

# Extrapolation of perturbation-theory expansions by self-similar approximants

S. GLUZMAN and V.I. YUKALOV

*Bogolubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, Russia*  
emails: [simon.gluzman@gmail.com](mailto:simon.gluzman@gmail.com), [yukalov@theor.jinr.ru](mailto:yukalov@theor.jinr.ru)

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The problem of extrapolating asymptotic perturbation-theory expansions in powers of a small variable to large values of the variable tending to infinity is investigated. The analysis is based on self-similar approximation theory. Several types of self-similar approximants are considered and their use in different problems of applied mathematics is illustrated. Self-similar approximants are shown to constitute a powerful tool for extrapolating asymptotic expansions of different natures.

**Key words:** Approximation with constraints; Approximation by arbitrary nonlinear expressions; Approximation to limiting values; Function-theoretic methods; Functional analytic methods of summability

## 1 Introduction

There exists a very old problem constantly met in various aspects of applied mathematics, which can be formulated as follows. Very often realistic problems are so complicated that they do not allow for exact solutions. It is standard for such problems to use some kind of perturbation theory [11, 17, 55]. Then one gets answers in terms of expansions in powers of a small parameter, or a small variable, say for  $x \rightarrow 0$ . However, often the problem of interest corresponds not to a small variable, but, rather the opposite, to large values of this variable; very often it is the infinite limit  $x \rightarrow \infty$  that is of maximum interest [41]. One could find this limit, provided the general formula of expansion terms would be given and the derived expansion would produce convergent series. None of these conditions is usually valid. As a rule, only a few expansion terms can be derived. In addition, the resulting series are divergent, being only asymptotic [16, 23]. Then the following question arises: How from the knowledge of several terms of an asymptotic expansion at a variable  $x \rightarrow 0$  could one find the limit corresponding to  $x \rightarrow \infty$ ?

One often extrapolates small-variable expansions by means of Padé approximants [5]. However, the straightforward use of these approximants yields

$$P_{M/N}(x) \sim x^{M-N} \quad (x \rightarrow \infty),$$

which, depending on the relation between  $M$  and  $N$ , can tend to:

- infinity (when  $M > N$ ),

- zero (when  $M < N$ ),
- a constant (if  $M = N$ ).

In that sense, the limit  $x \rightarrow \infty$  is not defined.

When the character of a large-variable limit is known, one can invoke the two-point Padé approximants [5]. However, the accuracy of the latter is not high and one confronts several difficulties:

- (1) Firstly of all, when constructing these approximants, one often obtains spurious poles yielding unphysical singularities [5], sometimes a large number of poles [61].
- (2) Secondly, there are the cases when Padé approximants are not able to sum perturbation series even for small values of an expansion parameter [64].
- (3) Thirdly, in the majority of cases, to reach a reasonable accuracy, one needs to have tens of terms in perturbative expansions [5], while often interesting problems provide only a few terms.
- (4) Fourthly, defining the two-point Padé approximants, one always meets an ambiguity in distributing the coefficients for deciding which of these must reproduce the left-side expansion and which the right-side series. This ambiguity worsens with the increase of approximants' orders, making it difficult to compose the two-point Padé tables. For the case of a few terms, this ambiguity makes the two-point Padé approximants practically inapplicable. For example, it has been shown [63] that, for the same problem, one may construct different two-point Padé approximants, all having correct left- and right-side limits, but differing from each other in the intermediate region by a factor of 40, which gives 1,000% uncertainty. This demonstrates that in the case of short series, the two-point Padé approximants do not allow one to get a reliable description.
- (5) Fifthly, the two-point Padé approximants cannot always be used for interpolating between two different expansions, but only when these two expansions have compatible variables [5]. When these expansions have incompatible variables, the two-point Padé approximants cannot be defined in principle.
- (6) Finally, interpolating between two points, one of which is finite and another is at infinity, one is able to characterize the large-variable limit of only rational powers [5].

Another method that allows for the extrapolation of divergent series is the optimized perturbation theory based on the introduction of control functions defined by an optimization condition and guaranteeing the transformation of divergent series into convergent series [66,67,82]. Since 1976, when the optimized perturbation theory was introduced [66,67], a number of variants of different control functions (see discussion in [81,82]) have been put forward. The Kleinert [39,41] variational perturbation theory, where control functions are introduced through a variable transformation and variational optimization conditions, is particularly worth mentioning. This method provides good accuracy for the extrapolation of weak-coupling expansions to the strong-coupling limit, especially when a number of terms in the weak-coupling perturbation theory are available [27].

In the present paper, we address the problem of extrapolating small-variable asymptotic expansions to their effective strong-coupling limits by employing another approach,

based on the self-similar approximation theory [68–71, 78–80]. The main difference of this approach from the optimized perturbation theory is that we possess the approximation methods without introducing control functions, which makes calculations essentially simpler. The self-similar approximation theory can be combined with the Kleinert variational perturbation theory [42]. This, however, also requires the introduction of variational control functions. In the present paper, however, we pay maximum attention to considering simpler ways not involving control functions.

There exists a principal problem, when one accomplishes an extrapolation in the case for which the exact solution is not known and only a few terms of the weak-coupling perturbation theory are available. This is the problem of reliability of obtained extrapolation. In such a case, it is important to be able to do extrapolation by several methods, and comparing their results. If these results yield close values, this suggests that the extrapolation is reliable.

In line with this idea, we aim at employing different variants of self-similar approximations, applying them to the same problems and comparing the results. If the approximants for a problem, obtained by different methods, are close to each other, this would suggest that the derived values are reliable.

We consider several variants of self-similar approximants for each problem and show that these are really close to each other, hence these can successfully extrapolate asymptotic expansions, valid at  $x \rightarrow 0$ , to their effective limits of  $x \rightarrow \infty$ . We especially concentrate on the strong-coupling limit, where approximate methods usually are the least accurate, leading to maximal errors. We show that, even in this least favourable situation, with just a few perturbative terms available, the self-similar extrapolation methods provide reasonable accuracy. For completeness, we also show that the self-similar methods allow us to construct approximants displaying good accuracy in the whole region of the studied variable. For instance, effective equations of state can be derived, these being in good agreement with experimental data.

Differences between the present paper and our previous papers are as follows:

- (i) We study several types of self-similar approximants and compare their accuracy, which allows us to draw conclusions on the reliability of the method.
- (ii) A large set of examples of different natures are analysed, demonstrating the generality of the method of self-similar approximants and their effectiveness for extrapolating different functions met in various problems of applied mathematics.
- (iii) We consider a new type of approximants resulting from a double self-similar renormalization and show how these improve the accuracy as compared with exact results, when these are available.
- (iv) We show an effective way for calculating large-variable critical exponents.
- (v) The method is shown to provide good accuracy for a whole range of variables. This is demonstrated by constructing the equation of state that exactly reproduces a phenomenological equation for quantum hard spheres.

## 2 Formulation of extrapolation problem

Suppose we are interested in the behaviour of a real function  $f(x)$  of a real variable  $x \in [0, \infty)$ . Also, let this function be defined by a complicated problem that does not allow

for an explicit derivation of the form of  $f(x)$ . What can only be done is use some kind of perturbation theory yielding asymptotic expansions representing the function

$$f(x) \simeq f_k(x) \quad (x \rightarrow 0) \quad (2.1)$$

at small values of the variable  $x \rightarrow 0$ , with  $k = 0, 1, \dots$  being the perturbation order. The perturbative series of the  $k$ th order can be written as an expansion in powers of  $x$  as

$$f_k(x) = f_0(x) \left( 1 + \sum_{n=1}^k a_n x^n \right), \quad (2.2)$$

where  $f_0(x)$  is chosen so that the series in the brackets would start with the term one. It is convenient to define the reduced expression

$$\bar{f}_k(x) \equiv \frac{f_k(x)}{f_0(x)} = 1 + \sum_{n=1}^k a_n x^n, \quad (2.3)$$

which will be subject to self-similar renormalization.

Note that practically any perturbative series can be represented in form (2.2). For instance, if we have a Laurent-type series

$$f_{m+k}(x) = \sum_{n=-m}^k c_n x^n,$$

it can be transformed to (2.2) by rewriting it as

$$f_{m+k}(x) = \frac{c_{-m}}{x^m} \left( 1 + \sum_{n=1}^{m+k} a_n x^n \right).$$

Here we consider the series in integer powers, or those that can be reduced to such, since this is the most frequent type of perturbation-theory expansions. Thus, the Puiseux expansion [60] of the type

$$f_k(t) = \sum_{n=n_0}^k c_n t^{n/m},$$

where  $n_0$  is an integer and  $m$  is a non-zero natural number, can be reduced to form (1.2) by the change of the variable  $t = x^m$ . It is possible to generalize the approach to the series of the type

$$f_k(x) = \sum_n^k c_n x^{\alpha_n} \quad (\alpha_n < \alpha_{n+1}),$$

with arbitrary real powers  $\alpha_n$  arranged in an ascending order. When  $\alpha_n$  pertains to an ordered group, the latter expression corresponds to the Hahn series [36, 49].

