

Article

Optimized Factor Approximants and Critical Index

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Abstract: Based on expansions with only two coefficients and known critical points, we consider a minimal model of critical phenomena. The method of analysis is both based on and inspired with the symmetry properties of functional self-similarity relation between the consecutive functional approximations. Factor approximants are applied together with various natural optimization conditions of non-perturbative nature. The role of control parameter is played by the critical index by itself. The minimal derivative condition imposed on critical amplitude appears to bring the most reasonable, uniquely defined results. The minimal difference condition also imposed on amplitudes produces upper and lower bound on the critical index. While one of the bounds is close to the result from the minimal difference condition, the second bound is determined by the non-optimized factor approximant. One would expect that for the minimal derivative condition to work well, the bounds determined by the minimal difference condition should be not too wide. In this sense the technique of optimization presented above is self-consistent, since it automatically supplies the solution and the bounds. In the case of effective viscosity of passive suspensions the bounds could be found that are too wide to make any sense from either of the solutions. Other optimization conditions imposed on the factor approximants, lead to better estimates for the critical index for the effective viscosity. The optimization is based on equating two explicit expressions following from two different definitions of the critical index, while optimization parameter is introduced as the trial third-order coefficient in the expansion.



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1. Introduction

Critical phenomena are found everywhere in quantum field theory, condensed matter physics, in equilibrium thermodynamics and non-equilibrium transport phenomena alike [1]. The challenge is to calculate and explain related critical indices for all such systems (at least for the most important), in the most transparent way based on the minimal information about the system.

Consider situation when the function $\Phi(x)$ of a real variable x exhibits critical behavior,

$$\Phi(x) \simeq A(x_c - x)^\alpha, \text{ as } x \rightarrow x_c - 0, \quad (1)$$

with a critical index α , and critical amplitude A at a finite critical point x_c . The definition covers the case of a negative and positive index.

The variable $x > 0$ represents, e.g., a coupling constant, inverse temperature or concentration of particles. For realistic physical systems with strong interactions one can develop some perturbation theory and learn their behavior at small variables. Most often one finds the divergent expansions, valid only for very small or very large x .

The case of convergent series in practice leads to a numerically convergent, truncated polynomial approximation [2]. However, there is still a problem of extrapolating outside of the region of numerical convergence, to the most interesting regime of the critical behavior.

Let us assume that some kind of perturbation theory is possible to develop, so that for a smooth function $\Phi(x)$, we have the asymptotic power series

$$\Phi(x) \sim \sum_{n=0}^{\infty} c_n x^n. \quad (2)$$

In practice we are dealing with (normalized to unity) truncation

$$\Phi_k(x) = 1 + \sum_{n=1}^k c_n x^n. \quad (3)$$

Our ultimate task is to transform the series (2) into analytical, convergent expressions by means of the so-called factor approximants [3].

One can consider the index k as the discrete time and view the truncated series (3) as the points of the trajectory of the dynamical system. After embedding the discrete system into continuous, one can define the velocity which governs the passage from one point to another. The stable fixed point of the dynamical system corresponds to zero velocity. Finding fixed points means that we found the sum (2) as $k \rightarrow \infty$. In practice, instead of zero velocity, we can define minimal velocity. There are two basic ways to approximate minimal velocity: in the form of a minimal difference between the adjacent approximations, or in the form of minimal derivative of each approximation. Moreover, to accelerate convergence one could introduce the so-called control functions and attempt to find them from the various conditions on the fixed point.

Such general formalization is due to V.I. Yukalov [4,5], and detailed referencing can be found in [6]. Minimal difference condition was applied in the form of equality by Kadanoff and Houghton in 1975 [7], and minimal sensitivity condition was invoked by Stevenson [8].

In the vicinity of the fixed point one can find the generic symmetry, called the functional self-similarity relation between the consecutive functional approximations. Due to the self-similarity, one can find the sought sum (fixed point) in the analytical form, as the factor approximant [3]. From the structure of factor approximant one can easily reach the critical index and treat it as an optimization parameter. Further imposition of the conditions on fixed points using critical index as a control parameter becomes particularly easy and leads to some transcendental equations [9].

The method of coherent anomaly suggested by M. Suzuki [10,11], is in the same spirit as any renormalization group (RG), but the flow of the sought quantity is considered with respect to the approximation parameter, discrete or continuous, just as in the general approach briefly discussed above. It allows to estimate critical indices but not the approximant valid for all regions, including the critical regime.

When dealing with criticality, the singular solutions emerge from factor approximants, and they correspond to critical points and phase transitions [3]. The case of singularity located at ∞ is easily derives from the factors. Factor approximants can do the same computational and intellectual work as Padè and *DLog*-Padè approximants [12,13]. The k -th order self-similar factor approximant reads as

$$\mathcal{F}_k^*(x) = c_0 \prod_{i=1}^{N_k} (1 + \mathcal{P}_i x)^{m_i}, \quad N_k = \frac{k}{2}, \quad k = 2, 4, \dots, \quad (4)$$

and the parameters \mathcal{P}_i and m_i are defined typically from k conditions. The necessary number of conditions typically is extracted from the conditions of asymptotic equivalence with the truncated series. However, nothing stops out from formulating additional constraints on the properties of the sought function or directly restricting the parameters of factor approximants. In our study, we are going to mix freely the type of conditions, keeping in mind only that their total number should be equal k .

The original intent behind the factor approximants is to calculate critical properties, such as critical exponents and thresholds, as well as reconstruct sought physical properties

over all relevant parametric regions [3]. When the truncated series is long, one would count on the accuracy to improve with increasing numbers of terms. Such an approach is conventional. However, it is very difficult to improve the quality of results produced by the factor approximants, when the truncated series are short.

Factor approximants were found to be amenable to optimization [9], but the techniques of [9] were never applied to actual calculation of the critical indices. One can think about the critical index as a control parameter needed to stabilize the divergent series, and find it from the optimization conditions, written as a minimal difference condition, or minimal derivative condition [1,14,15]. In such fashion, the so-called root approximants [16] were applied to the critical index calculations [6,17,18]. Root approximants are more suited technically to apply the minimal difference condition than minimal derivative condition.

Factor approximants were applied in conjunction with the minimal derivative condition [9]. In the case of factors it turned conceptually easier to come up with minimal derivative condition than with minimal difference. Besides, the minimal derivative condition preserves uniqueness of the parameters definition. Optimization conditions could be applied to the exponential and super-exponential approximants as well [17].

We consider below a minimal model of the critical phenomena based on expansions with only two coefficients and critical points. Some suggestions on improvement of the minimal case were advanced in [6,9]. For instance, one can use special variable transformation, or consider an index function instead of a parameter/critical index, see Section 4. Just like in the case of root approximants, one can consider the critical index as a control parameter, and intend to find it from the minimal derivative condition or minimal difference condition. Such conditions are going to be formulated and applied in current paper. It is essential that the optimization conditions are of non-perturbative nature.

The minimal derivative condition imposed on critical amplitude appears to bring the most reasonable, uniquely defined results. The minimal difference condition also imposed on amplitudes produces upper and lower bound on the critical index. While one of the bounds is close to the result from the minimal difference condition, the second bound is determined by the non-optimized factor approximant. One would expect that for the minimal derivative condition to work well, the bounds determined by the minimal difference condition should be not too wide.

In this sense the technique of optimization presented above is self-consistent, since it automatically supplies the solution and the bounds. In the case of effective viscosity of passive suspensions the bounds could be found that are too wide to make any sense from the either of the solutions. Therefore, we presented some other optimization conditions imposed on the factor approximants, which lead to the better estimates. The most natural approach is based on equating the results from two different definitions of the critical index, while optimization parameter is introduced as the trial third-order coefficient in the expansion.

