta = \frac{(n(n+1))}{2k}.
\]

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

\[
\gamma_0 = 1, \quad \Delta_0 = 0,
\]

\[
\gamma_1 = \frac{\eta}{k}, \quad \Delta_1 = \frac{1}{2k} \left( \eta^2 + l(l+1) \right).
\]

(4.28)

The solution of Eq. (4.18) can now be represented by the functions \( G_l(r) \) and \( F_l(r) \) by

\[
g_l(r) = \gamma_l F_l(r) + \delta_l G_l(r),
\]

(4.29a)

and

\[
\frac{d}{dr} g_l(r) = \gamma_l \frac{d}{dr} F_l(r) + \delta_l \frac{d}{dr} G_l(r).
\]

(4.29b)

From the knowledge of the numerical solutions of the differential equation at some point \( r_0 \), the coefficients \( \gamma_l \) and \( \delta_l \) are determined. The wave functions \( g_l(r) \) are then completely known for all \( r \geq r_0 \) by the functions \( F_l \) and \( G_l \) and therefore the coefficients \( \gamma_l \) 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 \( r \rightarrow \infty \). 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 \( F_l(r) \) and \( G_l(r) \) respectively, at small values of \( r \). The convergence of the truncated continued fraction can be tested by the Wronski-relations which is given by

\[
G_l(r) \frac{d}{dr} F_l(r) - F_l(r) \frac{d}{dr} G_l(r) = k.
\]

(4.30)

Numerical investigations have shown that for different values of \( V \) and \( \tau \) the functions \( F_l(r) \) and \( G_l(r) \) can be evaluated with the continued fraction expansion for \( r_0 \) given by

\[
r_0 \geq \frac{1}{2k} ( \eta^2 + l(l+1) ).
\]

(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 \( 10^{-5} \) for \( a_1 \) was required. Hereby we have used the parameters \( \eta = 10, \ k = 1 \) fm and angular momentum \( l = 0 \). The potential parameters are \( V_0 = 50 \text{ MeV} \) and \( \tau = 3 \).

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. 5. The number of terms required for a relative accuracy of 10^{-5} for the continued fraction expansion of F_l(r) and G_l(r) is shown as a function of r. The parameters used are: \( \eta = 10, \ k = 1 \text{fm}, \ l = 0, \ \text{V}_0 = 50 \text{ MeV} \) and \( \tau = 3 \).](image)
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 \( x(t) = \{ x_1(t), \ldots \} \) with a time-independent dissipative forward generator \( \Gamma \) [34–36]. If we study the linear response of the system to external dynamic forces \( F(t) \), the perturbed system can be described by a time-dependent generator \( \Gamma(t) \) of a non-stationary Markov process [35–36]:

\[
\hat{\Gamma}(t) = \Gamma + F(t) \Omega \text{ext},
\]

yielding the master equation for the perturbed probability \( \beta(x,t) \):

\[
\delta \beta(t) \delta x = \hat{\Gamma}(t) \beta(t).
\]

The stochastic operators \( \Gamma(t) \) and \( \Omega \) are in general dissipative linear integro-differential operators acting on probability functions. Using functional derivatives the linear response tensor \( \delta \beta(t) \delta x \) is then defined by the relation of the response of the state variables \( x(t) \):

\[
\delta \beta(t) \delta x = \frac{\delta F(t)}{\delta \beta(t)} \delta x \delta \beta(t).
\]

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 \( \beta_0(x) \) of the unperturbed Markov system

\[
\Gamma_0 \beta_0 = 0.
\]

The response tensor \( \delta \beta(t) \delta x \) can be expressed in the form of a generalized fluctuation-dissipation theorem first discussed by Hänggi and Thomas [30]. The theorem can be written as a correlation over the unperturbed stationary system

\[
\langle \delta \beta(t) \delta x \rangle = \Theta(t) \langle \delta x(t) \rangle - \langle \delta x(t) \rangle \langle \delta \beta(t) \delta x \rangle,
\]

where the time evolution of the conditional average is governed by the backward generator \( \Gamma^\ast \):

\[
\Gamma^\ast \langle x, y \rangle = \Gamma\langle y, x \rangle.
\]

