

Article

Continued Roots, Power Transform and Critical Properties

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Abstract: We consider the problem of calculation of the critical amplitudes at infinity by means of the self-similar continued root approximants. Region of applicability of the continued root approximants is extended from the determinate (convergent) problem with well-defined conditions studied before by Gluzman and Yukalov (Phys. Lett. A 377 2012, 124), to the indeterminate (divergent) problem by means of power transformation. Most challenging indeterminate for the continued roots problems of calculating critical amplitudes, can be successfully attacked by performing proper power transformation to be found from the optimization imposed on the parameters of power transform. The self-similar continued roots were derived by systematically applying the algebraic self-similar renormalization to each and every level of interactions with their strength increasing, while the algebraic renormalization follows from the fundamental symmetry principle of functional self-similarity, realized constructively in the space of approximations. Our approach to the solution of the indeterminate problem is to replace it with the determinate problem, but with some unknown control parameter b in place of the known critical index β . From optimization conditions b is found in the way making the problem determinate and convergent. The index β is hidden under the carpet and replaced by b . The idea is applied to various, mostly quantum-mechanical problems. In particular, the method allows us to solve the problem of Bose-Einstein condensation temperature with good accuracy.



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1. Introduction

Power transformation [1] could be combined with continued root approximants [2]. Through its application we intend to extend the applicability of the continued roots to a broader class of problems of finding the critical amplitudes and indices.

Generally speaking, the problem of finding the critical amplitudes is equivalent to calculating the constant value of the functions at infinity, another old problem existing in applied mathematics [3]. On the other hand, by applying the so-called D Log transformation, one can attack the problem of critical indices by means developed for the problem of critical amplitudes [4].

The self-similar continued roots were derived in [2] by systematically applying the algebraic self-similar renormalization to each and every level of interactions with their strength increasing, while the algebraic renormalization follows from the functional self-similarity principle implied in the space of approximations, as shown in [5]. In turn, power transformation can be viewed as an algebraic transformation applied to the continued root approximant as a whole.

Special features of the continued root approximants were also discussed in our recent work [6]. Mind that one can explicitly accomplish partial summation of the expression for the effective critical index in infinite order, and find an optimal value for the critical index in each order of perturbation theory [2].

The related body of work preceding or inspiring our own research, was performed by V.I. Yukalov in [7,8], by Kadanoff and Houghton in [9], by Stevenson [10], by M. Suzuki [11,12]

and H. Kleinert [13]. More information can be found in our recent papers [6,14,15]. Feynman’s inspirational ideas were documented in [16].

Formally, we are dealing with a real function $\phi(x)$ of a real variable $x \in [0, \infty)$. In practice, one is able to develop the perturbation theory which yields truncated asymptotic expansions representing the function

$$\phi(x) \simeq \phi_k(x) \quad (x \rightarrow 0) \tag{1}$$

at a small variable x , with $k = 0, 1, \dots$ standing for perturbation order.

Thus in k th order we are in possession of the truncated expansion in powers of x ,

$$\phi_k(x) = a_0 + \sum_{n=1}^k a_n x^n. \tag{2}$$

Unless otherwise stated the normalization $a_0 = 1$ is chosen. The truncated series (2) will be subjected to resummation. We are concerned with the typical power law behavior of the form

$$\phi(x) \simeq Bx^\beta \quad (x \rightarrow \infty), \tag{3}$$

and intend to calculate the constants B (critical amplitude) and β (critical index) based on the coefficients of the small variable expansion (2).

The amplitude is always positive. The critical exponent could be positive or negative. When the critical index is known one has to calculate only the amplitude.

In our preceding work [2], in low-orders we derived the following self-similar continued root approximants,

$$\begin{aligned} \mathcal{R}_1^*(x) &= (1 + A_1 x)^s, \quad \mathcal{R}_2^*(x) = (1 + A_1 x(1 + A_2 x)^s)^s, \\ \mathcal{R}_3^*(x) &= \left(1 + A_1 x(1 + A_2 x(1 + A_3 x)^s)^s\right)^s. \end{aligned} \tag{4}$$

The amplitudes A_k could be found iteratively. They are given in all orders by simple expressions:

$$\begin{aligned} A_1 &= \frac{a_1}{s}, \quad A_2 = \frac{a_1^2(-s) + a_1^2 + 2a_2s}{2a_1s^2}, \\ A_3 &= \frac{a_1^4(-(s-1))(s+1)(5s-3) + 12a_1^2a_2s(s^2-1) - 24a_1a_3s^3 + 12a_2^2(s-1)s^2}{12a_1s^3(a_1^2(s-1) - 2a_2s)}. \end{aligned} \tag{5}$$

The formulas (5) follow from the requirement of an asymptotic equivalence with the truncated series (2).

In general case we have

$$\mathcal{R}_k^*(x) = \left(1 + A_1 x(1 + A_2 x \dots (1 + A_k x)^s) \dots\right)^s, \tag{6}$$

with $k = 1, 2, \dots$. As $x \rightarrow \infty$

$$\mathcal{R}_k^* \simeq B_k x^{\beta_k},$$

with

$$\beta_k = s + s^2 + \dots s^k.$$

The critical amplitudes are given by the recursion

$$B_k = B_{k-1} A_k^{s^k}, \quad k = 1, 2, \dots,$$

with the initial condition $B_0 = a_0$.

With exactly found as $k \rightarrow \infty$, control parameter

$$s = \frac{\beta}{1 + \beta}, \quad \beta > -\frac{1}{2}, \tag{7}$$

the sequence of continued roots converges to the limit expression with the correct critical index β at infinity in the infinite order [2]. Of course, we have to know β in advance to make the formulas work.

The case when the inequality (7) is satisfied will be called *determinate*. In the opposite case, $\beta \leq -\frac{1}{2}$, we are dealing with a divergent *indeterminate* problem. The primary goal of the paper is to solve (approximately) the indeterminate problem. More precisely we would like to calculate the critical amplitudes and indices in such a case.