2. Optimization

We will try to reduce the problem of critical index to the problem of optimization already considered in [9]. First we recapitulate the main ideas of [9], and then apply them to the problem in the finite interval. Consider first the generic case when critical behavior occurs at infinity,

$$\Phi(x) \simeq Ax^\alpha, \text{ as } x \rightarrow \infty, \quad (5)$$

In the generic case the factor approximants give the critical index as the following sum

$$\sum_{i=1}^{N_k} m_i = \alpha_k.$$

where α_k stands for the approximate value for the critical index α arising in k -th order. In the low-orders, which are of a primary interest in the present paper, the factor approximants are simply expressed as follows,

$$\begin{aligned}\mathcal{F}_2^*(x) &= c_0(1 + \mathcal{P}_1x)^{\alpha_2} \\ \mathcal{F}_4^*(x) &= c_0(1 + \mathcal{P}_1x)^{m_1}(1 + \mathcal{P}_2x)^{\alpha_4 - m_1}.\end{aligned}\quad (6)$$

We consider the situation when all parameters except α_k , can be found for the asymptotic and alike conditions, and expressed as functions of only α_k . When the critical behavior occurs at infinity, the large-variable behavior of the factor approximants

$$\mathcal{F}_k^*(x, \alpha_k) \simeq A_k(\alpha_k) x^{\alpha_k}, \text{ as } x \rightarrow \infty, \quad (7)$$

is of primary interest. For instance,

$$\begin{aligned}A_2(\alpha_2) &= c_0(\mathcal{P}_1(\alpha_2))^{\alpha_2}, \\ A_4(\alpha_4) &= c_0(\mathcal{P}_1(\alpha_4))^{m_1(\alpha_4)}(\mathcal{P}_2(\alpha_4))^{\alpha_4 - m_1(\alpha_4)}\end{aligned}\quad (8)$$

The minimal difference condition from the paper [1], reduces to the condition on amplitudes,

$$\min_k |\mathcal{A}_{k+2}^*(\alpha_k) - \mathcal{A}_k^*(\alpha_k)|, \quad (k = 2, 4, \dots), \quad (9)$$

assuming that the critical indices are the same in corresponding approximants. In practice it leads to the equation on critical amplitudes in the two adjacent orders

$$A_{k+2}(\alpha_k) - A_k(\alpha_k) = 0. \quad (10)$$

The minimal derivative condition cannot be applied directly when the function either diverges or tends to zero. To apply this condition, we extract from the function non-divergent parts [1]. As $x \rightarrow \infty$, one can express the minimal derivative condition as follows,

$$\min_k \left| \frac{\partial}{\partial \alpha_k} \mathcal{A}_k(\alpha_k) \right|, \quad (k = 2, 4, \dots). \quad (11)$$

In the perfect case, but not always, the minimal difference condition reduces to the equation

$$\frac{\partial A_k(\alpha_k)}{\partial \alpha_k} = 0. \quad (12)$$

When one of the optimization conditions is resolved, the result of optimization should be substituted to the factor approximant, making it an optimized factor approximant.

The technique just discussed is applicable to polymers. Polymer properties give the most direct example of self-organized criticality, meaning the emergence of a power-law without any external tuning or phase transition implied. The subject of interest is geometrical quantity, but the corresponding critical index can be found as the particular case of the Wilson-Kadanoff statistical mechanics formalism [19], corresponding to a zero-component order parameter.

In the theory of polymer chains, the typical chain radius $\sqrt{\langle R^2 \rangle}$ dependence on the (large) number of monomers N composing the chain, is a power-law increase $\sqrt{\langle R^2 \rangle} \sim N^\nu$, with the critical index ν [20,21]. It is forbidden for the polymer segments to occupy the same space. As a consequence there is a swelling effect in $\langle R^2 \rangle$, when compared to the non-perturbed segments, quantified by the swelling factor $Y(g)$. As $g \rightarrow \infty$,

$$Y(g) \sim g^\alpha,$$

where g is the dimensionless coupling parameter [22]. For the swelling factor perturbation theory yields the expansion in powers of the dimensionless coupling parameter [22]. Consider the two-dimensional polymer coil [22], with

$$Y(g) \simeq 1 + \frac{1}{2} g - 0.12154525 g^2 + 0.02663136 g^3, \quad (13)$$

as $g \rightarrow 0$. The critical index at infinity α is considered to be known exactly, $\alpha = 1/2$ [20,21]. The indices are related, so that $\nu \equiv \frac{1}{2}(1 + \alpha) = \frac{3}{4}$.

Let us apply the optimization technique discussed above and compare results with non-optimized approximants, in the spirit of [9]. Non-optimized factor approximant constructed just like in [9],

$$Y^*(g) = \frac{(1 + g)^{0.500482}}{(1 + 15.3236g)^{0.0000314798}},$$

gives the critical index $\nu = 0.750225$ ($\alpha = 0.50045$). The error is very small, just 0.03%.

From the minimal derivative condition we find $\nu = 0.768$ ($\alpha = 0.535$), but the corresponding approximant has a non-physical singularity in the physical region, and we will consider the result as inferior.

From the minimal difference condition we obtain the critical indices $\alpha = 0.507006$, $\nu = 0.753503$, the error being just 0.467%.

The case of a three-dimensional polymer coil was extensively studied in [9]. We only note that the minimal difference condition brings a reasonable result of $\nu = 0.575$, slightly less than the minimal derivative result $\nu = 0.579$, and the non-optimized result $\nu = 0.61$. All results agree with the numerical result $\nu = 0.5886$ [23], as well as with other numerical calculations [24], which give slightly lower results, $\nu = 0.5877$, or 0.5876 [25].

To construct optimized factor approximants without any further assumptions, we needed three parameters, i.e., three coefficients c_i . In situations with finite critical points to be considered below we still keep the minimal number of parameters equal to three, but one of them will be the critical point by itself.

Working Formulas

The approach developed for the case of a critical point located at infinity can be applied with minor modifications when the critical point x_c is finite and its position is known, in conjunction with transformation

$$z = \frac{x}{x_c - x},$$

while $x = \frac{zx_c}{z+1}$. In the low-orders, the factor approximants in such case are given as follows,

$$\begin{aligned} \mathcal{F}_2^*(x) &= \left(1 + \mathcal{P}_1 \frac{x}{x_c - x}\right)^{-\alpha_2} \\ \mathcal{F}_4^*(x) &= \left(1 + \mathcal{P}_1 \frac{x}{x_c - x}\right)^{m_1} \left(1 + \mathcal{P}_2 \frac{x}{x_c - x}\right)^{-\alpha_4 - m_1}, \end{aligned} \tag{14}$$

assuming normalization to unity at $x = 0$.