As is known, the most difficult region for approximating is that of the large variable, where approximants are usually the least accurate. That is why our main interest here

will be the large-variable behaviour of the function, where its asymptotic form is

$$f(x) \simeq Bx^\beta \quad (x \rightarrow \infty). \tag{2.4}$$

The constant  $B$  is called the critical amplitude and the power  $\beta$  is the critical exponent.

After employing the self-similar renormalization for the reduced function (2.3), we get a self-similar approximant  $\bar{f}_k^*(x)$ , which gives a self-similar approximant

$$f_k^*(x) = f_0(x)\bar{f}_k^*(x) \tag{2.5}$$

for the sought function  $f(x)$ . Considering for the latter the limit  $x \rightarrow \infty$ , we find the related approximation for the critical amplitude and critical exponent. In many cases the exponent is known from other arguments. Then we need to find only the critical amplitude.

### 3 Variants of self-similar approximants

In the cases when one can compare the derived approximants with known expressions, one can easily evaluate the accuracy of the approximants. But how could we trust the approximants when no exact expression for the sought function is available? In that case, it would be desirable to have several variants of approximants in order to compare them with each other. If all of these give close results, this would suggest that the method is reliable.

Several types of approximants, based on the self-similar approximation theory, have been derived. We shall not repeat their derivation here. This can be found, along with all the details, in our previous publications. We shall just present the corresponding expressions and explain how these will be used for the problem of extrapolation to infinity.

#### 3.1 Self-similar factor approximants

Self-similar factor approximants have been introduced in [21, 77]. For the reduced expansion (2.3), the  $k$ th-order self-similar factor approximant reads as

$$\bar{f}_k^*(x) = \prod_{i=1}^{N_k} (1 + A_i x)^{n_i}, \tag{3.1}$$

where

$$N_k = \begin{cases} k/2, & k = 2, 4, \dots \\ (k + 1)/2, & k = 3, 5, \dots \end{cases} \tag{3.2}$$

and the parameters  $A_i$  and  $n_i$  are defined from the accuracy-through-order procedure by expanding expression (3.1) in powers of  $x$ , comparing the latter expansion with the given sum (2.3) and equating the like terms in these expansions. When the approximation order  $k = 2p$  is even, the above procedure uniquely defines all  $2p$  parameters. When

the approximation order  $k = 2p + 1$  is odd, the number of equations in the accuracy-through-order procedure is  $2p$ , which is by one smaller than the number of parameters. Then using the scale invariance arguments [83], one sets  $A_1 = 1$ , thus uniquely defining all parameters. Another way is to find one of the coefficients  $A_i$  from the variational optimization of the approximant [76]. Both these approaches give close results, although the scaling procedure of setting  $A_1$  to one is simpler.

With approximant (3.1), the self-similar approximant for the sought function (2.5) becomes

$$f_k^*(x) = f_0(x) \prod_{i=1}^{N_k} (1 + A_i x)^{n_i}. \quad (3.3)$$

If the zero-order factor has the large-variable form

$$f_0(x) \simeq Ax^\alpha \quad (x \rightarrow \infty), \quad (3.4)$$

then approximant (3.3) behaves as

$$f_k^*(x) \simeq B_k x^\beta \quad (x \rightarrow \infty). \quad (3.5)$$

Under a given exponent  $\beta$ , the powers  $n_i$  must satisfy the equality

$$\beta = \alpha + \sum_{i=1}^{N_k} n_i, \quad (3.6)$$

while the critical amplitude  $B$  is approximated by

$$B_k = A \prod_{i=1}^{N_k} A_i^{n_i}. \quad (3.7)$$

It is worth stressing that the factor  $f_0(x)$  in equation (3.3) is explicitly defined by the perturbative expansion (2.2), so it is known. The factor approximants (3.3) may have singularities when some  $A_i$  and  $n_i$  are negative. This makes it possible to associate such singularities with critical points and phase transitions. Investigation of the critical points and the related critical exponents, by means of the factor approximants, has been done in our previous papers [21, 75–77, 83].

### 3.2 Self-similar root approximants

The derivation of the self-similar root approximants can be found in [18, 82, 84]. The self-similar renormalization of the reduced expansion (2.3) yields

$$R_k(x) = (((\dots (1 + A_1 x)^{n_1} + A_2 x^2)^{n_2} + A_3 x^3)^{n_3} + \dots + A_k x^k)^{n_k}. \quad (3.8)$$

The  $k$ th-order approximant for the sought function then becomes

$$f_k^*(x) = f_0(x) R_k(x). \quad (3.9)$$

In Yukalov and Yukalova [82], it has been rigorously proved that the parameters  $A_i$  and  $n_i$  are uniquely defined, provided that  $k$  terms of the large-variable expansion at  $x \rightarrow \infty$  are known, and the condition  $pn_p - p + 1 = \text{const}$  holds for  $p = 1, 2, \dots, k - 1$ . Then expression (3.8) leads to

$$R_k(x) \simeq A_k^{n_k} x^{kn_k} \quad (x \rightarrow \infty). \tag{3.10}$$

With the given exponent  $\beta$ , the power  $n_k$  satisfies the relation

$$\beta = \alpha + kn_k \tag{3.11}$$

and the  $k$ th-order approximation for the critical amplitude is

$$B_k = AA_k^{n_k}. \tag{3.12}$$

### 3.3 Iterated root approximants

Self-similar root approximants are uniquely defined when their parameters are prescribed by the large-variable behaviour of the sought function. However, if we try to find these parameters from the small-variable expansion (2.2), then we meet the problem of multiple solutions [75]. To avoid this problem, one has to impose additional conditions on the parameters. Such a straightforward condition would be the requirement that all  $k$  terms in root (3.8) would contribute to the large-variable amplitude [20]. For this, it is necessary and sufficient that the internal powers  $n_j$  be defined as

$$n_j = \frac{j+1}{j} \quad (1 \leq j \leq k-1), \tag{3.13}$$

with the external power related to the exponent  $\beta$  as

$$n_k = \frac{\gamma}{k} \quad (\gamma = \beta - \alpha). \tag{3.14}$$

Then expression (3.8) becomes the iterated root approximant

$$R_k(x) = (((\dots(1 + A_1x)^2 + A_2x^2)^{3/2} + A_3x^3)^{4/3} + \dots + A_kx^k)^{\gamma/k}, \tag{3.15}$$

where all parameters  $A_j$  are uniquely defined by the accuracy-through-order procedure.

In the large-variable limit, equation (3.15) yields

$$R_k \simeq \frac{B_k}{A} x^\gamma \quad (x \rightarrow \infty), \tag{3.16}$$

with the critical amplitude

$$B_k = A((\dots(A_1^2 + A_2)^{3/2} + A_3)^{4/3} + \dots + A_k)^{\gamma/k}. \tag{3.17}$$

It may happen that the iterated root approximants are well defined up to an order  $k$ , after which they do not exist because some of the parameters  $A_p$  are negative. At the

same time, the higher-order terms of the perturbation-theory expansion can be available up to an order  $k + p$ . How then could we use these additional terms for constructing the higher-order approximants?

### 3.4 Corrected root approximants

Corrections to the iterated root approximants (3.15), employing the higher-order terms, can be constructed [20] by defining the corrected root approximants,

$$\tilde{R}_{k/p}(x) = R_k(x)C_{k/p}(x), \quad (3.18)$$

with the correction function

$$C_{k/p}(x) = 1 + d_{k+1}x^{k+1}(((\dots(1 + b_1x)^2 + b_2x^2)^{3/2} + b_3x^3)^{4/3} + \dots + b_{p-1}x^{p-1})^{-(k+1)/(p-1)}, \quad (3.19)$$

where  $p > 2$  and all parameters are defined from the accuracy-through-order procedure, when the terms of the expansion of form (3.18) are equated with the corresponding terms of the perturbation-theory expansion. Here, the critical exponent is defined by the iterated root approximant (3.16) so that the limit  $x \rightarrow \infty$  of the correction function is finite:

$$C_{k/p}(\infty) = 1 + d_{k+1}(((\dots(b_1^2 + b_2)^{3/2} + b_3)^{4/3} + \dots + b_{p-1})^{-(k+1)/(p-1)}). \quad (3.20)$$

The corresponding approximation for the sought function takes the form

$$f_{k/p}^*(x) = f_0(x)\tilde{R}_{k/p}(x). \quad (3.21)$$

Its large-variable behaviour is

$$f_{k/p}^*(x) \simeq B_{k/p}x^\beta \quad (x \rightarrow \infty), \quad (3.22)$$

with the corrected critical amplitude

$$B_{k/p} = AB_k C_{k/p}(\infty). \quad (3.23)$$

### 3.5 Self-similar power transforms

It is possible to get improvement of approximants by employing power transforms [19]. For this purpose, we define the power transform of the reduced expansion (2.3) as

$$P_k(x, m) \equiv \bar{f}_k^m(x), \quad (3.24)$$

which is expanded in powers of  $x$  giving

$$P_k(x, m) \cong \sum_{n=0}^k b_n(m)x^n. \quad (3.25)$$



After the self-similar renormalization of expansion (3.25), we get a self-similar approximant  $P_k^*(x, m)$ . We then accomplish the inverse transformation

$$\bar{F}_k(x, m) = [P_k^*(x, m)]^{1/m}. \tag{3.26}$$

The powers  $m_k = m_k(x)$  are defined by the variational condition

$$\frac{\partial \bar{F}_k(x, m)}{\partial m} = 0. \tag{3.27}$$

Finally, the corresponding approximation for the sought function is given by

$$f_k^*(x) = f_0(x)\bar{F}_k(x, m_k). \tag{3.28}$$

When we are interested in the large-variable limit, condition (3.27) reduces to the differentiation of only critical amplitude.