Similar indeterminate problem for the Padè approximants was discussed in [17,18]. Most intriguing quantum paradoxes could be associated with indeterminate moment problems [19]. Before proceeding to the indeterminate case, let us first illustrate the strength of continued roots for a couple of examples corresponding to the determinate problem.

2. Determinate Problem Examples

Harmonium. Let us consider the ground state energy of a 2-electron harmonium atom [20]. Such harmonium atom corresponds to the physical system of two electrons confined by the spherically symmetric harmonic potential, modeled by the Hamiltonian

$$\hat{H} = \frac{1}{2} \sum_{i=1}^2 \left(-\nabla_i^2 + \omega^2 r_i^2 \right) + \frac{1}{2} \sum_{i \neq j} \frac{1}{r_{ij}} . \tag{8}$$

The nondimensional variables are used, and $\frac{\omega^2}{2}$ stands for the harmonic oscillator force constant [20], while $r_i \equiv |\mathbf{r}_i|$, $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j|$.

By introducing the new variable $x \equiv \omega^{1/3}$, we arrive at the following truncation for the ground state energy of harmonium

$$e(x) \simeq 1.19055x^2(1 + 1.98734x + 0.102887x^2) \quad (x \rightarrow 0) .$$

As $x \rightarrow \infty$

$$e(x) \simeq Bx^3,$$

with $B = 3$. We have a determinate case with $\beta = 1$ and $s = 1/2$. It is then pretty much straightforward to calculate

$$B_1 = 2.37355, \quad B_2 = 2.85418, \quad B_3 = 2.93264.$$

The last estimate results from adding a trial value for the third-order coefficient, $a_3 = 0$. It brings the error of only 2.25%.

Fröhlich optical polaron. Consider the problem of the effective mass of the celebrated Fröhlich optical polaron. One can develop a perturbation theory in powers of the coupling constant g [21]. It reads as follows,

$$m(g) \simeq 1 + \frac{1}{6}g + 0.0236276g^2 \quad (g \rightarrow 0). \tag{9}$$

For large value of the coupling constant the effective mass behaves as a power law [21],

$$m(g) \simeq Bg^4 \quad (g \rightarrow \infty), \tag{10}$$

with the amplitude

$$B = 0.022702 . \tag{11}$$

We have a determinate case with $\beta = 4$ and $s = 4/5$. It is then pretty much straightforward to calculate

$$B_1 = 0.285106, \quad B_2 = 0.102836, \quad B_3 = 0.0252002.$$

The last estimate is obtained with $a_3 = 0$, bringing the error of 11%.

We had also studied the effect of adding one more trial term to the expansion for the ground state energy of the nonlinear Schrödinger model. Basic information concerning some mathematics and physical applications of the model could be found in [2]. The critical point is located at infinity, and

$$e(g) \simeq Bg^{2/3},$$

with $B = 3/2$. The expansion at small g is available up to the 5th order in the coupling constant g [2]. Let us add one more trial coefficient to the expansion at small g , i.e., $a_6 = 0$. After standard calculations we find an almost perfect numerical convergence to the value $B_6 = 1.50765$.

Also, the technique pertinent to the determinate case can be applied to the critical amplitudes of Schwinger model [22]. The ground state energy of the model [23], is known to decay as the power law

$$e(x) \simeq 0.6418x^{-1/3},$$

where x stands for the inverse coupling constant (see, e.g., [22] and references therein). After standard calculations with the second-order expansion at small x (see, e.g., [22] and referencing therein), we find some very reasonable estimates for the critical amplitude, $B_1 = 0.6403$, $B_2 = 0.5581$.

3. Indeterminate Problem Method

The fresh challenge starts when we are dealing with situations when $\beta \leq -1/2$. As of now we are confronted with an *indeterminate* problem as long as the continued roots are concerned. Mind that the key point for the effective solution of the determinate problem is our knowledge of β and the ability to express the control parameters s through β . Last but not least, the region of β allowing for convergence of continued roots, is strictly defined as is simply expressed by the expressions (7).

Our approach to the solution of the indeterminate problem is to replace it with the determinate problem, but with some unknown parameter b in place of the known β . The problem is going to be reduced to defining an additional condition(s) to find b , while making the problem convergent. But first we need to put β under the carpet and replace it by b . After b is found explicitly from optimization conditions, β is returned to play my means of inverse power transform.

We are going to approach the indeterminate problem my means of the power transforms [1,24,25]. First, we apply the power transform to the truncated expansion (2),

$$\hat{P}_k(x, b) \equiv (\phi_k(x))^{b/\beta} . \tag{12}$$

The transformed expression can be expanded in powers of x ,

$$\hat{P}_k(x, b) \simeq \sum_{n=0}^k c_n(b)x^n . \tag{13}$$

The expansion (13) is subjected to self-similar renormalization. We are supposed to arrive at an approximant $\mathcal{R}_k^*(x, b)$, and in our case to the self-similar continued root.

Then, we have to accomplish the inverse transformation

$$\hat{F}_k(x, b) = [\mathcal{R}_k^*(x, b)]^{\beta/b} . \tag{14}$$

Here

$$\mathcal{R}_k^*(x) = \left(1 + A_1(b)x \left(1 + A_2(b)x \dots \left(1 + A_k(b)x \right)^{s(b)} \right)^{s(b)} \dots \right)^{s(b)} .$$

As $x \rightarrow \infty$

$$\mathcal{R}_k^*(x, b) \simeq B_k(b)x^{b_k(b)},$$

with

$$b_k(b) = s(b) + s(b)^2 + \dots + s(b)^k,$$

and the intermediate amplitudes for the transformed sequence are given by the recursion

$$B_k(b) = B_{k-1}(b)A_k(b)^{s(b)^k}, \quad k = 1, 2, \dots,$$

with the initial condition $B_0 = 1$. With, supposedly found as $k \rightarrow \infty$, control parameter b , we have

$$s(b) = \frac{b}{1+b}, \quad b > -\frac{1}{2}. \tag{15}$$

And the sequence of continued roots $\mathcal{R}_k^*(x, b)$ converges to the limit power law expression $\mathcal{R}_\infty^*(x, b) \propto x^b$, with the index b as $x \rightarrow \infty$. Thus we formally reproduce the basic scheme of [2]. With the condition (15) the problem becomes *determinate* provided we can also supply the way to find b explicitly.