The critical amplitudes are modified accordingly,

$$\begin{aligned} A_2(\alpha_2) &= (\mathcal{P}_1(\alpha_2)x_c)^{-\alpha_2}, \\ A_4(\alpha_4) &= (\mathcal{P}_1(\alpha_4))^{m_1(\alpha_4)} (\mathcal{P}_2(\alpha_4))^{-\alpha_4 - m_1(\alpha_4)} x_c^{-\alpha_4}. \end{aligned} \tag{15}$$

Below, we consider the problem when only c_1, c_2 are available. Such scarcity of coefficients is not uncommon. In addition to optimization conditions, we have to impose another condition on parameters. E.g., following the scaling arguments (see [9] and references therein), we can set $\mathcal{P}_2 = 1$. Then

$$A_2(\alpha_2) = (\mathcal{P}_1(\alpha_2)x_c)^{-\alpha_2}, \quad \mathcal{P}_1(\alpha_2) = -\frac{c_1 x_c}{\alpha_2}, \tag{16}$$

and

$$A_4(\alpha_4) = (\mathcal{P}_1(\alpha_4))^{m_1(\alpha_4)} x_c^{-\alpha_4}, \tag{17}$$

while

$$P_1(\alpha_4) = \frac{x_c(c_1 + c_1^2 x_c - 2c_2 x_c)}{\alpha_4 + c_1 x_c}, \quad m_1(\alpha_4) = \frac{(\alpha_4 + c_1 x_c)^2}{-\alpha_4 + c_1^2 x_c^2 - 2c_2 x_c^2}.$$

The minimal difference optimization condition takes the following form

$$\min |\mathcal{A}_4^*(\alpha_2) - \mathcal{A}_2^*(\alpha_2)| \equiv \min |\mathcal{A}_4^*(\alpha) - \mathcal{A}_2^*(\alpha)|,$$

or

$$A_4(\alpha) - A_2(\alpha) = 0. \tag{18}$$

The minimal derivative condition also simplifies to

$$\min \left| \frac{\partial}{\partial \alpha} \mathcal{A}_4(\alpha) \right|. \tag{19}$$

The Equations (18) and (19) are to be solved numerically in each particular case.

3. Examples of Optimization

3.1. Susceptibility of the 2D Ising Model

Consider spin-1/2 Ising model characterized by the Hamiltonian [26]

$$\hat{H} = -\frac{J}{2} \sum_{\langle ij \rangle} s_i^z s_j^z \quad \left(s_j^z \equiv \frac{S_j^z}{S} \right) \tag{20}$$

on a lattice, with the ferromagnetic interaction of nearest neighbors, for spins $S_j^z = \pm 1/2$. The dimensionless interaction parameter is defined as

$$g \equiv \frac{J}{k_B T}. \tag{21}$$

On the square lattice, a high-temperature expansion of the susceptibility χ in powers of inverse temperature g could be obtained in rather high orders [26]. The starting terms of the expansion are given as follows,

$$\chi(g) = 1 + 4g + 12g^2 + O(g^3), \tag{22}$$

and $c_3 = \frac{104}{3}$. It is expected [27], that in the vicinity of the threshold

$$g_c = \left(\frac{2}{\log(1 + \sqrt{2})} \right)^{-1} \approx 0.440687,$$

the 2D susceptibility diverges as

$$\chi(g) \sim (g_c - g)^{-\gamma},$$

with exact $\gamma = \frac{7}{4}$.

Let us first find the non-optimized approximant $\mathcal{F}_2^*(g) = \left(1 + \mathcal{P}_1 \frac{g}{g_c - g} \right)^{-\alpha_2}$. The parameters \mathcal{P}_1, α_2 could be calculated only from the asymptotic equivalence with the expansion (22). In this way we find that $\gamma = 1.5758$.

From the minimal derivative condition we found a unique solution for the index, $\gamma = 1.773$. It appears to be close to the exact result. However, such an estimate pertains only to the critical point, and does not lead to the approximant valid for all relevant temperatures.

From the minimal difference condition we find two solutions for the index, $\gamma = 1.5758$, and $\gamma = 1.7628$. Effectively, by applying the minimal difference con-

dition we mix the two unique solutions obtained by the two preceding methods. The minimal difference condition gives slightly better estimates for the index, yet it is unable to decide which of the two estimates is better without additional information. It can be interpreted as a conservative method, which is able to give “only” lower and upper bound for the solution.

3.1.1. Formula for Susceptibility

Let us construct the expression for susceptibility valid for all $g > g_c$, inspired by Onsager’s exact solution for magnetization $M(g) = \sqrt[8]{1 - \frac{1}{\sinh(2g)}}$ [27]. Onsager understood that the critical index should enter the expression for all temperatures lower than critical, and that the problem of finding threshold is separable from the problem of finding critical indexes. The two ideas are implemented below for the susceptibility, leading to very accurate formulas. Root approximants, to a larger extent than any approximants, remind the Onsager exact solution, but are richer, allowing in principle, for correction-to-scaling terms [21].

Inspired by the Onsager formula for the low-temperature region $0 \leq g < g_c$, we suggest the following expression for the high-temperature region,

$$\chi_0(g) = \frac{(\sinh(g) \cosh(g))^{7/4}}{g^{7/4}(1 - \sinh(2g))^{7/4}},$$

to be employed as a zero-approximation for various corrected formulas for susceptibility. It is normalized to unity at $g = 0$.

The accurate and compact expression for the susceptibility arises when the zero-approximation $\chi_0(g)$ is corrected with account on the two leading terms in the expansion at small g

$$\chi_2(g) = \frac{0.434518(g + 0.631579) \sinh^{7/4}(2g)}{g^{7/4}(g + 0.923077)(1 - \sinh(2g))^{7/4}},$$

by multiplying with simplest diagonal Padé approximant. The formula can be viewed as “smart”, since it accurately “predicts” all remaining 21 coefficients from the high-temperature expansion [26], with average error of 0.92%.

The longer expression for the susceptibility can be found when $\chi_0(g)$ is corrected with account of the six leading terms in the expansion at small g

$$\chi_6(g) = \frac{0.363665(g + 0.538913)(g(g - 0.782611) + 0.477638) \sinh^{7/4}(2g)}{g^{7/4}(g(g - 0.083005) - 0.0890799) + 0.314863)(1 - \sinh(2g))^{7/4}},$$

by multiplying with corresponding diagonal Padé approximant. It accurately predicts all remaining 17 coefficients from the high-temperature expansion for the square lattice [26], with an average error of minuscule 0.022%.

3.2. (2 + 1)-Dimensional Ising Model

Let us also consider the so-called (2 + 1)-dimensional Ising model given by the Hamiltonian $\hat{H} = \sum_i (1 - \sigma_i^z) - g \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x - h \sum_i \sigma_i^x$, on a triangular lattice [28]. The (2 + 1) and three-dimensional isotropic Ising model (20) are believed to belong to the same universality class. For the former model we have an advantage of still being able to work on 2D lattice, while also avoiding the non-universal, confluent singularities [21,28].

Here i and j enumerate sites on the two-dimensional square lattice, $\langle ij \rangle$ denotes nearest-neighbor pairs, σ_i^α are the Pauli matrices, g corresponds to the dimensionless inverse temperature in the Euclidean formulation, and h is the magnetic field variable.

The second derivative of the ground state energy with respect to the magnetic field, as the magnetic field goes to zero, is called susceptibility. The susceptibility $\chi(g)$ diverges at a critical point $g_c \approx 0.20971$, as

$$\chi(g) \propto (g_c - g)^{-\gamma}, \quad (23)$$

with the critical index $\gamma \approx 1.24 - 1.25$ [28]. We recall that in generic notations (1), $\alpha \equiv -\gamma$.

The high-temperature expansion of the susceptibility yields [28] the truncated series in powers of g ,

$$\chi(g) \simeq 1 + 6g + 32.95g^2, \quad g \rightarrow 0. \quad (24)$$

Based on the threshold g_c and two known coefficients in the expansion, we can construct only a simple factor approximant, and reasonably estimate the critical index $\gamma \approx 1.32$.

From the minimal derivative condition we found a unique solution $\gamma = 1.25$. It appears to be close to the numerical results of [28]. From the minimal difference condition we find two solutions, $\gamma = 1.25$, and $\gamma = 1.32$. Such estimates are encouraging, but can not be extended further without knowing precisely the higher order coefficients, or some additional information from the critical region.