Hence the moments \( \mu_n \) can often be written more simply in terms of the backward generator \( \Gamma^\ast \):

\[
\mu_n = \langle \Gamma^\ast \mu_{n-1} \\Phi(x) \delta x \rangle
\]

where \( \Phi(x) \) is in general a non-linear fluctuation:

\[
\Phi(x) = \{ \Theta \beta_0 \mu \},
\]

with

\[
\langle \Phi(x) \rangle = \int \Phi(x) \beta_0(x) \delta x = 0.
\]
The Fourier transform of $\chi(\omega)$ is given by:

$$\chi(\omega) = \lim_{T \to \infty} \int_0^T \exp(i \omega \tau) \chi(\tau) \, d\tau,$$  

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

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

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 $\chi(\omega)$ of a general stationary correlation function $\chi(t)$. By applying the continued fraction method to Eq. (4.43) we obtain

$$\chi(\omega) = \chi' (\omega) + i \chi'' (\omega) = \frac{b_1}{z^2 + b_2} \ldots,$$

where $z = \frac{\omega}{\gamma}$ and $\gamma$ is the relaxation time.

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

$$\chi''(\omega) = \sum_{n=1}^{\infty} \frac{s_n}{\omega^{2n}}, \quad s_n = (-1)^{n+1} p_{2n+1}.$$  

For a one-dimensional Gaussian Markov process with a gradient type perturbation, $\chi''(\omega) = -\frac{\partial^2}{\partial \omega^2}$, the response function $\chi(\omega)$ can be written in terms of the relaxation rate $\gamma$ as

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

Using the moments

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

we have

$$s_1 = 1, \quad s_2 = \gamma, \quad \gamma = 0, \quad \gamma \geq 3,$$

which gives the exact result for Eq. (4.42)

$$\chi(\omega) = 1/(\omega_i + \gamma).$$

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

$$\chi(\omega) = \sum_{n=0}^{N} a_n \omega^{-n-1},$$

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

For all problems with a finite discrete state space of $S$ different states, the generator $\Gamma$ is an ordinary stochastic matrix $\Gamma$. 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 $-\Gamma$. 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 $\Gamma$. 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 $g_i(t)$ for a system prepared in a non-stationary state at time $t_0$ with the initial probability $p_0(t_0)$, can also be determined using the same technique. Using the propagator $\mathcal{R}(t) = \exp(\Gamma t)$ of the unperturbed master equation, the non-stationary probability at time $t$, $p(t)$, becomes

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

Hence, the moments $g_n(t_0)$ of the Taylor series for the relaxation function $g(t)$ are