To find final critical amplitudes we have to accomplish the inverse transformation (14). After the inverse transformation the sought approximation for original $\phi(x)$ is given by

$$\phi_k^*(x) = \hat{F}_k(x, b). \tag{16}$$

As $x \rightarrow \infty$

$$\phi_k^*(x) \simeq \hat{B}_k x^{\frac{\beta b_k}{b}},$$

with the sought critical amplitude expressed as follows,

$$\hat{B}_k = (B_k(b_k))^{\beta/b}.$$

The parameter b and powers b_k are defined by the variational condition

$$\frac{\partial \hat{B}_k(b)}{\partial b} = 0, \tag{17}$$

to be called the minimal derivative, or minimal sensitivity condition. Solving (17), we find some optimal $b = b^*$, and calculate the critical amplitude

$$\hat{B}_k = \hat{B}_k(b^*).$$

Equation (17) simply states that critical amplitude, a physical quantity, can not possibly depend on the formally introduced parameter of power transform.

We skip here explicitly mentioning that b^* is also dependent on the order k . If needed, such dependence can be made explicit.

4. Indeterminate Problem Examples

Consider first the toy model, expressed by the following function

$$\phi(x) = \frac{2}{(2x + 1)^{3/4} + 1}, \tag{18}$$

so that as $x \rightarrow 0$

$$\phi(x) \simeq 1 - 0.75x + 0.75x^2 - 0.859375x^3 + 1.07813x^4 - 1.44727x^5 + 2.04883x^6, \tag{19}$$

and as $x \rightarrow \infty$

$$\phi(x) \simeq 1.18921x^{-3/4}. \tag{20}$$

In the 4th order there are two good solutions

$$b^* = -0.280138, \hat{B}_4 = 1.20406; \quad b^* = -0.107597, \hat{B}_4 = 1.16005.$$

They do frame the exact result nicely, but the leftmost solution is much better in approximating the coefficient a_6 and should be preferred. The same logic will be followed in the forthcoming, more realistic examples, when the choice of the leftmost solution will be made.

Solving (17) in 5th order leads to the unique solution $b^* = -0.156158$, and $B = \hat{B}_5 = 1.18043$, a very accurate result for B .

One can approach the problem of finding b differently. Let us construct the approximant $[\mathcal{R}_5^*(x, b)]^{\hat{\beta}/b}$ in general form with arbitrary b , calculate the 6th order coefficient in the expansion as the function of b , compare it to the known a_6 and find b^* as the minimizer of the error in predicting a_6 . Following this line of calculations we find $b^* \approx -0.19986$, and $\hat{B}_{5+1} \approx 1.19101$.

Generally speaking, such approach could be coined as $k + 1$ optimization, when k asymptotic conditions are used to construct the approximant as the function of parameter b , but b is supposed to be found from minimizing the error in prediction of the known and purposely withheld $k + 1$ coefficient.

4.1. Bose-Einstein Condensation Temperature

From statistical physics we know how to find the Bose-Einstein condensation temperature T_0 of ideal uniform Bose gas [26]. It is also well-known that the ideal gas is unstable below the condensation temperature. One should explicitly introduce the atomic interactions and stabilize the system [27]. Introducing interactions also shifts the transition temperature to the value of T_c . The shift $\Delta T_c \equiv T_c - T_0$ appears to be linear in the parameter $\gamma \equiv \rho^{1/3} a_s$ (see, e.g., review [4] and paper [17]). Namely,

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

Here a_s stands for atomic scattering length, and ρ stands for gas density. Monte Carlo simulations (see [17] and multiple references therein), give $c_1 = 1.3 \pm 0.05$. Theoretically, the coefficient c_1 can be defined [28–30] as the strong-coupling limit

$$c_1 = \lim_{g \rightarrow \infty} c_1(g) \equiv B, \tag{21}$$

of a function $c_1(g)$ with the expansion at small g

$$c_1(g) \simeq 0.223286g - 0.0661032g^2 + 0.026446g^3 - 0.0129177g^4 + 0.00729073g^5, \tag{22}$$

in the effective coupling parameter g .

Since $\beta = -1$, the problem of finding B is undetermined. In the 4th order there are two good solutions

$$b^* = -0.30884, \hat{B}_4 = 1.30065; \quad b^* = -0.165796, \hat{B}_4 = 1.18522.$$

Both results agree rather well with other theoretical and numerical simulation estimates discussed extensively in [17]. But the leftmost solution as a less intrusive, being closer to the original value of -1 , should be preferred, the conclusion based also on the analogy with the toy model presented above.

In the same way one can find the values of c_1 for some other models. For instance, for the $O(1)$ field theory [29], it is represented by the following expansion at small g :

$$c_1(g) \simeq 0.334931g - 0.178478g^2 + 0.129786g^3 - 0.115999g^4 + 0.120433g^5.$$

Since $\beta = -1$ the problem of finding B is undetermined. In the 4th order there are two good solutions

$$b^* = -0.346347, \hat{B}_4 = 1.13982; \quad b^* = -0.166635, \hat{B}_4 = 0.998593.$$

Both results, especially the leftmost solution to be selected, agree with Monte Carlo numerical estimate $c_1 = 1.09 \pm 0.09$, discussed in [17].