### 3.6 Double self-similar approximants

Another way of improving the accuracy is by employing the procedure of self-similar renormalization twice. The fact that the accuracy does improve can be illustrated by the examples for which exact solutions are known.

The double renormalization is accomplished as follows. Firstly, renormalizing the reduced expansion (2.3), we construct the self-similar approximants (2.5). The approximants  $\bar{f}_k^*(x)$  form the approximation sequence  $\{\bar{f}_k^*(x)\}$ . Introducing the expansion function  $x(\varphi)$  by the equation

$$\bar{f}_1^*(x) = \varphi, \quad x = x(\varphi), \tag{3.29}$$

we define

$$y_k(\varphi) = \bar{f}_k^*(x(\varphi)). \tag{3.30}$$

By this definition, the sequence  $\{y_k(\varphi)\}$  is bijective to the sequence  $\{\bar{f}_k^*(x)\}$ . In view of equation (3.29), we have

$$y_1(\varphi) = \varphi. \tag{3.31}$$

Consider the sequence  $\{y_k(\varphi)\}$  as the trajectory of a dynamical system in discrete time, that is, of a cascade, with the initial condition (3.31). Embed this approximation cascade into an approximation flow:

$$\{y_k(\varphi) : k \in \mathbb{Z}_+\} \subset \{y(t, \varphi) : t \in \mathbb{R}_+\}, \tag{3.32}$$

where

$$\mathbb{Z}_+ \equiv \{0, 1, 2, \dots\}, \quad \mathbb{R}_+ \equiv [0, \infty),$$

so that the flow trajectory passes through all points of the cascade trajectory,

$$y(t, \varphi) = y_k(\varphi) \quad (t = k). \tag{3.33}$$

The evolution equation for the flow reads as

$$\frac{\partial}{\partial t} y(t, \varphi) = v(y), \quad (3.34)$$

with  $v(y)$  being the flow velocity.

Integrating the evolution equation (3.34) gives

$$\int_{y_k}^{y_k^*} \frac{dy}{v(y)} = \tau_k, \quad (3.35)$$

where  $y_k = y_k(\varphi)$ , and  $\tau_k$  is the minimal effective time necessary for reaching the approximate fixed point  $y_k^*(\varphi)$ . The latter, according to definition (3.30), is a twice renormalized self-similar approximant

$$y_k^*(\varphi) = \bar{f}_k^{**}(x(\varphi)). \quad (3.36)$$

Keeping in mind definition (3.30) also allows us to rewrite integral (3.35) as

$$\int_{\bar{f}_k^*}^{\bar{f}_k^{**}} \frac{d\varphi}{v_k(\varphi)} = \tau_k, \quad (3.37)$$

where

$$\bar{f}_k^* = \bar{f}_k^*(x), \quad \bar{f}_k^{**} = \bar{f}_k^{**}(x).$$

Assuming that we reach the quasi-fixed point in one step, we may set  $\tau_k = 1$ .

Employing in the evolution integral (3.37) the Euler discretization for the velocity

$$v_k(\varphi) = y_k(\varphi) - \varphi = \bar{f}_k^*(x(\varphi)) - \bar{f}_1^*(x(\varphi)) \quad (3.38)$$

and calculating this integral gives the twice renormalized approximant for the sought function

$$\bar{f}_k^{**}(x) = f_0(x) \bar{f}_k^{**}(x). \quad (3.39)$$

The large-variable limit of the latter

$$\bar{f}_k^{**}(x) \simeq B_k^* x^\beta \quad (x \rightarrow \infty) \quad (3.40)$$

defines the approximate expression for the critical amplitude  $B_k^*$ . Usually, integral (3.37) can be calculated only numerically.

In the following sections, the above methods of extrapolation will be illustrated by a number of examples of different nature, with emphasis on the large-variable limit  $x \rightarrow \infty$ . Analysing these examples, we shall pay maximum attention to the possibility of obtaining accurate approximate expressions by taking just a few terms in the small-variable expansions, bearing in mind that complicated realistic problems usually provide us with only a small number of terms of perturbation theory.

#### 4 Explicitly defined functions

In order to clearly demonstrate how the method works and to show that it really provides good accuracy, it is illustrative to start with functions whose explicit form is given.

This will allow us to easily evaluate the accuracy of approximants. The consideration of such simpler cases is necessary before considering the complicated problems whose exact solutions are not known, since only then it is possible to explicitly demonstrate the efficiency of the method and to evaluate what accuracy of the used approximants should be expected.

Variable  $x$  will be varying in the range  $[0, \infty)$ .

### 4.1 Function-1

Consider a function

$$f(x) = \frac{1}{2}(\sqrt{4+x} - 1), \tag{4.1}$$

which is of importance because of giving the golden ratio

$$\frac{1}{f(1)} = 1 + f(1) = 1.618034.$$

In its small-variable expansion

$$f_k(x) = \sum_{n=0}^k c_n x^n, \tag{4.2}$$

the first five coefficients are

$$c_0 = \frac{1}{2}, \quad c_1 = \frac{1}{8}, \quad c_2 = -\frac{1}{128}, \quad c_3 = \frac{1}{1024}, \quad c_4 = -\frac{5}{32768}.$$

Here  $f_0 = c_0$ .

Despite its simplicity, this function expansion is not trivial, since the first two coefficients are positive, after which they start alternating.

The large-variable behaviour

$$f(x) \simeq Bx^\beta = 0.5\sqrt{x} \tag{4.3}$$

shows that

$$B = 0.5, \quad \beta = 0.5.$$

Using the approximants described above, we fix exponent  $\beta$ , concentrating on the accuracy of calculating critical amplitude.

The method of factor approximants of Section 3.1 yields  $B_4 = 0.440$ . Power transforms of Section 3.5, with factor approximants, do not provide essential improvement. The optimization condition (3.27) results in two solutions for  $m$ , which yields for the amplitudes the values 0.416 and 0.455. The iterated root approximants of Section 3.3 give  $B_2 = 0.374, B_3 = 0.385, B_4 = 0.393$ . The corrected iterated roots of Section 3.4 give  $B_{2/2} = 0.422$ . Power transforms, with iterated roots, again yield two solutions for  $B_2$ , with the values 0.404 and 0.433. All these results are close to the Padé approximant,  $P_{2/2} = 0.433$ . Essential improvement of accuracy is achieved by double approximants in Section 3.6 on the basis of the iterated roots, giving  $B_4^* = 0.476$ .

### 4.2 Function-2

Let us take a more complicated function

$$f(x) = \frac{2}{\pi} \operatorname{arccot}(-x) \exp\left(1 - \frac{1}{1+x}\right). \quad (4.4)$$

In expansion (4.2), using the value  $\operatorname{arccot}(0) = \pi/2$ , we have

$$c_0 = 1, \quad c_1 = 1.637, \quad c_2 = 0.137, \quad c_3 = -0.364, \quad c_4 = -0.064.$$

Again  $f_0 = c_0$ . Here the first three coefficients are positive, while the next two are negative. The limit at infinity is

$$f(\infty) = 2e = 5.437, \quad (4.5)$$

where the equality  $\operatorname{arccot}(-\infty) = \pi$  is used.

The irregularity in the coefficient signs makes the extrapolation more difficult. The factor approximants give  $f_4^*(\infty) = 9.049$ . Power transforms, with the factor approximants, improve the result yielding the limit 5.192. Iterated roots give  $R_3(\infty) = 3.399$ ,  $R_4(\infty) = 3.547$ . Corrected iterated roots are close to the latter values:  $R_{2/2}(\infty) = 3.424$ . Power transforms, with iterated roots, give two values: 3.547 and 4.535. As we see, the power-transformed factor approximants are the most accurate.

### 4.3 Function-3

Expanding the function

$$f(x) = \frac{\operatorname{arccot}(-x)}{1 + e^{-x}}, \quad (4.6)$$

we get the coefficients

$$c_0 = \frac{\pi}{4}, \quad c_1 = \frac{1}{2} \left(1 + \frac{\pi}{4}\right), \quad c_2 = \frac{1}{4}, \quad c_3 = -\frac{1}{6} \left(1 + \frac{\pi}{16}\right), \quad c_4 = -\frac{5}{48}.$$

Here  $f_0 = c_0$ . Again, the first three coefficients are positive, while the next two are negative. The limit at infinity is

$$f(\infty) = \pi. \quad (4.7)$$

As in the previous case, the irregularity in the coefficient signs makes extrapolation difficult. For instance, Padé approximants fail, the best of them giving 1.414, which is rather far from limit (4.7). The factor approximants give  $f_4^*(\infty) = 4.759$ . The power-transformed factor approximants are more accurate, yielding the limit 3.142. Iterated roots are not good, with the limit 1.698. The power-transformed iterated roots give two solutions: 3.742 and 2.267. Thus, the power-transformed factor approximant, with the value 3.142, is the best.