$$g_n = \int_0^t g(s) (\Gamma^n p_0) \, ds, \quad n = 0, 1, \ldots.$$  

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-approximants, 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 the theory of Stieltjes series [38]. For a vectorial stochastic Markov process $\mathcal{M}(t) = (N(t), \ldots)$ which fulfills the strong detailed balance condition [35].
the real stochastic dissipative operator $\Gamma$ can be
symmetrized by
$$
\Gamma = \Gamma^* = \sum_{n=0}^{\infty} \xi_n \Gamma_n \xi_n^{\dagger},
$$
(5.1)
where $\Gamma_n$ again denotes the unique stationary
probability function. The symmetric dissipative
operator $\mathcal{P}$ may have eigenfunctions $\psi_n(x)$ and
self-adjoint $L \xi_0 \xi_0^{\dagger}$. Assuming that the set of eigen-
functions form a complete set (i.e. $\Gamma$ is even self-
adjoint)
$$
\delta(x - y) = \sum \frac{d^2}{\int \psi_n(x) \psi_n(y)}.
$$
(5.2)
we have for $\Gamma$ the spectral representation
$$
\Gamma = \sum \frac{d^2}{\int \psi_n(x) \psi_n^*(y)}.
$$
(5.3)
The stationary two-time joint-probability $p^{\omega}(a, y; x)$
then is
$$
p^{\omega}(a, y; x) = (p_n(a) p_n(y)) \frac{1}{2} 
\sum \frac{d^2}{\int \psi_n(x) \psi_n(y) \psi_n^{*}(x) \psi_n^{*}(y)},
$$
(5.4)
For an auto-correlation function $S(\tau)$ of any state
function $g(x)$,
$$
S(\tau) = \langle g(x(t)) g(x(0)) \rangle = \sum_{n=0}^{\infty} (-\frac{\tau}{\xi}) \frac{d_n^2}{\xi_n^{*}},
$$
(5.5)
the static moments,
$$
r_n = (-\frac{\tau}{\xi}) \frac{d_n^2}{\xi_n^{*}},
$$
(5.6)
can be expressed in terms of a Stieltjes integral by
using Eq. (5.4):
$$
r_n = \int \frac{d\nu(a)}{\nu(a)},
$$
(5.7)
where
$$
d\nu(a) \equiv d\nu \delta(|\lambda| - \nu) \{ \nu \xi^2 \psi_n^{*}(x) \}^2 \geq 0.
$$
(5.8)
In particular, $r_0$ is given by
$$
S(0) = r_0 = \sum_{\nu=0}^{\infty} \int \frac{d\nu}{\nu} \{ \nu \xi^2 \psi_n^{*}(x) \}^2 < + \infty,
$$
(5.9)
so that with Eq. (5.8) $p(\nu)$ is a bounded monotonic non-decreasing function. Therefore, the Laplace transform $S(\omega)$ for real $\omega$,
$$
S(\omega) = \frac{1}{\delta t} \int S(\tau) e^{-\omega \tau} \partial \omega > 0,
$$
(5.10a)
can be written with Eq. (5.3) as a Stieltjes series of the form
$$
S(a) = \sum_{\nu=0}^{\infty} (-\frac{\nu}{\xi})^n \nu_{an}^{n!},
$$
(5.10b)

The powerful methods developed for Stieltjes series
(58) can then be used directly. The function $S(\omega)$
then has a Stieltjes integral representation
$$
S(\omega) = \frac{d\nu(a)}{\omega - \nu} \partial \omega > 0.
$$
(5.11)
The Laplace transform $S(\omega)$ of the $n$-th time-
derivative of the auto-correlation $S(\tau)$ becomes
$$
S^{(n)}(\omega) = \omega^n S(n, \omega) - \sum_{m=0}^{n-1} \frac{n!}{m!} (-\omega^{-1})^m S(m, \omega) \partial \omega = 1, 2, ..., \partial \omega > 0.
$$
(5.12)
The functions $S^{(n)}(\omega)$ are for even $n$, a Stieltjes
series with $d\nu^{(n)}(a) = \omega^n d\nu(a)$ and for odd $n$, a
negative Stieltjes series. The Stieltjes series can be replaced by its "corresponding continued fractions" $c^{(n)}(\omega)$ of the R-form. If we consider a sequence of approximants $c^{(n)}(\omega)$, obtained by setting
$$
c^{(n+1)} = c^{(n)} - \cdots = 0
$$
the best upper and lower bounds are obtained.
This follows from Eq. (5.11) and Eqs. (5.17) to (5.19):
$$
c^{(n+1)}(\omega) \geq (-\omega) S^{(n)}(\omega) \geq c^{(n)}(\omega)
$$
(5.13)
for $n, k = 0, 1, \ldots$.
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
$$
c^{(n)}(\omega) = \frac{c^{(1)}}{c^{(1)} + \frac{c^{(2)}}{c^{(2)} + \frac{c^{(3)}}{c^{(3)} + \cdots}}}
$$
converges for all complex $z \in (-\infty, 0)$ uniformly
to a regular analytic function
$$
S(a) = \frac{d\nu(a)}{\omega} \partial \omega > 0, $z + \omega \quad \text{if} \quad x \in \mathbb{R} \quad \text{diverges},
$$
(5.15)
* Note that the function in Eq. (5.10b) is in general
not identical with the function in Eq. (5.11), but
represents an asymptotic series of the functions in
(5.14) and (5.15).
where
\[ b_1 = \frac{1}{c(z)}, \quad b_{n+1} = b_n^* c(z) c_n(z), \quad b_n = \frac{c_n(z)}{c_n(z) c(z)}, \quad (5.16) \]