Similarly, for yet different case of the $O(4)$ field theory, the following expansion was found in the paper [29],

$$c_1(g) \simeq 0.167465g - 0.0297465g^2 + 0.00700448g^3 - 0.00198926g^4 + 0.000647007g^5,$$

and for the indeterminate problem with $\beta = -1$, we calculate

$$b^* = -0.284207, \hat{B}_4 = 1.55037; \quad b^* = -0.162829, \hat{B}_4 = 1.44751.$$

The leftmost solution to be selected, agrees with Monte Carlo numerical estimate $c_1 = 1.6 \pm 0.1$, discussed in [17].

The problem of Bose-Einstein condensation temperature was somewhat elusive even for our most advanced technique of corrected approximants, requiring a non-trivial approach with control functions, but is captured with relative ease and with better accuracy by the power-transformed and optimized continued roots. Although the truncation is short it appears to be informative as one can think that the role of missing higher-order terms is successfully mimicked by the minimal derivative condition.

4.2. Lieb-Liniger Bose Gas

Consider a one-dimensional Bose gas with contact interactions quantified by the coupling parameter g . The ground-state energy of the Lieb and Liniger model [31], can be written as

$$E(g) \simeq g - \frac{4}{3\pi} g^{3/2} + \frac{1.29}{2\pi^2} g^2 - 0.017201g^{5/2} \quad (g \rightarrow 0). \quad (23)$$

In the limit of very large g , another expression

$$E(\infty) = \frac{\pi^2}{3} \approx 3.289868, \quad (24)$$

was found by Tonks and Girardeau.

In the variables $e(x) \equiv E(x^2)$, $g \equiv x^2$, the expansion (23) can be standardized, i.e.,

$$e(x) \simeq x^2 \left(1 - 0.424413x + 0.065352x^2 - 0.017201x^3 \right). \quad (25)$$

In this case $\beta = -2$, and we are dealing with the indeterminate problem.

Sometimes, the “inverse” approximant with $b = 1$, could give better results than transformed approximants. Taking the inverse of the sought quantity can possibly restore some lost exact asymptotic property as it happens in the theory of critical indices with the celebrated ϵ -expansion [5].

How to understand the case of $b = 1$? Mind that pretty much standard way to calculate the critical amplitude B was suggested in [3]. Let us calculate the critical amplitude B . First, let us apply the power transform with fixed power to obtain power-transformed series

$$T(x) = \phi(x)^{-1/\beta}.$$

The transformation excludes from consideration the x^β behavior at infinity. Thus we arrive to the following approximation to the critical amplitude

$$B = \lim_{x \rightarrow \infty} (xP_{n,n+1}(x))^{-\beta},$$

to be calculated by means of the standard Padé approximants $P_{n,n+1}(x)$, applied to the function $T(x)$ [3,32].

Any other approximants, including continued roots, with similar behavior at infinity could be employed [14,18,33]. The desired approximants to series $T(x)$ should behave

at infinity as x^{-1} . Such asymptotic form is required to guarantee the finite value for the critical amplitude B . From the standpoint of the continued roots approximants the problem appears as indeterminate.

We are concerned with application of the continued roots and would need to have at hand a determinate problem. Naively, one can simply take the inverse of $xT(x)$. In order for the inverse, $\frac{1}{xT(x)}$, to be able to calculate the finite value at infinity, the desired continued roots approximants to the series $T(x)^{-1}$ should behave at infinity linearly, as x^1 . Now, from the standpoint of the continued roots we arrive at the determinate problem. Here comes the explanation of the term “standard inverse”, or just “inverse”, through sketching the line of thought leading to the condition of $b = 1$.

In the case of Lieb-Liniger gas the “inverse” approximants with $b = 1$, give the best results, by far better than optimized approximants. We have numerically convergent sequence of critical amplitudes,

$$\hat{B}_1(1) = 2.3562, \hat{B}_2(1) = 3.20382, \hat{B}_3(1) = 3.25752,$$

only 0.98% off the exact Tonks-Girardeau result. Numerical convergence of the inverse scheme is controlled only through increasing order of approximants.

4.3. Calculation of the Wilson Loop

The following expression, containing the modified Bessel function of the first kind I_1

$$\phi(y) = \frac{2 \exp(-\sqrt{y}) I_1(\sqrt{y})}{\sqrt{y}}, \tag{26}$$

has a deep physical meaning. It can be interpreted as the $N = 4$ Super Yang-Mills circular Wilson loop [34].

Let us introduce the new variable $\sqrt{y} = x$. In terms of x ,

$$\phi(x) \simeq 1 - x + \frac{5x^2}{8} - \frac{7x^3}{24} + \frac{7x^4}{64} - \frac{11}{320}x^5, \quad x \rightarrow 0. \tag{27}$$

And as $x \rightarrow \infty$,

$$\phi(x) \simeq B x^{-3/2}.$$

Here the critical amplitude $B = \sqrt{\frac{2}{\pi}} \approx 0.797885$. In this case $\beta = -3/2$, and we once again have to solve the indeterminate problem.

The optimization based on the minimal derivative condition gives bad results in this case, with the best result of only $B \approx 0.595$ achieved.

The “inverse” approximants with $b = 1$, give good results, so that have numerically convergent sequence of critical amplitudes,

$$\hat{B}_1(1) = 0.805927, \hat{B}_2(1) = 0.782096, \hat{B}_3(1) = 0.779155,$$

$$\hat{B}_4(1) = 0.777479, \hat{B}_5(1) = 0.775124.$$

The error incurred by the last term in the sequence equals 2.85%.