Another critical index ν describes the so-called mass gap at zero magnetic field [28],

$$F(g) \sim (g_c - g)^\nu, \quad \text{as } g \rightarrow g_c - 0. \quad (25)$$

The gap is a difference between the energy of the first excited and ground state. For the triangular lattice

$$F(g) \simeq 1 - 3g - 3g^2, \quad \text{as } g \rightarrow 0. \quad (26)$$

Direct application of the second-order factor approximant to the expansion (26) gives $\nu = 0.6612$. The minimal sensitivity condition gives a unique result $\nu = 0.6263$. The minimal difference condition gives lower and upper bounds, $\nu = 0.6291$ and $\nu = 0.6612$. The results agree reasonably with the accepted numerical estimate for the index, $\nu \approx 0.63$ [21,28–30].

3.3. Critical Index in 2D Site Percolation

For 2D site percolation on the quadratic lattice, there is a minimal model known as the Lorenz 2D gas. It gives the expansion for conductivity in concentration of conducting sites. This minimal model is a simple statistic hopping model allowing both for analytical consideration and numerical simulations [31,32]. The test particle, or tracer, walks randomly, and the diffusion coefficient can be found. The diffusion ceases to exist at the critical density of the excluded sites. If f stands for the concentration of conducting or not excluded sites in the Lorenz model, then $x = 1 - f$ is the concentration of excluded sites. In the vicinity of the site percolation threshold x_c the conductivity behaves as

$$\sigma(x) \sim (x_c - x)^t, \quad \text{as } x \rightarrow x_c - 0, \quad (27)$$

with $x_c = 0.4073$, $t = 1.310$ [33,34].

Perturbation theory in powers of the variable $x = 1 - f$ gives [31] for the two-dimensional square lattice the expansion

$$\sigma(x) \simeq 1 - \pi x + 1.28588x^2, \quad \text{as } x \rightarrow 0. \quad (28)$$

Let us first find the non-optimized approximant $\mathcal{F}_2^*(x)$ directly from the asymptotic equivalence with the expansion (28). In this way we find that $t = 1.2142$.

From the minimal derivative (sensitivity) condition we found a unique solution $t = 1.2835$. It appears to be reasonably close to the numerically exact result. From the minimal difference condition we find two solutions, $t = 1.2142$, and $t = 1.2796$. Again, we have a mix of the two solutions obtained by the two preceding methods. Furthermore, the minimal derivative condition gives slightly better estimates for the index, it is unable to

give the approximation valid for all x . On the other hand minimal difference condition is able to give the lower and upper bounds for the solution.

3.4. 3D Conductivity for Site Percolation

For 3D site percolation on the cubic lattice, perturbation theory gives the following expansion for conductivity [35], $\sigma(f) \simeq f - 1.52f(1 - f)$. This expression can be re-written in the form

$$\sigma(x) \simeq 1 - 2.52x + 1.52x^2, \quad x \rightarrow 0. \quad (29)$$

in powers of variable $x = 1 - f$. It is also known that the three-dimensional site percolation conductivity problem, similarly to the two-dimensional one, exhibits the critical behavior [35–37] described by formula (27), with $x_c = 0.688$, $t = 1.9$ [34,38]. One can extract critical properties of the 3D case from the expansion (29). Technical part is accomplished exactly the same way as above.

The factor approximant asymptotically equivalent to the expansion (29), gives the critical index $t = 1.58$. Using minimal derivative condition, we get the critical index $t = 1.74$. By applying minimal difference condition, we calculate the lower bound $t = 1.58$ and the upper bound $t = 1.73$. The estimates are slightly lower than accepted values, but tend to agree better with the value of 1.6 from [35].

3.5. Compressibility Factor of Hard-Disks Fluids

The state of hard-disks fluids is described by the compressibility factor $Z = \frac{P}{\rho k_B T} = Z(f)$, $f \equiv \frac{\pi \rho}{4} a_s^2$. Here P stands for pressure, ρ is density, T is temperature, a_s is the disk diameter, and f is called packing fraction [6].

For low packing fraction, the compressibility factor is represented by the virial expansion

$$Z(f) \simeq 1 + 2f + 3.12802f^2, \quad f \rightarrow 0, \quad (30)$$

and much more terms are available [39,40]. The compressibility factor exhibits critical behaviour at a space filling $f_c = 1$, a

$$Z(f) \sim (f_c - f)^\alpha \quad (f \rightarrow f_c - 0), \quad (31)$$

with the parameter $\alpha = -2$ [41,42]. The value is widely accepted, but it is not proven to be an asymptotically exact value.

The non-optimized factor approximant asymptotically equivalent to the expansion (29), gives for the critical index $\alpha = -2.29363$. Using the minimal derivative condition, we get for the critical index $\alpha = -2$. By applying the minimal difference condition, we calculate the lower bound $\alpha = -2.29363$ and the upper bound $\alpha = -2$. Corresponding approximants can be expanded in powers f , and one can see that they give also reasonable bounds for the coefficients. Especially good is the upper bound, in agreement with an observation made in [42].

All methods based on very short series should be approached with caution. Indeed, the predictions based only on two starting coefficients and critical points can not be always true. However, in all particular cases of physical significance studied above they can be verified against experimental evidence. The minimal derivative condition appears to bring the most reasonable results and the bounds determined by the minimal difference condition are found to be not too wide. In this sense the technique of optimization presented above is self-consistent, since it automatically supplies the solution and the bounds.

However, in the case of effective viscosity to be considered in the next section, the bounds could be found that are too wide to make any sense from either of the solutions. Nevertheless, in Chapter 8 of the book [6], some other variants of the factor approximants were advanced. We anticipate that some other variants of optimization imposed on the factor approximants, can lead to better estimates. In the second part of the

paper we develop further, and apply such methods to several key problems in transport phenomena and statistical physics alike, all involving calculation of the critical properties.

4. Effective Viscosity of Passive Suspensions

Viscosity μ is a scalar quantifying the rheology of an isotropic Newtonian fluid. It establishes the proportionality between the macroscopic strain-rate and stress. Einstein's work in the field of viscous suspensions had inspired uncountable analytical expressions for the effective viscosity of suspensions. His seminal work [43] remains one their most quoted and not less important than Maxwell's, in the theory of effective properties.

Effective viscosity for isotropic suspensions μ_e is the multiplier, by which the average rate of strain is multiplied to result in the average stress. The fundamental homogenization proposition [43], requires that the viscous energy dissipation rate of the suspension must be equal to the dissipation rate of the effective homogeneous fluid. Such definition gives the effective viscosity, and is applicable for any volume fractions. The definition is applicable to both passive and active, bacterial suspensions. For special bacterial suspensions the effective viscosity may become negative.

The effective viscosity of random suspensions of hard spheres with the stick boundary conditions, is expressed as the expansion in the volume fraction of hard spheres f . For the low deformation rate one can produce the following expansion

$$\frac{\mu_e}{\mu} \simeq 1 + c_1 f + c_2 f^2, \quad f \rightarrow 0, \quad (32)$$

for the effective viscosity of a suspension [44]. The higher order coefficients depend on the location of particles. This implies that it is impossible to write a universal formula for c_3 and a universal formula for 2D suspensions valid within the precision $O(f^3)$ [6]. The value $c_1 = \frac{5}{2}$ was eventually derived by Einstein [43]. Because of energy dissipation on individually considered spheres the effective viscosity linearly increases with f , and does not depend on their size.