The asymptotic expansion of \( S(z) \) is then given by a series like that of Equation (5.104). If the sum in Eq. (5.16) converges, the continued fraction is divergent for all \( z \in C \).

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

\[
\sum_{n=0}^{2M} \frac{c_n(z)}{c_n(z) c(z)} f(r_n) = \sum_{n=0}^{2M} \frac{c_n(z)}{c_n(z) c(z)} f(r_n) + \sum_{n=0}^{2M} \frac{c_n(z)}{c_n(z) c(z)} f^{(2M)}(r_n) \quad (5.17)
\]

Using the orthogonal transformation matrix \( \tilde{U} \), the parameters \( \gamma_{ij}^{(k)} \) are then given by the eigenvalues
\[
\gamma_{ij}^{(k)} = \langle \tilde{U}^{-1} \tilde{M} \tilde{U} \rangle_{ij} \quad (5.23)
\]

and the weight factors by
\[
\tilde{C}_m^{(k)} = \sqrt{\gamma_{m}^{(k)}} \tilde{U}^{(k)}_{m} \quad (5.23)
\]

The odd parameters are obtained by setting the \( \gamma_{ij}^{(k)} \) in the original matrix \( \tilde{M} \) equal to zero.

By using the Taylor series for the auto-correlation function
\[
S(r) = \sum_{k=0}^{\infty} \sum_{n=0}^{\infty} r^k \sigma_n r_n \quad (5.35)
\]

we find together with \( \xi_r \), (5.3) for the n-th time derivative of \( S(r) \)
\[
\frac{d\xi_r}{dt^n} = \langle -\gamma_{n}^{(k)} \rangle_1^{(k)} r^n \quad (5.26)
\]

Using the quadrature formulas with \( f(u) = e^{-u} \), the best upper and lower bounds become
\[
\sum_{k=0}^{\infty} \frac{1}{k!} \gamma_{k}^{(k)} \exp \left( -\gamma_{k}^{(k)} \right) \geq \langle -\gamma_\infty \rangle_1^{(k)} \frac{d\xi_r}{dt^n} \quad (5.27)
\]

or
\[
\int_{0}^{\infty} f(u) g^{(k)}(u) \frac{du}{u} = \sum_{k=0}^{\infty} \frac{1}{k!} \gamma_{k}^{(k)} \frac{d^{k+1}}{dt^{k+1}} \left. \frac{d\xi_r}{dt^n} \right|_{t=\infty} \quad (5.18)
\]

where \( \xi (0, \infty) \) and the coefficients \( \langle k \rangle \) are all positive for a monotonic decreasing bounded function \( g^{(k)}(u) \). The parameters in Eqs. (5.17) and (5.18) can be found from the finite approximates
\[
d_1^{(k)}(u) = \sum_{k=0}^{\infty} \frac{1}{k!} \gamma_{k}^{(k)} \frac{d^{k+1}}{dt^{k+1}} \left. \frac{d\xi_r}{dt^n} \right|_{t=\infty} \quad (5.19)
\]

and
\[
d_{2M-1}^{(k)}(u) = \sum_{k=0}^{\infty} \frac{1}{k!} \gamma_{k}^{(k)} \frac{d^{k+1}}{dt^{k+1}} \left. \frac{d\xi_r}{dt^n} \right|_{t=\infty} \quad (5.19)
\]

with
\[
g^{(k)}(u) = 0 \quad (5.21)
\]