One can approach the problem of finding b differently, following the pass already outlined above. Let us construct the approximant $[\mathcal{R}_4^*(x, b)]^{\beta/b}$ in general form with arbitrary b , calculate the 5th order coefficient in the expansion as the function of b , compare it to the known a_5 and find b^* as the minimizer of the error in predicting a_5 . Following this line of calculations we find $b^* \approx 0.902075$, and $\hat{B}_{4+1} \approx 0.794868$. Such an approach, coined as $4 + 1$ scheme, brings the error of only 0.38%.

Convergence is not always as fast as in the examples presented above. For instance, in the correlation function of random branched polymers discussed in [4,18], we encounter much slower convergence when a similar methodology is applied with a comparable

number of terms in the expansion. Typical remedies include adding more terms when possible, and applying different optimized approximations, or even introducing control functions instead of control parameters [17,18]. Generally speaking, a similar to very slow convergence problem of barren information plateaus is met in quantum machine learning [35].

4.4. Hard-Core Scattering Problem

The problem of calculating the scattering length of a repulsive square-well potential [36], can be reduced to calculation of the integral

$$S(y) = \int_0^y \left(\frac{\sin t}{t^3} - \frac{\cos t}{t^2} \right) dt, \tag{28}$$

with the exact limit

$$S(\infty) = \pi/15.$$

Using the variable $y = \sqrt{x}$, one can find as $x \rightarrow 0$,

$$S(x) \simeq \sqrt{x} \left(\frac{1}{9} - \frac{x}{135} + \frac{x^2}{2625} - \frac{4x^3}{297675} + \frac{2x^4}{5893965} - \frac{x^5}{166080925} + \frac{x^6}{10672286625} \right). \tag{29}$$

We see that the problem of calculating critical amplitude

$$B = \pi/15 \approx 0.20944,$$

can be reduced to the indeterminate problem with $\beta = -1/2$.

The method of minimal derivative severely underestimates the amplitude, giving the estimate $\hat{B} \approx 0.1$. On the other hand, the “inverse” approximants with $b = 1$, give a numerically convergent sequence of critical amplitudes

$$\begin{aligned} \hat{B}_1(1) &= 0.15462, \hat{B}_2(1) = 0.185754, \hat{B}_3(1) = 0.203357, \\ \hat{B}_4(1) &= 0.212125, \hat{B}_5(1) = 0.216145. \end{aligned}$$

The error incurred by the last term in the sequence equals 3.2%.

Let us explore the 4 + 1 scheme and construct the approximant $[\mathcal{R}_4^*(x, b)]^{\beta/b}$ following the same route as in the previous example. Following this line of calculations we find $b^* \approx 1.0045$, and $\hat{B}_{4+1} \approx 0.211961$. The 4 + 1 scheme brings the error of 1.2%.

When the 6th-order coefficient a_6 in the expansion in the variable y is available as well, one can extend the calculations to 4 + 2, meaning that one should predict both 5th and 6th order coefficients, calculate the error for each of them (not forgetting to take the absolute value of differences), and take their simple average. By minimizing such defined average error of predicting the two withheld coefficients one can attempt to find b . Following the idea we find $b^* \approx 1.0518$, and $\hat{B}_{4+2} \approx 0.210248$. Such an approach could be coined as 4 + 2, and it brings the error of only 0.39%.

5. Indeterminate Problem Calculation of Critical Exponents

Critical exponents can be found by using the very same techniques as employed above for the critical amplitudes. Consider the following limit-case

$$\phi(x) \simeq Bx^\beta \quad (x \rightarrow \infty),$$

representative to the critical phenomena. The critical exponent β can be expressed formally as the following limit

$$\beta = \lim_{x \rightarrow \infty} x \frac{d}{dx} \ln \phi(x) \equiv \lim_{x \rightarrow \infty} x \psi(x), \tag{30}$$

where

$$\psi(x) \equiv \frac{d}{dx} \ln \phi(x),$$

as shown in [4,37,38]. In terms of the small-variable truncation $\phi_k(x)$, we can express the truncated *DLog* function $\psi_k(x)$,

$$\psi_k(x) = \frac{d}{dx} \ln \phi_k(x).$$

In turn, it can be expanded in powers of x ,

$$\psi_k(x) = \sum_{n=0}^k d_n x^n. \tag{31}$$

But for large $x \rightarrow \infty$

$$\psi(x) \simeq \beta x^\delta,$$

where the “amplitude” is the sought critical index β , and the “critical index” $\delta \equiv -1$.

Thus a critical index could be expressed as an amplitude for some extrapolation problem. The problem of finding the critical index β appears to be always indeterminate. It is analogous to the indeterminate problem of finding critical amplitude with known critical index $\equiv -1$. We are going to calculate the critical index routinely, by applying to the obtained expansion (31) the methods developed above for the indeterminate problem for the critical amplitudes.

To warm up let us consider first the toy model, described by the function

$$\phi(x) = \frac{\sqrt{1+2x} + 1}{2}, \tag{32}$$

which can be interpreted as the generalized Flory equation of state in the theory of 2D polymer coils [33]. For small x the following expansion can be easily established,

$$\phi(x) \simeq 1 + \frac{x}{2} - \frac{x^2}{4} + \frac{x^3}{4} - \frac{5x^4}{16} + \frac{7x^5}{16},$$

while for large x we have a power law

$$\phi(x) \sim \sqrt{x}.$$

Method of optimization based on the minimal derivative requirement gives the best results

$$\hat{\beta}_2(-0.28681) = 0.441731, \quad \hat{\beta}_3(-0.15899) = 0.435746, \quad \hat{\beta}_4(-0.32889) = 0.467625, \\ \hat{\beta}_5(-0.252525) = 0.465299,$$

with an error of 6.5%. The $k + 1$ optimization fails to bring the real solution, and the inverse approximants give inferior results, with the best result $\hat{\beta}_4(1) = 0.338866$ being far off the target value.