The expansion (32) is available only up to the second order term inclusively, as $f \rightarrow 0$. For the second-order coefficient c_2 , several estimates are available [44,45]. In particular, Batchelor [45] gives $c_2 = 6.2$, Wajnryb and Dahler [44] give the exact $c_2 = 5.9147$ [44]. The result for c_2 includes the hydrodynamic contribution as well as contribution from the strong Brownian motion of the particles. The effective shear viscosity grows rapidly with increasing volume fraction, because it is harder to shear a dense suspension, since particles have less room to move past each other. There is a power-law divergence of the viscosity in the vicinity of the maximal volume fraction value f_c

$$\frac{\mu_e}{\mu} \simeq A(f_c - f)^{-\mathcal{S}}, \quad \text{as } f \rightarrow f_c.$$

The value of the critical exponent $\mathcal{S} \simeq 2$ is currently accepted and it is believed that $f_c = 0.637$ [46,47]. As explained in [48], such value of f_c corresponds to the experiments with the most rapid compression of the hard-sphere liquid. It is even suggested to consider such divergence as an universal power law with the value of $\mathcal{S} = 2$ [49].

The "universality" of the critical index with the value of $\mathcal{S} = 2$ [49], may be very well related to a certain protocol, while the whole spectrum of values, between the value corresponding to regular suspension $\mathcal{S} = 1$ [50], and fully random systems can be observed.

The methodology of Section 2 can be applied to the expansion (32), but the bounds that it produces, $\mathcal{S} \approx 1.593$ and $\mathcal{S} \approx 2.753$ are rather distant. We have to apply some further modifications of the optimization conditions to the factor approximants in order to have tighter bounds on the solution.

Yet, non-optimized factor approximants give quite sensible estimates for the index in different theoretical setups. Remarkably, that without any serious deliberations, we can construct rather the simplest factor approximant,

$$\frac{\mu_e(f)}{\mu} = \mathcal{F}_4^*(f) = (1 - 1.56986f)^{-2.00267}(1 + f)^{-0.643908},$$

based only the threshold f_c and two known coefficients c_1 and c_2 , and quite well estimate the critical index, $\mathcal{S} = 2.00267$. Furthermore, vice versa, using the value of index $\mathcal{S} = 2$, one obtains an excellent value of $f_c = 0.63647$ for the threshold.

We had also considered the following modified factor approximant [6,51]

$$\mathcal{F}^*(f) = \left(1 + \mathcal{P}_1 \frac{(f/f_c)^{1/2}}{1 - (f/f_c)^{1/2}}\right)^{\mathcal{S}-m} \left(1 + \mathcal{P}_2 \frac{(f/f_c)^{1/2}}{1 - (f/f_c)^{1/2}}\right)^m, \tag{33}$$

which brought $\mathcal{S} \approx 2.036$.

Yet different technique of the index function $\mathcal{S}(f)$ [6], with the following ansatz

$$\frac{\mu_e(f)}{\mu} = \left(1 - \frac{f}{f_c}\right)^{-\mathcal{S}(f)},$$

allowed to estimate the critical index. Here we use an approximate index function

$$\mathcal{S}(f) = \frac{2c_1^2 f_c^2}{(c_1^2 - 2c_2) f f_c + c_1(f + 2f_c)},$$

and find $\mathcal{S}(f_c) = \mathcal{S} \approx 2.02$. Such estimates do look encouraging, but can not be understood or extended further without knowing precisely at least one, higher order coefficient.

We would like to get a better idea why low-order factor approximants can produce the value of index around 2. For the factor approximants we have to develop some special techniques for accelerating their convergence, different from methods developed for root approximants [1,6]. Obviously, optimization conditions should be imposed and they ought be different from the conditions already tried in the previous sections. The problem can be also understood in terms of accelerating convergence of the *DLog* Padé approximants, closely related to the factor approximants. We are primarily interested in the case of truncated series with just two non-trivial terms. We would like to anticipate what would happen to the results if some higher-order terms are added.

Let us apply the methodology presented in Chapter 1 of the book [6]. Presentation below will be accomplished in terms of effective viscosity, but can be applied without much ado to similar problems of permeability, susceptibility and so on.

Assume that we were able to develop two different approximants for the effective viscosity, $\Phi(f)$ and $\Psi(f)$. Each of them is able to calculate the critical index and both approximations respect asymptotically, as $f \rightarrow 0$, the same asymptotic expansion with N terms available. In addition they also behave critically as $f \rightarrow f_c$. With known critical point f_c , the value of critical index \mathcal{S}_Φ and \mathcal{S}_Ψ estimated from the two approximants could be different. However, one can always expect that the estimates are close. We intend to capitalize from the latter observation. Let us try to increase accuracy further by adding formally additional terms to the expansion and finding the parameters with such terms by requiring that the two estimates for the critical index would become as close as possible.

Indeed, let us introduce a higher-order term to the expansion for the viscosity $\mu_N(f)$ at small f , namely

$$\mu_{N+1}(f) = \mu_N(f) + af^{N+1},$$

with unknown trial parameter a . The parameter has to accelerate convergence of the series. The formulas presented below are quite general, but will be applied specifically to the very old problem of the effective viscosity of suspensions. The case to be studied corresponds to

$N = 2$, and $c_2 = 5.9147$. Despite very hard efforts by many researchers over considerable time, the higher-order terms are still not available.

We stress, here, that a is just some parameter introduced to accelerate convergence of the original truncated series. To find a explicitly we have to formulate an additional optimization condition, akin to the optimization conditions exploited above. The value of a estimated from resummation, may have nothing to do with the true coefficient c_{N+1} . One can expect that introducing a into consideration will change the value of either of critical indices, moving the indices to the same unknown values

$$\mathcal{S}_\Phi \rightarrow \mathcal{S}_{\Phi,N+1}(a), \quad \mathcal{S}_\Psi \rightarrow \mathcal{S}_{\Psi,N+1}(a). \tag{34}$$

The two particular algorithms are supposed to lead to the analytical expressions for the approximants of higher order, $\Phi_{N+1}(f, a)$ and $\Psi_{N+1}(f, a)$. The value of $\mathcal{S}_{N+1}(a)$ could be found analytically from the explicit formulas for the approximants. Then, by minimizing the difference

$$|\mathcal{S}_{\Phi,N+1}(a) - \mathcal{S}_{\Psi,N+1}(a)|, \tag{35}$$

we can compute the parameter a . Naturally, one would prefer the equality

$$\mathcal{S}_{\Phi,N+1}(a) = \mathcal{S}_{\Psi,N+1}(a). \tag{36}$$

When the equality is not possible, one would fall back on the minimal difference condition (35).

The two approximations, $\Phi(f)$ and $\Psi(f)$, could be seen as the two different versions of factor approximants [52]. Introducing also the free parameter a , we can write explicitly

$$\begin{aligned} \Phi_3(f, a) &= 1 + c_1 f \left(1 + p(a) \frac{f}{f_c - f} \right)^{\mathcal{S}_{\Phi,3}(a)}, \\ \mathcal{S}_{\Phi,3}(a) &= \frac{c_2^2 f_c}{-2ac_1 f_c + 2c_1 c_2 + c_2^2 f_c}, \end{aligned} \tag{37}$$

and

$$\begin{aligned} \Psi_3(f, a) &= (1 + p_1(a) f)^{m_1(a)} \left(1 - \frac{f}{f_c} \right)^{-\mathcal{S}_{\Psi,3}(a)}, \\ \mathcal{S}_{\Psi,3}(a) &= \frac{f_c^3 (3ac_1 + c_2 (c_1^2 - 4c_2))}{f_c^2 (3a + c_1^3 - 3c_1 c_2) + 2f_c (c_1^2 - 2c_2) + c_1}. \end{aligned} \tag{38}$$

Our primary mission to find analytically the critical indices from two different approximations is accomplished. However, the rest of parameters from (37), (38) not shown here, can be expressed in a closed form as well. Since we are talking about the effective viscosity, the physical quantity divergent at the critical point, the parameter $\mathcal{S}_{\Phi,3}(a)$ expresses the critical index, which could be compared with $\mathcal{S}_{\Psi,3}(a)$.