### 4.4 Debye–Hückel function

The Debye–Hückel function

$$D(x) = \frac{2}{x} - \frac{2}{x^2}(1 - e^{-x}) \tag{4.8}$$

appears in the theory of strong electrolytes [45]. Its expansion gives the sign-alternating coefficients

$$c_0 = 1, \quad c_1 = -\frac{1}{3}, \quad c_2 = \frac{1}{12}, \quad c_3 = -\frac{1}{60},$$

$$c_4 = \frac{1}{360}, \quad c_5 = -\frac{1}{2520}, \quad c_6 = \frac{1}{20160}.$$

Here,  $f_0 = c_0$ .

The large-variable behaviour is

$$D(x) \simeq \frac{2}{x} \quad (x \rightarrow \infty). \tag{4.9}$$

Factor approximants give  $B_4 = 1.640$ . The power-transformed factor approximants result in  $B_5 = 1.779$ . Corrected factor approximants yield  $B_{2/2} = 1.642$ . Iterated roots result in  $B_2 = 2.449$ ,  $B_3 = 2.229$ ,  $B_4 = 2.127$ . For corrected iterated roots, we have  $B_{1/2} = 1.611$ ,  $B_{1/3} = 1.841$ ,  $B_{1/4} = 1.934$ ,  $B_{2/2} = 1.130$ ,  $B_{2/3} = 1.712$ ,  $B_{2/4} = 1.811$ . The power-transformed iterated roots in the fourth order give two solutions: 1.993 and 2.049. The best two-point Padé approximant  $P_{2/2}$  gives the critical amplitude 1.333, which is much worse than the self-similar approximants of the same fourth order.

### 4.5 Stirling function

The Stirling series expansion for the function

$$f(x) = \frac{1}{\sqrt{2\pi}} e^{1/x} x^{1/x} \Gamma\left(1 + \frac{1}{x}\right) \tag{4.10}$$

can be written as

$$f_k(x) = \frac{1}{\sqrt{x}} \left(1 + \sum_{n=1}^k a_n x^n\right), \tag{4.11}$$

with the coefficients

$$a_1 = \frac{1}{12}, \quad a_2 = \frac{1}{288}, \quad a_3 = -\frac{139}{51840},$$

$$a_4 = -\frac{571}{2488320}, \quad a_5 = \frac{163879}{209018880}, \quad a_6 = \frac{5246819}{75246796800},$$

$$a_7 = -\frac{534703531}{902961561600}, \quad a_8 = -\frac{4483131259}{86684309913600}.$$

Here,  $f_0 = 1/\sqrt{x}$ .

The limit at infinity is

$$f(\infty) = \frac{1}{\sqrt{2\pi}} = 0.398942. \tag{4.12}$$

Factor approximants yield the limit  $f_6^*(\infty) = 0.454$ . The power-transformed factor approximants improve the accuracy, giving  $f_5^*(\infty) = 0.406$ . Iterated roots result in  $B_2 = 0.485$ ,  $B_3 = 0.422$ , but the fourth-order approximant is complex. Corrected iterated roots give the limit  $B_{2/1} = 0.408$ ,  $B_{2/2} = 0.312$ ,  $B_{2/3} = 0.405$ . Padé approximants are essentially worse.

## 5 Functions defined through integrals

Many functions are defined by means of integral representations. Expansions of such functions often result in strongly divergent series. However, self-similar approximants provide rather accurate extrapolation from the zero variable to its infinite limit.

### 5.1 Integral-1

Consider the integral

$$f(x) = (1 + 2x) \int_0^{\infty} \frac{e^{-t}}{1 + x^2 t^2} dt. \quad (5.1)$$

Its expansion in powers of  $x$  contains the coefficients

$$\begin{aligned} c_0 = 1, \quad c_1 = 2, \quad c_2 = -2, \quad c_3 = -4, \quad c_4 = 24, \\ c_5 = 48, \quad c_6 = -720, \quad c_7 = -1440, \quad c_8 = 40320, \quad c_9 = 80640. \end{aligned}$$

The general expressions for the latter are

$$c_{2n} = (-1)^n (2n)!, \quad c_{2n+1} = (-1)^n 2(2n)!.$$

The limit of equation (5.1) at infinity is

$$f(\infty) = \pi. \quad (5.2)$$

Factor approximants yield  $f_4^*(\infty) = 1.965$ ,  $f_5^*(\infty) = 2.015$ , demonstrating good numerical convergence, e.g. giving in the ninth order the limit 3.113. Iterated roots lead to  $R_2(\infty) = 1.754$ ,  $R_3(\infty) = 2.071$ , but the higher-order approximants are complex. The power-transformed iterated roots in the fourth order give two solutions: 1.971 and 2.071. Corrected iterated roots in the fourth order give 2.582 and display good numerical convergence in higher orders. Padé approximants of the same order are less accurate, for instance,  $P_{2/2} = 1.875$ .

### 5.2 Complimentary error function

The complimentary error function

$$f(x) = \operatorname{erfc}(-x) \quad (5.3)$$

is expressed through the error function as

$$\operatorname{erfc}(x) \equiv 1 - \operatorname{erf}(x),$$

the error function being

$$\operatorname{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt.$$

Hence, function (5.3) is defined by means of the integral

$$\operatorname{erfc}(x) \equiv \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt.$$

Expanding equation (5.3), we get the coefficients

$$c_0 = 1, \quad c_1 = 1.12838, \quad c_2 = 0, \quad c_3 = -0.37613, \quad c_4 = 0.$$

The limit at infinity is

$$f(\infty) = 2. \tag{5.4}$$

All self-similar approximants give close results. Thus, factor approximants yield  $f_4^*(\infty) = 3.772$ . Iterated roots give  $R_3(\infty) = 2.382$ . Power-transformed iterated roots of the fourth order have two solutions: 2.305 and 3.739. Taking into account more expansion terms results in better accuracy. Thus,  $f_5^*(\infty) = 2.629$ .

### 5.3 Integral-2

The function

$$f(x) = \frac{\operatorname{erfc}(-x)}{1 + e^{-x}} \tag{5.5}$$

is defined through the integral representation for the complimentary error function considered in the previous section. The coefficients of the corresponding expansion are

$$c_0 = \frac{1}{2}, \quad c_1 = 1, \quad c_2 = 1.62838, \quad c_3 = -0.41779, \quad c_4 = -0.23508.$$

The limit at infinity is

$$f(\infty) = 2. \tag{5.6}$$

Factor approximants overestimate the limit, yielding  $f_3^*(\infty) = 5.052$ ,  $f_5^*(\infty) = 3.286$ . Power-transformed factor approximants, on the other hand, underestimate it, giving to the fourth order 1.392. Iterated root approximants lead to  $B_3 = 1.371$ ,  $B_4 = 1.893$ . Power-transformed iterated roots to the fourth order give the limit 1.684. In the same order, Padé approximants give 1.027. Iterated root approximants here are the most accurate.

The large-variable behaviour of functions (5.3) and (5.5) involves exponentials. Therefore the accuracy of approximations can be essentially improved by employing exponential self-similar approximants [74]. However, here we limit ourselves by the analysis of approximants described in Section 3.

### 5.4 Mittag–Leffler function

A particular case of the Mittag-Leffler function

$$E(x) = e^{x^2} \operatorname{erfc}(x), \tag{5.7}$$

which is expressed through the complimentary error function, appears in the model of anomalous diffusion [58]. The small-variable expansion yields the coefficients

$$c_0 = 1, \quad c_1 = -\frac{2}{\sqrt{\pi}}, \quad c_2 = 1, \quad c_3 = -\frac{4}{3\sqrt{\pi}}, \quad c_4 = \frac{1}{2}.$$

In the large-variable limit, one has

$$E(x) \simeq \frac{B}{x} \quad (x \rightarrow \infty), \quad (5.8)$$

with the critical amplitude

$$B = \frac{1}{\sqrt{\pi}} = 0.56419. \quad (5.9)$$

Factor approximants give in the fourth order  $B_4 = 0.511$ . The same result holds for the corrected factor approximants  $B_{2/2} = 0.511$ . Power-transformed factors yield, in the fourth order, the amplitude 0.541. Iterated roots lead to  $B_1 = 0.886$ ,  $B_2 = 0.741$ ,  $B_3 = 0.680$ ,  $B_4 = 0.650$ . Corrected iterated roots give in the fourth order 0.403. Power-transformed iterated roots yield three solutions, all being close to 0.641. The accuracy improves when more terms in the expansion are taken into account. For instance, the factor approximants in the sixth order give  $B_6 = 0.532$ .

## 6 Anharmonic and nonlinear models

Divergent series often appear in applying perturbation theory to anharmonic and non-linear models that are typical for many problems in physics and chemistry. In these problems, perturbation theory is usually done with respect to a parameter called the *coupling parameter* which characterizes the strength of interactions or anharmonicity of an external field.