5.1. Polymer Coil

Consider the three-dimensional polymer coil, characterized by a nondimensional interaction parameter g [39,40]. In the strong-interaction limit $g \rightarrow 0$ one expects the power law behavior for the swelling factor

$$Y(g) \simeq Bg^\beta \quad (g \rightarrow \infty), \tag{33}$$

with the reference value of critical exponent $\beta = 0.3544$, found numerically in [40]. Perturbation theory developed for the swelling factor in [39], leads to the truncated expansion

$$Y(g) \simeq 1 + \frac{4}{3}g - 2.075385396g^2 + 6.296879676g^3 - 25.05725072g^4 + 116.134785g^5 - 594.71663g^6 \quad (g \rightarrow 0). \quad (34)$$

Following the main scheme of indeterminate problem we obtain with the power-transformed self-similar continued roots after optimization with the minimal derivative condition,

$$\hat{\beta}_3(-0.19071) = 0.3675, \quad \hat{\beta}_4(-0.09925) = 0.3599, \quad \hat{\beta}_5(-0.2134) = 0.36513.$$

The 4 + 1 optimization scheme gives close result $\hat{\beta}_{4+1}(-0.14425) = 0.3647$, while the “inverse” approximants scheme converges rapidly to the inferior result $\hat{\beta}_3(1) = 0.3074$. The higher-order results appear to be complex.

5.2. Quartic Oscillator

The quantum anharmonic oscillator with the Hamiltonian

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

where g is a positive parameter of anharmonicity, is widely studied in quantum mechanics and approximation theory. The Hamiltonian is known to result in a strongly divergent perturbation theory. For the ground-state energy it yields [41,42] the truncated series

$$e_k(g) \simeq \sum_{n=0}^k a_n g^n, \quad (35)$$

in rather high orders, with only the few starting coefficients shown below:

$$a_0 = \frac{1}{2}, \quad a_1 = \frac{3}{4}, \quad a_2 = -\frac{21}{8}, \quad a_3 = \frac{333}{16}, \quad a_4 = -\frac{30885}{128},$$

$$a_5 = \frac{916731}{256}, \quad a_6 = -\frac{65518401}{1024}, \quad a_7 = \frac{2723294673}{2048}.$$

The strong-coupling limit is a power law

$$e(g) \sim g^\beta \quad (g \rightarrow \infty), \quad (36)$$

while the critical exponent $\beta = 1/3$.

Following the main scheme of indeterminate problem we obtain with the power-transformed self-similar continued roots after optimization with the minimal derivative condition,

$$\hat{\beta}_3(-0.22740) = 0.274960, \quad \hat{\beta}_4(-0.16085) = 0.282615, \quad \hat{\beta}_5(-0.28985) = 0.311653,$$

$$\hat{\beta}_6(-0.23515) = 0.312131,$$

with the error of 6.36%. Two other schemes fail to produce a convergent sequence (“inverse” scheme), or generate complex numbers (5 + 1 scheme). Even better accuracy can be achieved when much more terms from the expansion (35) are accounted for, as discussed in the Section 6. Higher-order potentials can be of interest as well [43,44].

5.3. Nonlinear Schrödinger Model

We can also calculate the critical exponent for the one-dimensional nonlinear Schrödinger model with the following nonlinear Hamiltonian

$$\hat{H}_{NLS} = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} x^2 + g|\psi|^2, \quad (37)$$

for the wave function $\psi(x)$ of the Bose-condensed atoms in a harmonic trap, where g is the effective coupling.

The expansion of the ground state energy $e(g)$ for small g

$$e_5(g) = 1 + g - \frac{1}{8}g^2 + \frac{1}{32}g^3 - \frac{1}{128}g^4 + \frac{3}{2048}g^5, \tag{38}$$

was obtained first in [43]. The critical point is located at infinity, with the ground state energy behaving as

$$e(g) \sim g^\beta,$$

with the exponent $\beta = 2/3$. Let us again add one more trial coefficient, $a_6 = 0$, to the expansion at small g .

After standard calculations with 3 + 1 optimization scheme we find rather good estimate $\hat{\beta}_{3+1}(0.271135) = 0.67592$, bringing the error of 1.39%,

Following the scheme of indeterminate problem and the “inverse” scheme we obtain with the power-transformed self-similar continued roots

$$\begin{aligned} \hat{\beta}_1(1) &= 0.632456, \hat{\beta}_2(1) = 0.581431, \hat{\beta}_3(1) = 0.589432, \\ \hat{\beta}_4(1) &= 0.607582, \hat{\beta}_5(1) = 0.625906, \end{aligned}$$

with the best estimate giving an error of 6%. The method of optimization based on the minimal derivative condition gives “only” $\hat{\beta} \approx 0.55$.

Along the same lines one can also consider the Bose-condensate within spherically-symmetrical traps. It is modeled by the effective Hamiltonian

$$\hat{H}_r = \frac{1}{2} \left(-\frac{d^2}{dr^2} + r^2 \right) + \frac{g}{4\pi r^2} \chi^2, \tag{39}$$

for the radial part of the condensate wave function $\chi(r)$ [45].

The energy of the ground state can be approximated by the truncated expansions

$$e(c) \simeq \frac{3}{2} + \frac{1}{2}c - \frac{3}{16}c^2 + \frac{9}{64}c^3 - \frac{35}{256}c^4 \quad (c \rightarrow 0), \tag{40}$$

and

$$e(c) \sim c^\beta \quad (c \rightarrow \infty), \tag{41}$$

with the index $\beta = \frac{2}{5}$, and $c = \frac{g}{(2\pi)^{3/2}}$.

Following the main scheme of indeterminate problem we obtain with the power-transformed continued roots after optimization with the minimal derivative condition,

$$\hat{\beta}_2(-0.261315) = 0.40692, \hat{\beta}_3(-0.127056) = 0.386405.$$

with the error of 3.34% in the latter case. The standard inverse scheme brings the results by far inferior.