We stress that the principal novelty consists of finding and comparing the two approximants of the same order, based on the very same information, but expressing the sought quantity differently. Naturally, one would expect that the problem could be solved by more than one method, but at least by two, and they both can be made convergent to some rather close results. We are simply trying to find the control parameter which would make sure that the results for the critical index are close indeed.

Below, in all other examples, we are going to discuss the divergent quantities, such as the effective viscosity, and assume that proper inverse transformation of the original truncated series could be accomplished. Generally speaking, one can also introduce yet additional control parameters by means of the power transform defined in [52]. Considering the inverse means settling down for some plausible choice of the power transform as explained in [52]. However, in all cases to be considered such a choice is justifiable, because the bounds produced by the optimization conditions discussed above will be respected.

Power-transformation can be also seen as leading to the general class of continued root approximants [53,54]. The continued roots are special among the self-similar approximants, since they can be considered as the direct generalization of the diagonal Padé approximants

and continuous fractions. They also allow for partial summation in infinite order. Such explicitly accomplished summation gives an optimal value for the critical index in each order of perturbation theory. For such uniquely found values one can easily, in an iterative way, calculate critical amplitudes for several important problems of quantum mechanics and statistical physics [53]. It still remains to find out how to apply the continued roots to the critical indices calculations.

There are some other transformations available, such as Tukey ladder [55], and Box-Cox transformation [56]. The former transformation was extended to obtain the so-called additive approximants [6,57]. The latter transformation, also known as replica-trick, in conjunction with some optimization conditions led to the popular concept of highly optimized tolerance (HOT) [58]. HOT, together with another general framework for generating critical phenomena, called self-organized criticality (SOC), is used to obtain power-laws with (HOT) or without (SOC) tuning to any critical point.

The equality of the two expressions for the index leads in the case of viscosity to a quadratic equation with two non-physical complex-conjugated solutions for a . However, turning to the minimization condition gives $a = 12.1821$. Then there are following two values for the index,

$$\mathcal{S}_{\Phi,3}(a) \approx 1.71, \quad \mathcal{S}_{\Psi,3}(a) = 2.08.$$

Their average gives $\mathcal{S} \approx 1.9 \pm 0.2$. The factor approximant of the type preferred in the current work, can be found explicitly,

$$\Psi_3(f) = (1 - 1.56986f)^{-2.08445}(1 + 0.57281f)^{-1.34824},$$

with the critical index $\mathcal{S} = 2.08$, rather close to 2, as we hoped. Application of the *DLog* Padé technique [17,18], gives a much larger result of 2.75.

The methodology discussed above requires only to develop two explicit expressions for the critical index. They should contain optimization parameters, obtained from two different approximations, but based on the same asymptotic input. For instance, one can resort to the two different definitions of the critical index, as first suggested in [6].

We recall from [6,59], that since $\mu_e(f) \propto (f_c - f)^\alpha$, with $\alpha = -\mathcal{S}$, the critical index could be expressed equivalently as shown below,

$$\begin{aligned} \alpha &= \lim_{f \rightarrow f_c} \frac{(f-f_c)\mu'_e(f)}{\mu_e(f)}, \text{ or} \\ \alpha &= 1 + \lim_{f \rightarrow f_c} \frac{(f-f_c)\mu''_e(f)}{\mu'_e(f)}. \end{aligned} \tag{39}$$

The two expressions, $\frac{\mu'_e(f)}{\mu_e(f)}$, $\frac{\mu''_e(f)}{\mu'_e(f)}$, can be expanded as $f \rightarrow 0$,

$$\begin{aligned} \frac{\mu'_e(f)}{\mu_e(f)} &\simeq c_1 + f(2c_2 - c_1^2) + f^2(3a + c_1^3 - 3c_1c_2), \\ \frac{\mu''_e(f)}{\mu'_e(f)} &\simeq \frac{2c_2}{c_1} + f\left(\frac{6a}{c_1} - \frac{4c_2^2}{c_1^2}\right). \end{aligned} \tag{40}$$

The task at hand consists of finding such approximants to (40), which satisfy simultaneously both kind of asymptotic expressions (39) and (40). From the longer series from (40), we suggest to extract the following Padé approximant

$$\begin{aligned} P_{1,2}(f, a) &= \frac{p_1 + p_2(a)f}{(1 - p_3(a)f)(f_c - f)}, \quad p_1 = c_1f_c, \\ p_2(a) &= \frac{c_1f_c(3af_c + 2c_2) - c_1^3f_c + c_1^2(c_2f_c^2 - 1) - 4c_2^2f_c^2}{c_1^2f_c + c_1 - 2c_2f_c}, \\ p_3(a) &= -\frac{3af_c + c_1^3f_c + c_1^2 - 3c_1c_2f_c - 2c_2}{c_1^2f_c + c_1 - 2c_2f_c}. \end{aligned} \tag{41}$$

From the shorter series from (40), one can find the simplest diagonal Padé approximant

$$P_{1,1}(f, a) = q_1(a) + \frac{q_2(a)}{f_c - f}, \tag{42}$$

$$q_1(a) = \frac{-6ac_1f_c + 2c_1c_2 + 4c_2^2f_c}{c_1^2}, \quad q_2(a) = \frac{2f_c^2(3ac_1 - 2c_2^2)}{c_1^2}.$$

It is crucial to obtain explicitly the limits expressing the critical index (39). The value of parameter a has to be found simply by equating the two expressions for the index, or just minimizing the difference between them. By minimizing the latter difference

$$\left| q_2(a) - 1 - \left(\frac{p_1 + p_2(a)f_c}{1 - p_3(a)f_c} \right) \right|,$$

we estimate $a \approx 12.5913$. The estimate leads to the following two solutions for the index, $S \approx 2.18$, $S \approx 2.34$, which follow from the approximants (42) and (41), respectively. After integration, the approximant (41) leads to a factor approximant and to the critical index $S \approx 2.34$.

A novel suggestion is put forward below. One can think about a middle-of-the road approach, when there are two different *DLog* approximants, expected to give equal value to the critical index. The critical index is expressed conventionally as

$$S = \lim_{f \rightarrow f_c} \frac{(f_c - f)\mu'_e(f)}{\mu_e(f)}.$$

To such end, in addition to the approximant (41), we can develop also the following iterated root approximant [6]

$$\mathcal{R}_2(f, a) = \sqrt{v_0 + \frac{v_1f}{f_c - f} + \frac{v_2(a)f^2}{(f_c - f)^2}}, \tag{43}$$

$$v_0 = c_1^2, \quad v_1 = -2c_1f_c(c_1^2 - 2c_2),$$

$$v_2(a) = f_c(6ac_1f_c + 3c_1^4f_c + 2c_1^3 - 10c_1^2c_2f_c - 4c_1c_2 + 4c_2^2f_c).$$

The corresponding limits for the two approximants could be found explicitly. Thus, the value of parameter a could be found by demanding the equality of the limit-expressions for the critical index. The equality condition

$$f_c \sqrt{v_2(a)} = \frac{p_1 + p_2(a)f_c}{1 - p_3(a)f_c},$$

brings in the case of viscosity, two close solutions for the parameter, $a \approx 12.182$ and $a \approx 12.498$, giving $S \approx 2.08$ and $S \approx 2.26$.

Thus, we are to conclude that the estimates based on factor approximants deduced from the short truncated series including only c_1 and c_2 , are robust. It means that the values for critical index would weakly depend on addition of an extra, third-order term to the original expansion, and the knowledge of the third-order coefficient could be superseded by imposing some general-type optimization conditions of a non-perturbative nature. With or without such addition, the value of the critical index is of the order of 2. The higher order coefficients c_i appear to be redundant as long as one is concerned with the correct estimates for the critical index S [51].