### 6.1 Zero-dimensional anharmonic model

This is one of the simplest models that, at the same time, demonstrates mathematical features typical of many problems in chemistry and physics. The partition function of this model reads as

$$Z(g) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \exp(-x^2 - gx^4) dx, \quad (6.1)$$

where  $g \in [0, \infty)$  is a dimensionless coupling parameter. The weak-coupling perturbation theory yields the series

$$Z_k(g) = \sum_{n=0}^k c_n g^n, \quad (6.2)$$

with the coefficients

$$c_n = \frac{(-1)^n}{\sqrt{\pi} n!} \Gamma\left(2n + \frac{1}{2}\right).$$



Explicitly, the first few coefficients are

$$c_0 = 1, \quad c_1 = -\frac{3}{4}, \quad c_2 = \frac{105}{32},$$

$$c_3 = -\frac{3465}{128}, \quad c_4 = \frac{675675}{2048}.$$

In the strong-coupling limit,

$$Z(g) \simeq Bg^{-1/4} \quad (g \rightarrow \infty), \tag{6.3}$$

with

$$B = 1.022765. \tag{6.4}$$

Fixing the exponent  $\beta$ , we calculate the critical amplitude  $B_k$ , comparing it with the known exact value from equation (6.4). Factor approximants give the fourth order  $B_4 = 0.838$ . Corrected factor approximants, to the same order, yield  $B_{2/2} = 1.131$ . Iterated root approximants give  $B_2 = 0.760$ , but the higher-order approximants are complex. Corrected iterated roots result in  $B_{2/2} = 0.678$ . Power-transformed iterated roots of the fourth order produce two solutions: 0.879 and 0.971. As we see, the best accuracy is provided by the corrected factor approximants and power-transformed iterated roots.

### 6.2 One-dimensional anharmonic oscillator

The anharmonic oscillator is described by the Hamiltonian

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + gx^4, \tag{6.5}$$

in which  $x \in (-\infty, +\infty)$  and  $g$  is a positive anharmonicity parameter. The perturbation theory for the ground-state energy yields [24] the series

$$E_k(g) = \sum_{n=0}^k c_n g^n, \tag{6.6}$$

with the coefficients

$$c_0 = \frac{1}{2}, \quad c_1 = \frac{3}{4}, \quad c_2 = -\frac{21}{8}, \quad c_3 = \frac{333}{16}, \quad c_4 = -\frac{30885}{128}.$$

The strong-coupling limit is

$$E(g) \simeq 0.667986g^{1/3} \quad (g \rightarrow \infty). \tag{6.7}$$

Factor approximants give  $B_3 = 0.750$ ,  $B_5 = 0.725$ ,  $B_7 = 0.712$ . Corrected factor approximants yield  $B_{3/4} = 0.728$ . The power-transformed factor approximant of the fourth order gives 0.681. Iterated root approximants result in  $B_2 = 0.572$ ,  $B_3 = 0.855$ , but the fourth-order approximant is complex. Corrected iterated roots give  $B_4 = 0.587$ , and power-transformed iterated roots, 0.665. The latter value is the closest to the exact amplitude in equation (6.7).

Comparing these results with those obtained by means of the Kleinert variational perturbation theory [27], we see that the latter provides better accuracy. However, we would like to recall that our main aim in the present paper is to test the methods of the self-similar approximation theory, without involving the introduction of variational or other control functions, and based on just a few initial terms of the perturbation theory. Although, in our case, the accuracy is lower than in the Kleinert method, the calculations are much simpler.

### 6.3 Scalar field theory

Consider the so-called  $m\phi^2$  quantum field theory on a  $d$ -dimensional cubic lattice with lattice spacing  $a$ . The free energy of the system can be expressed [6] as the integral

$$f(x) = x \exp \left\{ 2 \int_0^\infty e^{-t} \ln [e^{-xt} I_0(xt)] dt \right\}, \quad (6.8)$$

where  $I_0(\cdot)$  is the modified Bessel function of zero order and  $x = 1/ma^2$ . Expanding the integral in powers of the variable  $x$  yields the series

$$f_k(x) = x \left( 1 + \sum_{n=1}^k a_n x^n \right), \quad (6.9)$$

with the coefficients

$$a_1 = -2, \quad a_2 = 3, \quad a_3 = -\frac{10}{3}, \quad a_4 = \frac{29}{12},$$

$$a_5 = -\frac{11}{10}, \quad a_6 = \frac{391}{180}, \quad a_7 = -\frac{2389}{630}.$$

When passing to continuous space, one takes the limit  $a \rightarrow 0$ , which means that  $x \rightarrow \infty$ . The sought continuous-space limit is

$$f(\infty) = \frac{e^\gamma}{2\pi} = 0.28347. \quad (6.10)$$

Factor approximants of the fourth order give the limit 0.322 and power-transformed factor approximants, 0.333. Iterated root approximants yield  $f_2^*(\infty) = 0.408$ ,  $f_3^*(\infty) = 0.377$ ,  $f_4^*(\infty) = 0.365$ . Their accuracy can be improved by taking more terms in expansion (6.9), e.g.  $f_{12}^*(\infty) = 0.280$ . Corrected iterated roots give  $f_{2/2}^*(\infty) = 0.266$ , and power-transformed iterated roots of the fourth order lead to 0.356 and 0.347. The best Padé approximant, up to the fifth order, gives  $P_{2/3} = 0.326$ . For these low orders, the most accurate is the corrected root approximant  $f_{2/2}^*(\infty) = 0.266$ .

### 6.4 Nonlinear Schrödinger equation

The nonlinear Schrödinger equation serves as a basic tool for modelling several different problems, such as those of waves on the surface of a deep fluid [85], electromagnetic waves in fibre optics [29] and the Bose–Einstein condensates [57, 72, 73]. For the last case,

it is often called the Gross–Pitaevskii equation, although Bogolubov was the first to write down this equation for the Bose systems in his famous *Lectures on Quantum Statistics* published in 1949 [7] and wrote on it many times since (see, e.g. [9, 10]). This equation for non-equilibrium superfluids was also studied in [8]. The one-dimensional stationary nonlinear Schrödinger equation for Bose condensed atoms in a harmonic trap reads

$$\hat{H}_{NLS}\psi = E\psi, \tag{6.11}$$

with the nonlinear Hamiltonian

$$\hat{H}_{NLS} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + g|\psi|^2. \tag{6.12}$$

Here,  $g$  is a dimensionless coupling parameter. The energy levels can be represented in the form

$$E(g) = \left(n + \frac{1}{2}\right) f(g), \tag{6.13}$$

where  $n = 0, 1, 2, \dots$  is a quantum index labelling the eigenvalues. Employing the optimized perturbation theory for the function  $f(g)$ , as in [84], gives the expansion

$$f_k(g) = 1 + \sum_{n=1}^k a_n z^n \tag{6.14}$$

in powers of the effective coupling

$$z \equiv \frac{J_n}{n + 1/2} g,$$

in which

$$J_n \equiv \frac{1}{2^n \pi n!} \int_{-\infty}^{\infty} \exp(-2x^2) H_n^4(x) dx,$$

with  $H_n(\cdot)$  being a Hermite polynomial. The coefficients in expansion (6.14) are

$$a_1 = 1, \quad a_2 = -\frac{1}{8}, \quad a_3 = \frac{1}{32}, \quad a_4 = -\frac{1}{128}.$$

Then for the strong-coupling limit, we have

$$f(g) \simeq \frac{3}{2} z^{2/3} \quad (z \rightarrow \infty). \tag{6.15}$$

Hence, the critical amplitude is  $B = 3/2$ .

Factor approximants give  $B_4 = 1.496$ , which is very close to 1.5. Corrected factor approximants, to the fourth order, yield 1.451 and power-transformed factor approximants, 1.477. Iterated roots result in  $B_2 = 1.379$ ,  $B_3 = 1.415$ ,  $B_4 = 1.435$ . Corrected iterated roots give  $B_{2/2} = 1.492$  and power-transformed iterated roots, 1.426. For the double self-similar approximant, based on iterated roots, we get  $B_4^* = 1.498$ . The latter is slightly better than the value  $B_4 = 1.496$ , given by the factor approximant, but calculating the doubly renormalized approximants is essentially more complicated. Of course, calculations,

employing any of the self-similar approximants, are much less time-consuming than the direct solution of the nonlinear differential equation (6.11).

## 7 Problems in many-body theory

Perturbation theory in many-body problems is usually accomplished with respect to the coupling parameter characterizing the interaction strength. However, this coupling parameter is often rather large. Moreover, perturbative expansions practically always yield divergent series for any finite value of the coupling parameter. Another difficulty is that the many-body problems, as a rule, are so much complicated that they allow one to calculate only a few low-order terms of perturbation theory. We show here that self-similar approximants allow for an effective extrapolation of such short series, giving good accuracy even in the extreme case of infinitely strong coupling.

### 7.1 Lieb–Liniger Bose gas

Lieb and Liniger [48] have considered a one-dimensional Bose gas with contact interactions. The ground-state energy of the gas can be written as an expansion with respect to the coupling parameter as

$$E(g) \simeq g - \frac{4}{3\pi} g^{3/2} + \frac{1.29}{2\pi^2} g^2 - 0.017201g^{5/2}. \quad (7.1)$$

In the strong-coupling limit, we have the Tonks–Girardeau expression

$$E(\infty) = \frac{\pi^2}{3} = 3.289868. \quad (7.2)$$

By the change of the variables

$$e(x) \equiv E(x^2), \quad g \equiv x^2, \quad (7.3)$$

expansion (7.1) reduces to the form

$$e(x) \simeq x^2(1 + a_1x + a_2x^2 + a_3x^3), \quad (7.4)$$

in which

$$a_1 = -\frac{4}{3\pi} = -0.424413, \quad a_2 = \frac{1.29}{2\pi^2} = 0.065352, \quad a_3 = -0.017201.$$

The fourth-order term can be set as having  $a_4 = 0$ .