5.4. Scalar Field Theory

Consider free energy $f(x)$ of the $m\varphi^2$ quantum field theory. It is defined on a d -dimensional cubic lattice with lattice spacing a [3]. In terms convenient for the further analysis, it could be expressed through the modified Bessel function of zero order

$$\frac{f(x)}{x} \equiv \phi(x) = \exp \left\{ 2 \int_0^\infty e^{-t} \ln [e^{-xt} I_0(xt)] dt \right\}. \tag{42}$$

The variable x is expressed through the lattice spacing, and $x = 1/ma^2$. The integral can be expanded in powers of the variable x , i.e.,

$$\phi(x) \simeq 1 - 2x + 3x^2 - \frac{10x^3}{3} + \frac{29x^4}{12}. \tag{43}$$

In order to pass to the continuous limit, we have to take explicitly the limit $a \rightarrow 0$ ($x \rightarrow \infty$). In the continuous limit the selected part of the free energy is characterized by the following power law:

$$\phi(x) \sim x^\beta,$$

with $\beta = -1$.

The “inverse” approximants with $b = 1$, give good results, so that we have a numerically convergent sequence of critical indices,

$$\hat{\beta}_1(1) = -1.41421, \hat{\beta}_2(1) = -1.07457, \hat{\beta}_3(1) = -0.975575.$$

The higher-order calculations lead to complex results for the index. The error incurred by the last term in the sequence equals 2.2%.

From the standard calculations with 3 + 1 optimization scheme we find rather good estimate $\hat{\beta}_{3+1}(0.5502) = -1.02113$, bringing the error of 2%, while the optimization scheme based on minimal derivative condition fails to produce the solutions to the optimization problem.

6. Discussion

In most general form the continued roots can be expressed

$$R_k^*(x) = \left(1 + A_1 x (1 + A_2 x \dots (1 + A_k x)^{s_1})^{s_2} \dots \right)^{s_k}, \tag{44}$$

with all different “amplitudes” A_k and sub-“indices” s_k [2]. When interested in the critical amplitudes B it is natural to concentrate only on “amplitudes” A_k and set all sub-“indices” to equal value of s . Such an idea amounts to the well-defined convergence of continued roots, while not necessarily ensuring existence of real solutions in arbitrary orders.

On other hand, when interested in direct calculations of critical indices β one can try to impose simplifying conditions on “amplitudes” A_k , setting them all to the same value of A . Such complementary approach ensures existence of real solutions and leads to the following approximants

$$r_k^*(x) = \left(1 + A x (1 + A x \dots (1 + A x)^{s_1})^{s_2} \dots \right)^{s_k}, \quad k = 1, 2, \dots, \tag{45}$$

with

$$r_1^*(x) = (1 + A x)^{s_1}, \quad r_2^*(x) = (1 + A x (1 + A x)^{s_1})^{s_2},$$

$$r_3^*(x) = \left(1 + A x (1 + A x (1 + A x)^{s_1})^{s_2} \right)^{s_3}.$$

Elementary power-counting leads to explicit expressions for the critical indices β_i . In low-orders we have simple expressions

$$\beta_2 = (1 + s_1)s_2, \quad \beta_3 = (1 + (1 + s_1)s_2)s_3, \quad \beta_4 = (1 + (1 + (1 + s_1)s_2)s_3)s_4,$$

and so on. One can see that

$$\beta_4 = s_4 + s_4s_3 + s_4s_3s_2 + s_4s_3s_2s_1,$$

meaning that the critical index by itself is being represented as an expansion in the sub-“indices”.

The latter formula can be easily generalized to an arbitrary order,

$$\beta_k = s_k + s_k s_{k-1} + s_k s_{k-1} s_{k-2} + \dots + s_k s_{k-1} s_{k-2} \dots s_1, \tag{46}$$

(with $s_0 \equiv 0$). Note that the case of $\beta = 0$ can be treated as well.

Remarkably, the critical index can be expressed from the continued roots in two different ways. In addition to the Formula (30) we have the expansion in sub-“indices” (46). As a consequence, there are two complementary ways, expressed in the Formulas (6) and (45), to approximate the complete expression (44). One can even think that the two approaches are applicable to different physical situations. Detailed study of the ansatz (45) and its comparison with the ansatz (6), will be presented elsewhere.

In the second order, at the level of β_2 , the idea of expansion in sub-indices was realized in [46]. The approximants (45) should be combined with minimal-sensitivity conditions with the outer index s_k considered as an optimization parameter. Positive A is guaranteed, and the Formula (47) simply propagates A to arbitrary orders. Minimal-sensitivity conditions could be imposed directly on the expression for the critical index [46]. Mind that all previous approaches considered critical amplitude as the subject of optimization [6,47–49]. One can hope that a direct optimization of the critical indices is going to improve accuracy of the indices estimations.

We only note here that in the case of susceptibility χ of a three-dimensional Ising model on the simple cubic lattice [6,50–52], the technique based on the approximants (45) appears rather successful. Its application leads to the following expression for the $\chi(g)$

$$\chi(g) = \left(1 + \frac{1.07347g}{(0.221655-g) \left(\frac{1.07347g}{(0.221655-g) \left(\frac{1.07347g \left(\frac{0.23794}{0.221655-g} - 0.073471 \right) + 0.213426}{0.221655-g} + 1 \right) + 1 \right) + 1.14257} \right)^{0.0185894} \right)^{1.2389}, \tag{47}$$

where $g = \frac{1}{k_B T}$, and critical point $g_c \approx 0.221655$. Formula (47) is written for the variable $z(g) = \frac{g}{g_c - g}$.

The critical index $-\beta \equiv \gamma = 1.2478$, can be deduced from (47). It appears to be in a reasonable agreement with various numerical estimates, $\gamma \approx 1.24$, compiled in [53]. The Formula (47), is based only four starting terms from the expansion for the susceptibility [50], but it is able to predict the remaining 21 coefficients with very good average accuracy of 0.596%.