In our opinion, the optimization based on equating the two different definitions of the critical index expressed by formula (39), is the most natural, since it allows to reduce the problem only to the Padé approximants. If required such an approach can be extended to higher orders. The method is applied below to a few more examples.

5. Permeability

The permeability is defined to quantify the amount of viscous fluid flow through a porous medium assuming that a macroscopic pressure gradient is applied to the system [6]. Precise definitions and general discussion of the critical properties of permeability in porous media, including flow in various channels, can be found in Chapter 7 of the book [6].

Let us consider the case of the two-dimensional channel bounded by the surfaces $z = \pm b (1 + \epsilon \cos x)$, where ϵ is termed waviness. The permeability $K(\epsilon)$ behaves critically [1,6,60]. Precisely, it is expected to tend to zero,

$$K(\epsilon) \sim (\epsilon_c - \epsilon)^\kappa, \text{ as } \epsilon \rightarrow \epsilon_c - 0, \tag{44}$$

with $\epsilon_c = 1, \kappa = \frac{5}{2}$.

Iterative perturbation theory gives an expansion for permeability in powers of ϵ [2,6,17,60], to be truncated to make it applicable. For $b = 0.5$, the permeability can be expanded as follows,

$$K(\epsilon) \simeq 1 - 3.14963 \epsilon^2 + 4.08109 \epsilon^4, \text{ as } \epsilon \rightarrow 0, \tag{45}$$

and an inverse of permeability is given as follows,

$$K(\epsilon)^{-1} \simeq 1 + 3.14963 \epsilon^2 + 5.83908 \epsilon^4, \text{ as } \epsilon \rightarrow 0. \tag{46}$$

The methodology of Section 2 can be formally applied to the expansion (46), but the bounds that it produces, $\kappa \approx 2.184$ and $\kappa \approx 3.14$, are far too distant. We have to apply some other method based on the factor approximants in order to have tighter bounds on the solution.

The method based on comparison of the definitions for the critical index expressed by Formula (39), gives a good estimate $\kappa = 2.45854$. The found value of $a = 9.0332$ well agrees with the numerically “exact” value of the third coefficient in the expansion 9.0281 [2]. The permeability has the form of factor approximant

$$K^*(\epsilon) = \frac{0.990781(1 - \epsilon^2)^{2.45854}}{(\epsilon^2 + 0.986508)^{0.68177}},$$

and we also found that the higher order coefficients are approximated quite well. There is also the second solution which is plagued by a competing singularity at positive ϵ , leading to the bad estimate for the index. Besides, it does not fit within the bounds given above. The solution chosen above does not have any extra singularity for positive ϵ .

The permeability can be expanded as follows (for $b = 0.25$) [2],

$$K(\epsilon) \simeq 1 - 3.03748 \epsilon^2 + 3.54570 \epsilon^4, \text{ as } \epsilon \rightarrow 0. \tag{47}$$

The inverse can be readily obtained,

$$K(\epsilon)^{-1} \simeq 1 + 3.03748 \epsilon^2 + 5.68058 \epsilon^4, \text{ as } \epsilon \rightarrow 0. \tag{48}$$

The methodology of Section 2 can be applied to the expansion (46), but the bounds that it produces, $\kappa \approx 2.342$ and $\kappa \approx 3.037$, are too distant. We have to apply again the method based on comparison of the two definitions for critical index expressed by Formula (39). It gives a rather good estimate $\kappa = 2.548$, falling well within the bounds given by the optimized factor approximants. The estimate of $a = 8.8751$ agrees well with the numerical $c_3 = 8.81972$ [2]. The following factor approximant

$$K^*(\epsilon) = \frac{1.10387(1 - \epsilon^2)^{2.54786}}{(\epsilon^2 + 1.18558)^{0.580484}},$$

gives the expression for permeability. We found also that the higher order coefficients are approximated quite well. Again we select the solution which does not have any extra singularity for positive ϵ . Beside, such solutions bring the estimate well outside of the bounds.

Brinkman’s formula for the permeability $k(p)$ of a porous aggregates is known as the function of porosity p (see, e.g., [61]),

$$k(p) = \frac{1}{18}(-3\sqrt{\frac{8}{1-p}} - 3 + \frac{4}{1-p} + 3).$$

In order to bring it to the standard form, let us change the variable, so that $p = 1 - x^2$, and consider the function $f(x) = (\frac{9}{2}x^2k(1 - x^2))^{-1}$.

As $x \rightarrow 0$

$$f(x) \simeq 1 + \frac{3}{\sqrt{2}}x + \frac{15}{4}x^2. \tag{49}$$

As $x \rightarrow x_c = \sqrt{\frac{2}{3}} \approx 0.816497$,

$$f(x) \sim (x_c - x)^{-t},$$

with $t = 2$ [61]. Here t corresponds to the critical index for the conductivity for the 3D percolation model of the type discussed above.

The methodology of Section 2 can be applied to the expansion (49), but the bounds that it produces, $t \approx 1.732$ and $t \approx 2.049$ are still too distant. We have to apply some other modifications to the factor approximants in order to have tighter bounds on the solution.

The method based on comparison of the two definitions for critical index expressed by Formula (39), gives $a = 6.0091$, with a very tight range for the index, defined by $t = 1.998$ and $t = 2.011$. Their average $t \approx 2$. Furthermore, our estimate for the third order coefficient turns out to be only slightly different from the exact number 5.9662. One can also obtain the complete expression

$$f^*(x) = \frac{0.000023987(11.7659 - x)^{4.14914}}{(0.816497 - x)^{2.01998}},$$

and find that the higher order coefficients are being approximated rather well.

6. Critical Indices for 3D Ising Model

Consider the ferromagnetic three-dimensional Ising model with the Hamiltonian (20), but being studied now on a simple cubic lattice. The dimensionless interaction parameter is defined as in (21).

One of the most studied in the physics of critical phenomena is the critical index ν , which characterizes the divergence of critical length. However, there are no explicitly written, high-temperature series for such index in [26]. Still, the index ν can be deduced from the series for the so-called second moment of correlation function $\mu_2(g)$ [26,62]. For small g , in normalized form, it is given as follows

$$\mu_2(g) \simeq 1 + 12g + \frac{290g^2}{3} + 664g^3 + \frac{62402g^4}{15} + \frac{369128g^5}{15} + \frac{8801924g^6}{63}, \tag{50}$$

and close to the critical point $g_c = 0.22165463(8)$ [63,64], it diverges

$$\mu_2(g) \sim (g_c - g)^{-(2\nu+\gamma)}, \tag{51}$$

with the critical index $\alpha = -(2\nu + \gamma)$. From the reference values of [21,30], it follows that $\alpha \approx -2.5$.

We find that the method of optimized factors approximants described in the Section 2, generates rather reasonable bounds, $\alpha \approx -2.66$ and $\alpha \approx -2.443$. Let us try to improve even further on those estimates.

The method of optimization based on the equation arising from the two different definitions for the critical index expressed by Formula (39), generates two solutions. From the two solutions we choose the one with better physical properties in the physical region and falling well within the bounds. Namely, we obtain

$$\mu_2^*(g) = \frac{0.029942g(0.472675 + g)^{0.342708}}{(0.221655 - g)^{2.49915}}, \tag{52}$$

with an exceptionally good estimate for the index $\alpha \approx -2.4992$.