Different self-similar approximants yield close results. The most accurate among these correspond to iterated root approximants displaying fast numerical convergence:  $E_2^*(\infty) = 8.713$ ,  $E_3^*(\infty) = 4.765$ ,  $E_4^*(\infty) = 3.2924$ . The last expression provides very good accuracy when compared with the exact value (7.2).

### 7.2 Bose–Einstein condensation temperature

The Bose-Einstein condensation temperature of ideal uniform Bose gas in three-dimensional space is known to be

$$T_0 = \frac{2\pi\hbar^2}{mk_B} \left[ \frac{\rho}{\zeta(3/2)} \right]^{2/3}, \tag{7.5}$$

where  $m$  is atomic mass and  $\rho$  is the gas density. The ideal gas is, however, unstable below the condensation temperature [73]. Atomic interactions stabilize the system and shift the transition temperature by the amount

$$\Delta T_c \equiv T_c - T_0. \tag{7.6}$$

This shift, at asymptotically small gas parameter

$$\gamma \equiv \rho^{1/3} a_s, \tag{7.7}$$

in which  $a_s$  is atomic scattering length, behaves as

$$\frac{\Delta T_c}{T_0} \simeq c_1 \gamma \quad (\gamma \rightarrow 0). \tag{7.8}$$

The Monte Carlo simulations [1, 2, 30, 56, 59] give

$$c_1 = 1.3 \pm 0.05. \tag{7.9}$$

At the same time, the coefficient  $c_1$  can be defined [32–34] as a strong-coupling limit

$$c_1 = \lim_{g \rightarrow \infty} c_1(g) \equiv B \tag{7.10}$$

of a function  $c_1(g)$  that is available only as an expansion in an effective coupling parameter

$$c_1(g) \simeq b_1 g + b_2 g^2 + b_3 g^3 + b_4 g^4 + b_5 g^5, \tag{7.11}$$

where

$$b_1 = 0.223286, \quad b_2 = -0.0661032, \quad b_3 = 0.026446, \\ b_4 = -0.0129177, \quad b_5 = 0.00729073.$$

Expansion (7.11) can be represented as

$$c_1(g) \simeq b_1 g (1 + a_1 g + a_2 g^2 + a_3 g^3 + a_4 g^4), \tag{7.12}$$

with the coefficients

$$a_n \equiv \frac{b_{n+1}}{b_1} \quad (n = 1, 2, 3, 4).$$

Padé approximants do not provide good accuracy, the best of them gives  $c_1(\infty) = 0.985$ . Factor approximants, to the third order, yield  $B_3 = 1.025$ . At the fourth order, factor approximants give  $B_4 = 1.096$  if one of the parameters  $A_i$  is set to one, and 1.446 if it

is defined by the variational procedure. On average, the latter values give  $B_4 = 1.271$ . Iterated roots result in  $B_2 = 1.383$  to the second order and  $B_3 = 0.854$  to the third order; the fourth-order approximant is complex. Corrected iterated roots give  $B_{1/2} = 0.924$ ,  $B_{1/3} = 1.289$ ,  $B_{2/2} = 1.309$ . Power-transformed iterated roots give two solutions: 1.227 and 1.388, which on average makes 1.308. The corrected iterated root  $B_{2/2} = 1.309$  produces the most accurate result, practically coinciding with that found by the Monte Carlo simulations [1, 2, 30, 56, 59]. Kastening [32–34], using the Kleinert variational perturbation theory involving seven loops, found the value  $1.27 \pm 0.11$ , which is close to our results.

### 7.3 Unitary Fermi gas

The ground-state energy of a dilute Fermi gas can be obtained by means of perturbation theory [4, 38] with respect to the effective coupling parameter

$$g \equiv |k_F a_s|, \quad (7.13)$$

where  $k_F$  is the Fermi wave number, and  $a_s$  is the atomic scattering length. This perturbation theory yields the expansion

$$E(g) \simeq c_0 + c_1 g + c_2 g^2 + c_3 g^3 + c_4 g^4, \quad (7.14)$$

with the coefficients

$$c_0 = \frac{3}{10}, \quad c_1 = -\frac{1}{3\pi}, \quad c_2 = 0.055661,$$

$$c_3 = -0.00914, \quad c_4 = -0.018604.$$

The scattering length and, respectively, the effective coupling parameter (7.13) can be varied by means of the Feshbach resonance techniques in a rather wide range, including  $g \rightarrow \infty$ . The latter limit corresponds to the system called a unitary Fermi gas. Numerical calculations [3, 12] yield

$$E(\infty) = 0.132. \quad (7.15)$$

Expansion (7.14) can be rewritten in the form

$$E(g) \simeq c_0(1 + a_1 g + a_2 g^2 + a_3 g^3 + a_4 g^4), \quad (7.16)$$

in which

$$a_n \equiv \frac{c_n}{c_0} \quad (n = 1, 2, 3, 4).$$

Factor approximants give  $E_4^*(\infty) = 0.174$  and corrected factor approximants give 0.143. Power-transformed factor approximants yield 0.162. Iterated roots give  $E_3^*(\infty) = 0.169$ ,  $E_4^*(\infty) = 0.163$ . Corrected iterated roots result in  $E_{1/2}^*(\infty) = 0.103$  and power-transformed iterated roots result in 0.163. Doubly renormalized iterated roots improve the limit to 0.146. Padé approximants are not accurate, the best of them giving  $P_{2/2} = 0.170$ .

### 7.4 One-dimensional Heisenberg antiferromagnet

The ground-state energy of an equilibrium one-dimensional Heisenberg antiferromagnet can be represented [25] as the infinite time limit for the energy  $E(t)$  of a non-equilibrium antiferromagnet. At small time  $t \rightarrow 0$ , one has an expansion

$$E(g) \simeq -\frac{1}{4} \left( 1 + \sum_{n=1}^4 a_n t^n \right), \tag{7.17}$$

with the coefficients

$$a_1 = 4, \quad a_2 = -8, \quad a_3 = -\frac{16}{3}, \quad a_4 = 64.$$

In the other limit, this ground-state energy was calculated by Hulthen [26] exactly as

$$E = E(\infty) = -0.4431. \tag{7.18}$$

We apply the self-similar approximations to extrapolate the small-time expansion (7.17) to the infinite time limit  $t \rightarrow \infty$  determining  $E(\infty)$ .

Factor approximants yield  $E_4^*(\infty) = -0.570$ , with power-transformed factor approximants resulting in practically the same value. Corrected factor approximants give  $E_{2/2}^*(\infty) = -0.211$ . Corrected iterated roots also underestimate the limit, giving  $-0.254$ . Iterated roots give  $E_3^*(\infty) = -0.511$ ,  $E_4^*(\infty) = -0.482$ . Power-transformed iterated roots yield  $-0.475$ . The best Padé approximant is  $P_{2/2} = -0.329$ . The most accurate here is the power-transformed iterated root approximant  $E_4^*(\infty) = -0.475$ .

### 7.5 Fröhlich optical polaron

The ground-state energy of the Fröhlich optical polaron in the weak-coupling perturbation theory [43,63] reads as

$$E(g) \simeq -g(1 + a_1g + a_2g^2), \tag{7.19}$$

with the coefficients

$$a_1 = 1.591962 \times 10^{-2}, \quad a_2 = 0.806070 \times 10^{-3}.$$

In the strong-coupling limit, the asymptotic behaviour of the ground-state energy has been found by Miyake [51,52] in the form

$$E(g) \simeq Bg^2 \quad (g \rightarrow \infty), \tag{7.20}$$

with the amplitude

$$B = -0.108513. \tag{7.21}$$

Since just a few terms in the perturbative expansion are available, the Padé approximants are not applicable at all, yielding unreasonable values for the amplitude by many orders differing from equation (7.21). Self-similar approximants give more realistic values. Thus, factor approximants give for the amplitude  $B$  the value 0.061 and iterated roots the value

0.049. The doubly renormalized iterated roots improve the accuracy, giving the value 0.1287 for the amplitude.

## 8 Characteristics of polymer systems

Polymers are rather complicated molecules and are highly important in many branches of physics and chemistry. As a rule, their characteristics are calculated by means of perturbation theory with respect to a small parameter, although in reality this parameter can be quite large. Self-similar approximants can successfully extrapolate these characteristics to arbitrary values of the parameters, including asymptotically large values.