The second comment is on the subject of long series. When dealing with long series one is confronted with very cumbersome expressions for the amplitude to be optimized. Instead, one can adopt the following strategy motivated by the Tukey approach to the definition of powers of the Tukey’s ladder of powers [24].

Let us fix the value of $b = b^*$ plausibly, considering it as equal to some “vulgar” fraction, chosen based on the experience gained from optimization of shorter series. In all orders let us evaluate corresponding amplitudes, or critical indices for such selected b^* . Mind that computations with fixed b^* are easy to perform because of the iterated structure of the continued roots. In fact, let us select a few trial values for b^* .

Let us analyze the convergence of the sequences of such calculated values. If there are a few possible choices of b^* leading to a numerically convergent series in some order to

some values, let us analyze the quality of the approximants corresponding to such found values by attempting to predict the coefficients from the series not involved in construction of the approximant.

Finally, let us find the approximant (and corresponding b^*) with the best predictive abilities. To this end find the maximal error incurred in predicting the coefficients and select the approximant with the smallest maximal error. One can also use another selection criteria, e.g., the average error in prediction of some plausible number of coefficients.

For the toy model (18) we found the value of $b^* = -\frac{3}{7}$, which brings good, clear numerical convergence and predictability. The following sequence of value was found,

$$\begin{aligned}\hat{\beta}_1 &= 0.654827, \hat{\beta}_2 = 0.372624, \hat{\beta}_3 = 0.600457, \hat{\beta}_4 = 0.420037, \\ \hat{\beta}_5 &= 0.553834, \hat{\beta}_6 = 0.451467, \hat{\beta}_7 = 0.528073, \hat{\beta}_8 = 0.470503, \\ \hat{\beta}_9 &= 0.51406, \hat{\beta}_{10} = 0.481738, \hat{\beta}_{11} = 0.506438, \hat{\beta}_{12} = 0.488313, \\ \hat{\beta}_{13} &= 0.502313, \hat{\beta}_{14} = 0.492167, \hat{\beta}_{15} = 0.500111.\end{aligned}$$

Convergence to the value of 0.5 is fast enough and evident. The last value brings a small error of just 0.022%. Corresponding to the last point approximant, is able to predict at least eight more coefficients with average error of 0.00025% and maximal error of 0.0011%. It appears to be quite good and better in prediction than others considered for some other trial values of b^* .

Rate of convergence is controlled by the proximity to the boundary point $b = -1/2$, and decreases as we approach it. Further away from this point rate increases, but the error can increase as well. Some balancing acts, though, help to combine reasonable convergence rate with good accuracy.

In the important case of the quartic oscillator discussed above, both good convergence and good predictive abilities are achieved for $b^* = -1/3$. We find the following sequence of critical indices,

$$\begin{aligned}\hat{\beta}_1 &= 0.111199, \hat{\beta}_2 = 0.609154, \hat{\beta}_3 = 0.239164, \hat{\beta}_4 = 0.396971, \\ \hat{\beta}_5 &= 0.303855, \hat{\beta}_6 = 0.349685, \hat{\beta}_7 = 0.325101, \hat{\beta}_8 = 0.337622, \\ \hat{\beta}_9 &= 0.331129, \hat{\beta}_{10} = 0.334455, \hat{\beta}_{11} = 0.332753, \hat{\beta}_{12} = 0.333624, \\ \hat{\beta}_{13} &= 0.333182, \hat{\beta}_{14} = 0.333408, \hat{\beta}_{15} = 0.333293, \hat{\beta}_{16} = 0.333341.\end{aligned}$$

Convergence to the value of 0.33 is fast and evident. The last value brings a minuscule error of just 0.00027%. Corresponding to the last point approximant, is able to predict six more coefficients with average error of 0.2% and maximal error of 0.77%. It appears to be quite good and better in prediction than others considered for some other trial values of b^* . The convergence of the method is much faster than for the method of corrected approximants [14,33], or for the fractional-calculus applied together with Padé approximants [37,38].

The techniques for calculation of critical amplitude can be useful for solving ODE's, such as celebrated Gross-Pitaevskii equation for the wave function of vortex in Bose condensate (see, e.g., [43,54,55] and references therein), where in the course of computations appears the unknown parameter c with the linear term for small distances from the vortex origin. On the other hand, the expansion of the wave function at large distances from the origin is well defined, albeit it appears to be strongly divergent [43]. The problem of calculating c from the known three starting terms at large distances, can be reduced to the indeterminate problem and the $3 + 1$ method gives $c \approx 0.578$, while purely numerical methods give $c \approx 0.583$ [56,57]. Mind that for ODE accuracy of various approximations could be checked by direct substitution and quantified by their defect [55].

7. Concluding Remark

We conclude that the most challenging, indeterminate for the continued roots problem of calculating critical amplitudes and indices, can be successfully attacked by performing proper power transformation. The region of applicability of the continued root approximants can be successfully extended from the determinate (convergent) problem studied in [2] with well-defined conditions to the indeterminate (divergent) problem by means of a two-ways power transformation [1].

Notwithstanding the somewhat tedious technical details, our approach to the solution of the indeterminate problem consists in replacing it with the determinate problem, with some unknown control parameter b in place of the known critical index β . From optimization conditions b is found in the way making the problem determinate and convergent. By means of the power transform the index β is hidden under the carpet and replaced by b . But there is a cost incurred by the transformation, since we are dealing now with the whole spectrum of b , while for the determinate problem all parameters are defined uniquely by simple formulas. Instead, we should solve the optimization problem.

The problem of finding the critical indices by means of the continued roots given by the expression (6) is always indeterminate and is solved by analogy to the indeterminate problem of finding critical amplitudes. One can think that various potentials leave an undeniable weak imprint at the energy level of a quantum harmonic oscillator which can be read with good accuracy by means of special techniques.

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