The factor approximant can be expanded at small g , giving

$$\mu_2^*(g) \simeq 1 + 12g + 96.6667g^2 + 661.578g^3 + 4132.28g^4 + 24350g^5 + 137786g^6.$$

One can readily verify that the coefficients in the exact and approximate expansions agree well with each other. The average error of the four estimated coefficients is less than 1%. So, the higher-order coefficients appear to be somewhat excessive and reverting to the low-order calculations is reasonable. General idea of expressing the higher-order coefficients through the low-order coefficients from the approximate formulas is ascribed to Feynman [65], as a smart alternative to brute force calculations.

One can compute yet another thermodynamic characteristic, $\chi_0^{(2)}$, the second derivative of the susceptibility with respect to a weak external magnetic field [26]. It is expected to diverge at critical point as $\chi_0^{(2)} \sim (g_c - g)^{-\gamma_4}$, with the critical index $\gamma_4 = \gamma + 2\Delta$, where Δ is the so-called gap exponent. From the estimates of Δ , one can find more of the different critical indices [21,62].

In order to find the critical index for the gap Δ , in a weak external magnetic field, one can study the critical behavior of the ratio $\frac{\chi_0^{(2)}(g)}{\chi(g)}$,

$$\frac{\chi_0^{(2)}(g)}{\chi(g)} \sim (g_c - g)^{-2\Delta},$$

divergent at the critical point. On the other hand, at small g one can deduce from the series written down in [26], that

$$\frac{\chi_0^{(2)}(g)}{\chi(g)} \simeq 1 + 18g + 180g^2.$$

Furthermore, again, we find that although the methodology of optimized factor approximants from Section 2 can be applied with ease, the bounds that it produces, $\Delta \approx 1.282$ and $\Delta \approx 1.995$, are far too distant. We once again have to apply some other method based on the factor approximants in order to have tighter bounds on the solution.

Method of optimization arising from the two different definitions for critical index expressed by Formula (39), gives a rather good estimate for the parameter $a = 1449.63$. It deviates from the exact third-order coefficient $c_3 = 1464$ by less than 1%. We obtain also a rather reasonable estimate for the gap index $\Delta = 1.54408$, only by 1.34%, deviating from the reference value of $\Delta = 1.565 \pm 0.004$ [66].

Formula for 3D Susceptibility

Consider the susceptibility of the three-dimensional ferromagnetic Ising model on a simple cubic lattice. The susceptibility is expected to diverge at a critical point $g_c = 0.22165463(8)$, known with high numerical precision [63,64], so that

$$\chi(g) \sim (g_c - g)^{-\gamma}, \tag{53}$$

with the critical index $\gamma = 1.237 - 1.244$, known from various numerical and theoretical estimates [21,29,30]. The high-temperature expansion of the susceptibility yields [26] the series in powers of inverse temperature g ,

$$\chi(g) = 1 + 6g + 30g^2 + 148g^3 + 706g^4 + \frac{16804}{6}g^5 + \frac{42760}{3}g^6 + \frac{7744136}{105}g^7 + \frac{35975026}{105}g^8 + \dots \quad (g \rightarrow 0). \tag{54}$$

Let us construct the expression for susceptibility in the high-temperature region $g > g_c$, inspired by Onsager’s exact solution low-temperature magnetization for the 2D Ising model [27], following the same idea as above, expressed in Section 3.1.1.

We start with zero-approximation (to be corrected) for susceptibility,

$$\chi_0(g) = \frac{0.180568 \sinh^{1.24}(3.97634g)}{g^{1.24}(1 - \sinh(3.97634g))^{1.24}}.$$

suggested by analogy to the derivation in 2D case from Section 3.1.1. It is normalized to unity as $g \rightarrow 0$ and designed to possess the correct leading asymptotic behaviors and correct threshold. The simplest expression for the susceptibility is corrected with account on the two leading terms in the expansion at small g

$$\chi_2(g) = \frac{(0.594439g + 0.387033) \sinh^{1.24}(3.97634g)}{g^{1.24}(g + 2.14342)(1 - \sinh(3.97634g))^{1.24}},$$

by multiplying $\chi_0(g)$ with simplest diagonal Padé approximant. It accurately predicts all remaining 23 coefficients from the high-temperature expansion [26], with an average error of 0.61%.

The longer expression for the susceptibility is obtained when $\chi_0(g)$ is corrected with account on the nine leading terms in the expansion at small g

$$\chi_9(g) = \frac{g(g((-1.34728g - 0.61183)g - 0.435938) + 0.0240448) + 0.0353811}{(g(g(g(g(g + 0.306749) - 0.14492) - 0.519154) - 0.0137897) + 0.0353811)(1 - \sinh(3.97634g))^{1.24}}, \tag{55}$$

by multiplying zero-approximation with corresponding non-diagonal Padé approximant $P_{4,5}$. It accurately “predicts” all remaining 16 coefficients from the high-temperature expansion [26], with average error of 0.018%. In the latter case we employed the following, simpler “ground-state”

$$\chi_0(g) = \frac{1}{(1 - \sinh(3.97634g))^{1.24}}.$$

It also possesses the correct leading asymptotic behaviors and correct threshold.

7. Conclusions

Factor approximants are amenable to optimization and can be successfully applied to the critical phenomena. The critical index by itself serves as a control parameter to be calculated from the optimization condition.

We limit ourselves to the minimal model of critical phenomena based on expansions with only two coefficients and critical points. Factor approximants are asymptotically equivalent to such series. The approximants are optimized by complementing them with various natural optimization conditions of non-perturbative nature. The role of control parameter is played by the critical index by itself. The minimal derivative condition imposed on critical amplitude appears to bring the most reasonable, uniquely defined results. For the minimal model it is not feasible to apply some other known technique for upper and lower bounds evaluation [67–69], but for longer expansions the non-diagonal Padé approximants can be useful [6].

The minimal difference condition imposed on the critical amplitudes produces upper and lower bound on the critical index. While one of the bounds is close to the result from

the minimal difference condition, the second bound is determined by the non-optimized factor approximant. One would expect that for the minimal derivative condition to work well, the bounds determined by the minimal difference condition should be not too wide. In such a sense the technique of optimization presented above is self-consistent, since it automatically supplies the solution and the bounds.

In the case of effective viscosity of passive suspensions the bounds could be found that are too wide to make any sense from either of the solutions. Some other variants of the factor approximants were shown to give rather good estimates. Therefore, we designed some other optimization conditions imposed on the factor approximants, leading to better estimates. The most appealing approach is based on equating the results from two different definitions of the critical index, while optimization parameter is introduced as the trial third-order coefficient in the expansion.

All techniques for calculation of the critical index presented in the paper appear powerful, but there is no such thing as the best method for all problems. The problem consists of finding the best method for each concrete physical problem. From the standpoint of the method of corrected approximants [6,18,57,70], it is also important to form properly the starting approximation based on a small number of terms, to be corrected by means, e.g., of the diagonal Padé approximants into very high orders.

Methods of calculation based on optimized factors are applied and results presented for critical indices of several key models of conductivity and viscosity of random media. The results for Ising model in two and three dimensions, permeability in two-dimensional channels are discussed as well.

Accurate calculations with short truncated series become possible in some important cases, because the higher-order coefficients appear to be redundant close to the critical point, and critical indices could be estimated from only two low-order coefficients by imposing some universal conditions of non-perturbative nature. Self-similarity with addition of minimal derivative conditions successfully replaces the higher-order terms. The redundancy (independence of the critical indices from the higher-order coefficients c_n) plays the same role as the requirement of independence of the critical phenomena on the interactions at finer scales. Exclusion of such interactions and scales leads to the celebrated constructive renormalization group in Wilson–Kadanoff formulation [19,27].

The redundancy allows us to deduce compact formulas for all regions, not only calculate the critical index. Concrete derivation of such formulas is presented for the susceptibility of the Ising model in 2D and 3D cases.

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