### 8.1 Randomly branched polymers

Many characteristics of polymers are expressed through their structure factors. The structure factor of three-dimensional branched polymers is given [44,50] by the confluent hypergeometric function

$$S(x) = F_1 \left( 1 ; \frac{3}{2} ; \frac{3}{2} x \right), \quad (8.1)$$

in which  $x$  is a dimensionless wave-vector modulus. The long-wave expansion

$$S(x) \simeq c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 \quad (8.2)$$

contains the coefficients

$$c_0 = 1, \quad c_1 = -1, \quad c_2 = 0.6, \quad c_3 = -0.257143, \quad c_4 = 0.085714.$$

In the short-wave limit, one has

$$S(x) \simeq \frac{B}{x} \quad (x \rightarrow \infty), \quad (8.3)$$

with the amplitude

$$B = \frac{1}{3}. \quad (8.4)$$

The reconstruction of the short-wave amplitude by Padé approximants leads to senseless negative values. Factor approximants give  $B_4 = 0.097$ , and the power-transformed factors yield two solutions: 0.179 and 0.329. Iterated roots, at low orders, overestimate the amplitude, giving  $B_2 = 0.745$ ,  $B_3 = 0.642$  and  $B_4 = 0.590$ . The same happens for the power-transformed roots yielding the values close to 0.6. However, the higher orders of the iterated roots converge to value (8.4). For instance, the seventh-order iterated root approximant gives a very good accuracy, with  $B_7 = 0.330$ .

### 8.2 Fluctuating fluid string

There exists an important class of systems, called fluid membranes [62], which finds wide applications in chemistry, biology, medicine and in a variety of technological applications. Firstly, let us consider a model of a fluid string that is a cartoon of a one-dimensional



membrane oscillating between two rigid walls [14, 15]. The free energy of the string coincides with the ground-state energy of a quantum particle in a one-dimensional rigid potential [31, 40]. This energy, as a function of a finite wall stiffness  $g$ , can be represented as

$$E(g) = \frac{\pi^2}{8g^2} \left( 1 + \frac{g^2}{32} + \frac{g}{4} \sqrt{1 + \frac{g^2}{64}} \right). \tag{8.5}$$

The low-stiffness expansion results in

$$E_k(g) = \frac{\pi^2}{8g^2} \left( 1 + \sum_{n=1}^k a_n g^n \right), \tag{8.6}$$

with the coefficients

$$a_1 = \frac{1}{4}, \quad a_2 = \frac{1}{32}, \quad a_3 = \frac{1}{512}, \quad a_4 = 0,$$

$$a_5 = -\frac{1}{131072}, \quad a_6 = 0, \quad a_7 = \frac{1}{16777216}.$$

The case of interest corresponds to rigid walls, when the stiffness tends to infinity. For such rigid walls, the energy is

$$E(\infty) = \frac{\pi^2}{128} = 0.077106. \tag{8.7}$$

Padé approximants are not applicable for this problem, giving negative values of large-stiffness energy. Factor approximants give positive values, although overestimating the energy, e.g.  $E_4^*(\infty) = 0.15$ . Iterated roots yield  $E_2^*(\infty) = 0.039$ ,  $E_3^*(\infty) = 0.051$  and  $E_4^*(\infty) = 0.058$ . Corrected iterated roots give  $E_{2/2}^*(\infty) = 0.169$  and power-transformed iterated roots,  $E_4^*(\infty) = 0.065$ . Taking more terms in the expansion improves the accuracy. Thus, iterated roots of higher orders yield  $E_5^*(\infty) = 0.062$ ,  $E_6^*(\infty) = 0.065$  and  $E_7^*(\infty) = 0.067$ . The most accurate result is obtained by employing the doubly renormalized iterated roots, giving  $E_2^{**}(\infty) = 0.07237$ . The variational perturbation theory to the sixth order gives [35] the value 0.076991.

### 8.3 Fluctuating fluid membrane

In the case of a two-dimensional membrane, its pressure can be calculated by perturbation theory with respect to wall stiffness [35], which yields

$$p_k(g) = \frac{\pi^2}{8g^2} \left( 1 + \sum_{n=1}^k a_n g^n \right), \tag{8.8}$$

with the coefficients

$$a_1 = \frac{1}{4}, \quad a_2 = \frac{1}{32}, \quad a_3 = 2.176347 \times 10^{-3},$$

$$a_4 = 0.552721 \times 10^{-4}, \quad a_5 = -0.721482 \times 10^{-5}, \quad a_6 = -1.777848 \times 10^{-6}.$$

The rigid-wall limit, calculated by means of the Monte Carlo simulations [22], is found to be

$$p(\infty) = 0.0798 \pm 0.0003. \quad (8.9)$$

Padé approximants are again not applicable, resulting in negative values of pressure. Factor approximants of low orders overestimate the limit, e.g. the fourth order giving 0.312. To higher orders, factor approximants become slightly better, but still overestimating the pressure. Iterated roots of low orders give  $p_2^*(\infty) = 0.039$ ,  $p_3^*(\infty) = 0.053$  and  $p_4^*(\infty) = 0.061$ , and power-transformed iterated roots in the fourth order give 0.068. Taking into account all available coefficients improves the results. For instance, in the case of the iterated roots, we have  $p_5^*(\infty) = 0.067$ ,  $p_6^*(\infty) = 0.071$ . Doubly renormalized iterated roots give  $p_3^{**}(\infty) = 0.0792$ , which is the most accurate result. This is to be compared with the value of 0.0821 from the variational perturbation theory [35], which overestimates the Monte Carlo result (8.9).

#### 8.4 Two-dimensional polymer chain

An important characteristic of polymer chains is their expansion factor, that is, the ratio of the mean-square end-to-end distance of the chain, with interactions between its segments, to the value of the mean-square end-to-end distance of the chain, without such interactions. Two-dimensional polymers are often met in chemistry and biology. For such polymers, perturbation theory with respect to weak interactions can be developed [53, 54] and, in a certain limiting case, can be reduced to a series in a single dimensionless interaction parameter  $g$ . For a two-dimensional polymer chain, perturbation theory results [53] in the expansion factor,

$$F(g) \simeq 1 + \sum_{n=1}^4 a_n g^n, \quad (8.10)$$

with the coefficients

$$a_1 = \frac{1}{2}, \quad a_2 = -0.12154525, \quad a_3 = 0.02663136, \quad a_4 = -0.13223603.$$

In the strong-interaction limit [47], one has

$$F(g) \simeq Bg^\beta \quad (g \rightarrow \infty), \quad (8.11)$$

with the critical exponent

$$\beta = 1. \quad (8.12)$$

One also considers the critical index

$$\nu \equiv \frac{1}{2} \left( 1 + \frac{\beta}{2} \right), \quad (8.13)$$

which here is  $\nu = 0.75$ .

Calculating the critical amplitude, we have the following. Factor approximants are complex, but the power-transformed factor approximant at the fourth order gives 0.31. Iterated roots yield  $B_2 = 0.08$ , with the higher orders being complex. The corrected iterated

roots yield  $B_{2/2} = 0.09$ . The exact value of the amplitude  $B$  is not known, because of which we cannot evaluate the accuracy of approximants. But, as we see, all approximants give the values of order 0.1.

### 8.5 Three-dimensional polymer coil

In the case of a three-dimensional polymer coil, perturbation theory [53] for the expansion factor leads to series (8.10), however with the coefficients

$$a_1 = \frac{4}{3}, \quad a_2 = -2.075385396, \quad a_3 = 6.296879676,$$

$$a_4 = -25.05725072, \quad a_5 = 116.134785, \quad a_6 = -594.71663.$$

The strong-coupling limit [54] is

$$F(g) \simeq 1.531g^{0.3544} \quad (g \rightarrow \infty), \tag{8.14}$$

which yields for the critical index (8.13)  $\nu = 0.5866$ . Numerical fitting [54] for the whole range of interactions results in the formula

$$F(g) = (1 + 7.524g + 11.06g^2)^{0.1772}. \tag{8.15}$$

Employing four terms in a weak-coupling expansion gives for the factor approximants the amplitude  $B_4 = 1.548$ , and for power-transformed factor approximants, 1.535. Iterated roots yield  $B_2 = 1.543$ ,  $B_3 = 1.549$ ,  $B_4 = 1.538$ . Corrected iterated roots result in  $B_{2/2} = 1.544$  and power-transformed iterated roots result in  $B_4 = 1.535$ . Doubly renormalized iterated roots give 1.530. Higher-order approximants improve the results, but already at the fourth order all these approximants are close to the numerical value,  $B = 1.531$ . The accuracy of Padé approximants is several orders worse [21].

## 9 Calculation of critical exponents

In the previous sections, we have concentrated on the calculation of critical amplitudes, with known critical exponents, by extrapolating the small-variable perturbative expansions to the large-variable limit, employing the techniques of self-similar approximants. Now we show how the critical exponents can also be found by using these techniques.

### 9.1 Scheme of general approach

When a function, for asymptotically large variable, behaves as

$$f(x) \simeq Bx^\beta \quad (x \rightarrow \infty), \tag{9.1}$$

then the critical exponent can be represented by the limit

$$\beta = \lim_{x \rightarrow \infty} x \frac{d}{dx} \ln f(x). \tag{9.2}$$

Assuming that the small-variable expansion for the function is given by the sum  $f_k(x)$ , as in equation (2.2), we have the corresponding small-variable expression for the critical exponent

$$\beta_k(x) = x \frac{d}{dx} \ln f_k(x), \quad (9.3)$$

which can be expanded in powers of  $x$ , leading to

$$\beta_k(x) = \sum_{n=0}^k b_n x^n. \quad (9.4)$$

Applying the method of self-similar approximants to expansion (9.4), as has been done above, we get a self-similar approximant  $\beta_k^*(x)$  whose limit, being by definition finite,

$$\beta_k^*(x) \rightarrow \text{const} \quad (x \rightarrow \infty),$$

gives us the sought approximate expression for the critical exponent

$$\beta_k^* = \lim_{x \rightarrow \infty} \beta_k^*(x). \quad (9.5)$$

Note that the value of the critical amplitude  $B$  does not need to be considered at all. Below we illustrate this method of calculating critical exponents by concrete examples.