Following Gordon [35] a direct calculation of the parameters in Eqs. (5.17) and (5.18) consists in a diagonalisation procedure for the symmetric tridiagonal matrix \( \tilde{M} \):

\[
\tilde{M} = \begin{pmatrix}
0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & \gamma_{2M}^{(k)}
\end{pmatrix}
\]

(5.22)
The relations in Eqs. (5.27) and (5.13) also have a wide application in equilibrium statistical thermodynamics, where the following fluctuation-dissipation-theorem holds [16, 35, 36]
\[ \chi(t) = -\frac{\partial}{\partial t} S(t). \]  
(5.28)

Here, \( \beta \) denotes the Boltzmann factor. In addition, the Fourier transform \( \chi(\omega) = -\beta \cdot S(\omega) \) follows as a consequence of the Kramers-Kronig relation the sum rule
\[ -\beta \int S(\omega) d\omega = \int \chi''(\omega) d\omega, \]
(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 \( p(N) \) 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 \( p(N, t) \) is given by the Fokker-Planck equation
\[ \frac{\partial p(N, t)}{\partial t} = \frac{\partial}{\partial N} \left( A(N) p(N, t) \right) - \frac{\partial}{\partial N} \left( D(N) \frac{\partial p(N, t)}{\partial N} \right). \]
(5.30)

This system obeys a strong detailed balance condition yielding for the probability current \( I(N) \):
\[ I(N) = A(N) p_{Nu}(N) - \frac{\partial}{\partial N} \left( D(N) \frac{\partial p(N, t)}{\partial N} \right) = 0. \]
(5.31)

The symmetric operator \( T \) becomes in this case
\[ T = -\frac{\partial}{\partial N} \left( D(N) \frac{\partial}{\partial N} \right) \]
\[ = -\frac{\partial}{\partial N^2} \left( A(N) + \frac{\partial}{\partial N} A(N) \right), \]
(5.32)

with
\[ A(N) = A(N) = -\epsilon D(N) \frac{\partial}{\partial N}. \]
(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 \[ 40 \]
\[ A(N) = A(N) + 4 \left[ p(N) \right] - \epsilon D(N) = \eta(N) + \epsilon D(N). \]
(5.34)

\[ D(N) = D(N) + \frac{\partial}{\partial N} \left( N^2 \right) + \left[ \epsilon(N) + \epsilon(N) \right]. \]
(5.35)

The Euler current \( \epsilon \) and the thermal current \( \eta \) tend to discharge the diode capacitance, whereas the linear current \( \epsilon \) and the supply current \( \eta \) (pump parameter) tend to charge the diode capacitance. The auto-correlation function \( S(t) \) of the fluctuations of the charge number \( N \) on the diode capacitance is then
\[ S(t) = \langle \Delta N(t) \Delta N(0) \rangle, \]
(5.36)

with
\[ \Delta N(t) = N(t) - \langle N \rangle_{e} \]
(5.37)

The results in Eq. (5.27) can now be applied directly using the moments
\[ \rho_0 = \langle \langle \Delta N(0) \rangle^{n} \rangle_{e} \]
(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 \( S(t) \) are given by
\[ \rho_0 = S(0) \geq S(t) \]
(5.39)

\[ \geq S(0) \exp \left( -\frac{t}{\rho_0} \right), \quad \tau \geq 0. \]
(5.40)

Using the first four moments \( \rho_0, \rho_1, \rho_2, \rho_3 \) we find
\[ \rho_2 / \rho_1 - \rho_3 / \rho_2 - \rho_3 / \rho_2 - \rho_3 / \rho_2 \quad \rho_2 / \rho_1 - \rho_3 / \rho_2 - \rho_3 / \rho_2 \]
(5.41)

\[ \rho_0 \geq S(t) \geq \rho_0 \left( 1 - \alpha \right) \quad \exp \left( -\gamma t \right) \quad \exp \left( -\gamma t \right), \]
(5.42)

with \( \alpha, \gamma \) 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 Riken-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 [22] and on diffusion in periodic 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 restate 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 Eolmann equation [42].

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

[34] H. Haken, Rev. Mod. Phys. 47, 67 (1978).