## 9.2 One-dimensional anharmonic oscillator

Let us consider, as in Section 6.2, the model of a one-dimensional anharmonic oscillator whose mathematical structure is typical for many applied problems, yielding strongly divergent perturbation series.

The exact critical exponent, as follows from equation (6.7), is

$$\beta = \frac{1}{3}.$$

In addition to the coefficients  $c_n$  of Section 6.2, we shall analyse the higher-order terms of sum (6.6), with the coefficients

$$c_5 = \frac{916731}{256}, \quad c_6 = -\frac{65518401}{1024}, \quad c_7 = \frac{2723294673}{2048},$$

$$c_8 = -\frac{1030495099053}{32786}, \quad c_9 = \frac{54626982511455}{65536}, \quad c_{10} = -24478940702.8.$$

Employing the scheme of Section 9.1, we find, for the critical exponent, the factor approximants  $\beta_4^* = 0.241$ ,  $\beta_7^* = 0.303$  and  $\beta_8^* = 0.282$ . Iterated roots result in  $\beta_2^* = 0.397$ ,  $\beta_3^* = 0.181$ , but  $\beta_4^*$  is complex. Corrected iterated roots yield  $\beta_{2/2}^* = 0.307$ ,  $\beta_{2/3}^* = 0.328$ ,  $\beta_{2/4}^* = 0.310$ ,  $\beta_{2/5}^* = 0.346$  and  $\beta_{2/6}^* = 0.305$ . Power-transformed roots give two solutions: 0.156 and 0.238. Doubly renormalized iterated roots of the second order lead to 0.319. As we see, the self-similar approximants are rather accurate, being close to 0.3.

### 9.3 Three-dimensional polymer coil

As another example, we consider the three-dimensional polymer coil of Section 8.5. The exponent found numerically, according to equation (8.14), is

$$\beta = 0.3544.$$

Following the scheme of Section 9.1, we obtain the self-similar approximants for critical exponent. Factor approximants yield  $\beta_3^* = 0.343$ ,  $\beta_4^* = 0.346$  and  $\beta_5^* = 0.349$ . Iterated roots result in  $\beta_2^* = 0.345$ ,  $\beta_3^* = 0.343$ ,  $\beta_4^* = 0.351$  and  $\beta_5^* = 0.349$ . Power-transformed iterated roots give two solutions: 0.285 and 0.349, and corrected iterated roots give  $\beta_{1/4}^* = 0.348$ ,  $\beta_{2/2}^* = 0.345$ ,  $\beta_{3/2}^* = 0.349$ . Doubly renormalized iterated roots yield  $\beta_4^{**} = 0.353$ ,  $\beta_5^{**} = 0.355$ . All these approximants are close to the numerical value  $\beta = 0.3544$ .

### 10 Equation of state

The problems, considered in the previous sections, were related to the cases when it was necessary to find the large-variable behaviour of the studied functions. However, generally, the self-similar approximation theory allows us to derive approximants valid for a whole range of the variable. To illustrate this, we show below how it is possible to construct an equation of state, providing a good description in the whole region of densities.

Let us consider a system of quantum hard spheres [37] characterized by the *s*-wave scattering length  $a_s$  corresponding to the diameter of a hard sphere. The ground-state energy, in the limit of low density  $\rho \rightarrow 0$ , is given [46] by the asymptotic expression

$$\frac{E}{N} \simeq 2\pi \frac{\rho a_s}{m} \left( 1 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a_s^3} \right), \tag{10.1}$$

where  $m$  is the sphere mass. The density can increase up to the value  $\rho_0$ , when the system of the spheres becomes close packed. For a primitive hexagonal close packing, such as producing a face-centred cubic arrangement,

$$\rho_0 = \frac{\sqrt{2}}{a_s^3}. \tag{10.2}$$

In the close-packed limit, the energy behaves as

$$\frac{E}{N} \simeq \frac{B}{2m} \left( \rho^{-1/3} - \rho_0^{-1/3} \right), \tag{10.3}$$

with the experimental value

$$B \equiv 2^{2/3} \pi^2 \tag{10.4}$$

found by Cole [13].

To rewrite the low-density asymptotic expression in a more convenient way, we introduce the variable  $x$  by the relation

$$\frac{\rho}{\rho_0} = \frac{x^6}{(1+x^2)^3}. \tag{10.5}$$

As is seen,  $x \rightarrow 0$  when  $\rho \rightarrow 0$  and  $x \rightarrow \infty$  when  $\rho \rightarrow \rho_0$ . With the new variable, expansion (10.1) for  $x \rightarrow 0$  takes the form

$$\frac{E}{N} \simeq 2\pi \frac{\rho_0 a_s}{m} x^6 \left( 1 - 3x^2 + \frac{128}{15\sqrt{\pi}} \sqrt{\rho_0 a_s^3} x^3 + 6x^4 - \frac{192}{5} \sqrt{\rho_0 a_s^3} x^5 \right), \quad (10.6)$$

while the close-packed limit reads as

$$\frac{E}{N} \simeq \frac{\pi^2}{ma_s^2} x^4 \quad (x \rightarrow \infty). \quad (10.7)$$

Using the iterated root approximant of the second order for expansion (10.6), we get

$$\frac{E_2^*}{N} = 2\pi \frac{\rho_0 a_s}{m} x^6 (1 + A_2 x^2)^{-1}, \quad (10.8)$$

with  $A_2 = 2\sqrt{2}/\pi$  corresponding to limit (10.7). Inverting the change of the variable (10.5), we return to the initial variable, that is, to density, obtaining the equation of state

$$\frac{E_2^*}{N} = 2\pi \frac{\rho a_s}{m} \left[ 1 - \left( \frac{\rho}{\rho_0} \right)^{1/3} \right]^{-2} \left[ 1 + b \left( \frac{\rho}{\rho_0} \right)^{1/3} \right]^{-1}, \quad (10.9)$$

in which

$$b = \frac{2\sqrt{2}}{\pi} - 1. \quad (10.10)$$

This equation *exactly* coincides with the empirical equation, called the modified London equation [65], which is in very good agreement with the Green function Monte Carlo computer simulations for the many-body hard-sphere fluid [28]. Higher orders of the self-similar iterated root approximants, as we have checked, do not essentially change the accuracy of the equation of state (10.9) that already gives a perfect agreement with computer simulations.

## 11 Conclusions

We have considered the problem of extrapolating perturbation-theory expansions, obtained for asymptotically small variable  $x \rightarrow 0$ , to the large-variable limit  $x \rightarrow \infty$ . For this purpose, we have applied the theory of self-similar approximations, concentrating on six different variants, resulting in self-similar factor approximants (Section 3.1), self-similar root approximants (Section 3.2), iterated root approximants (Section 3.3), corrected root approximants (Section 3.4), self-similar power-transformed approximants (Section 3.5) and doubly renormalized self-similar approximants (Section 3.6).

Padé approximants are shown to be much less accurate than the self-similar approximants, and often not applicable at all. In some cases, more refined techniques, such as the Kleinert variational perturbation theory, employing control functions introduced through a variable transformation, can give better accuracy, although they are essentially more complicated. However, our main aim here has been the analysis of the validity of the approximants that could provide good accuracy, at the same time being sufficiently simple for calculations and yielding explicit analytical formulas.

In order to demonstrate the wide applicability of the self-similar approximants, we treated a number of examples of rather different nature. In the majority of cases, the approximants yield close results and provide good accuracy of extrapolation. In general, their accuracy is essentially higher than that of Padé approximants. In some cases, the latter are not applicable at all, giving qualitatively wrong results, while self-similar approximants do work in such cases.

Comparing different variants of the analysed self-similar approximants, we see that power-transformed approximants often lead to multiple solutions for the sought parameters, because of which they are less convenient than other approximants enjoying unique solutions. The doubly renormalized approximants, although improving the final results, are cumbersome, allowing only for their complicated numerical calculation. The self-similar factor approximants and iterated root approximants seem to be the most convenient approximants for the purpose of the considered extrapolation.

Having to hand several methods of self-similar extrapolation is important because of the following reason. A problem under consideration can be so complicated that the exact answer is not known and only a few terms of perturbation theory are available, then it is rather difficult to judge the accuracy of the approximation used. However, if different methods give close results, this serves as an argument that the obtained approximations are reliable.

Finally, we have considered problems whose large-variable behaviour is of power-law type. We are aware that there exists another class of problems possessing exponential behaviour and also demonstrating the Stokes phenomenon. For the problems of this class, it is necessary to use another variant of the self-similar approximation theory, involving self-similar exponential approximants [74,84]. These, as has been demonstrated in the cited papers, make it possible to derive accurate approximations for the functions of exponential behaviour as well as to treat problems accompanied by the Stokes phenomenon. We do not address such problems here but have been studied in our previous papers [74,84].

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