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Variational approximations and mean-field scaling theory

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Abstract. It is shown that 'mean-field finite-size scaling theory' can be adjusted and applied to sequences of approximations that do not obey the well known power laws of finite-size scaling. The proposed modification of the theory seems to be well directed to the sequence of Baxter's variational approximations. This sequence of approximations shows a novel feature according to which exponential laws appear in places where power laws should be expected, but the modified scaling theory still yields relations from which non-classical critical exponents can be estimated. Thus, two techniques for the estimation of the critical exponent β are suggested from the finite-order variational approximations. These techniques are applied to the zero-field Ising model on the square lattice using the systematic series of the Baxter–Tsang systems and excellent estimates of β are obtained correct up to 13 significant figures.

1. Introduction

We report here an application on 'finite-size scaling' techniques to the sequence of variational approximations of Baxter [1–3] for the zero-field Ising model on the square lattice.

Following the notions of mean-field finite-size scaling theory or coherent-anomaly method (CAM) of Suzuki [4–7] we provide substantial evidence that the variational method of Baxter may yield the best practical estimation of the critical exponent of spontaneous magnetization β. Thus, the present investigation is a test of two techniques for the estimation of the critical exponent β. The first of these techniques is the above-mentioned coherent-anomaly method of Suzuki and the second is a new proposal for an apparently more effective method based on estimates of spontaneous magnetization at the exact critical temperature.

The method is applied to the zero-field case using a simplification of Baxter's method developed by Tsang [8]. The sequence of approximations is generated by solving numerically Baxter–Tsang systems. Sequences of estimates are obtained for spontaneous magnetization at the exact critical temperature, for the approximate critical temperature and analysing the data close to these for the associated 'classical amplitudes'.

In section 2, the ideas of Suzuki [4–7] and the formulation of finite-size scaling theory of Fisher [9–11] are studied and extended in a fashion that permits exponential factors to replace the commonly used power laws. Section 3 briefly describes Baxter–Tsang systems. A parametric representation of the method together with an analysis of our numerical results are presented in section 4 where the necessity of the above-mentioned generalization to include exponential factors becomes obvious. Finally our conclusions are summarized in section 5.

2. Generalized mean-field approximations and scaling theory

Suzuki [4–7] has proposed a powerful method for the study of critical phenomena which is called the coherent-anomaly method (CAM). The method estimates critical exponents by using a sequence of mean-field approximations, called also 'canonical approximations' [6], which exhibit classical behaviour in finite-order. This method has been applied to various critical phenomena including two- and three-dimensional Ising models [4–7, 12–14], quantum spin systems [15], spin glasses [16], percolation [16], and so on.

Here we discuss the basic idea of Suzuki and focus upon the estimation of the critical exponent β for which Baxter's approximations will prove to provide the most efficient 'canonical sequence'. We assume that the 'canonical sequence' of approximations has the following three properties:

(i) In order n the approximation shows a critical temperature $T_{c,n}$ and

$$\lim_{n\to\infty} T_{c,n} = T_c^* \tag{1}$$

where T_c^* is the exact critical temperature of the real (infinite) Ising system.

(ii) The spontaneous magnetization $m(n, T)$ for all finite-order approximations exhibit classical behaviour with an exponent $\bar{\beta} = \frac{1}{2}$, i.e.

$$m(n, T) \sim \bar{m}_n(\varepsilon_n(T))^{\bar{\beta}} \qquad T \to T_{c,n} \tag{2}$$

where

$$\varepsilon_n(T) = \left| \frac{T_{c,n} - T}{T_{c,n}} \right|. \tag{3}$$

In the limit $n \to \infty$ the true critical behaviour is obtained and the critical exponent (2D Ising) is $\beta = 1/8$, i.e.

$$m(T) \sim (\varepsilon(T))^{\beta} \qquad T \to T_c^* \tag{4}$$

with

$$\varepsilon(T) = \left| \frac{T_c^* - T}{T_c^*} \right|. \tag{5}$$

(iii) A third assumption not considered by Suzuki but useful for our purpose concerns spontaneous magnetization at the exact critical temperature, i.e., it is assumed that T_c^* is approached from above ($T_{c,n} > T_c^*$) and therefore $m(n, T_c^*)$ exists, i.e.

$$m(n, T_c^*) \neq 0 \qquad n \neq \infty. \tag{6}$$

According to Suzuki [4] the amplitude $\bar{m}_n$ of the classical singularity and the approximate critical temperature have the following n-dependence

$$\bar{m}_n \sim n^{(\bar{\beta}-\beta)/\nu} \tag{7}$$

$$T_{c,n} \sim T_c^* + a n^{-1/\nu} \tag{8}$$

with the expectation that ν is the critical exponent of the correlation length, i.e.

$$\xi \sim |T - T_c^*|^{-\nu}. \tag{9}$$

However, Suzuki [4, 13] eliminates from (7) and (8) the $n^{1/\nu}$-dependence and the following asympotic relationship is assumed:

$$\bar{m}_n \sim \left(\frac{T_{c,n} - T_c^*}{T_c^*}\right)^{\beta - \bar{\beta}}. \tag{10}$$

Thus, one may define successive estimates of β by

$$\beta_{\bar{m}}(n+1, n) = \bar{\beta} + \frac{\log(\bar{m}_{n+1}/\bar{m}_n)}{\log(\Delta T_{c,n+1}/\Delta T_{c,n})} \tag{11}$$

where

$$\Delta T_{c,n} = (T_{c,n} - T_c^*)/T_c^* \tag{12}$$

and expect that

$$\lim_{n\to\infty} \beta_{\bar{m}}(n+1, n) = \beta. \tag{13}$$

These formulae are the basic ingredients of CAM and as pointed out by Suzuki [4–7] are inspired by Fisher's finite-size scaling theory, to which we now turn, assuming that the finite-size scaling hypothesis can be extended to a sequence of canonical approximations.

Following Barber [11] we give here two formulations of the finite-size scaling hypothesis for spontaneous magnetization. First we assume that

$$m(n, T) \sim n^{\omega} Q(n^{1/\nu}\varepsilon(T)) \qquad n\to\infty,\ \varepsilon(T)\sim 0 \tag{14}$$

and in order to reproduce the true critical behaviour (4) we require that in the limit $n\to\infty$

$$Q(x) \sim x^{\beta} \qquad \text{as } x\to\infty. \tag{15}$$

So that the true critical behaviour is reproduced if

$$\omega = -\beta/\nu. \tag{16}$$

In finite-order we expect a classical behaviour so we require

$$Q(x) \sim (x_c - x)^{\bar{\beta}} \qquad x\to x_c \tag{17}$$

where

$$x_c = n^{1/\nu}\Delta T_{c,n} \tag{18}$$

to obtain

$$m(n,T)\sim n^{(\dot\beta-\beta)/\nu}\left(\frac{T_{c,n}}{T_c^*}\right)^{\dot\beta}(\varepsilon_n(T))^{\dot\beta}\qquad T\to T_{c,n} \tag{19}$$

which implies for the amplitude $\bar{m}_n$ a relation asymptotically equivalent to (7), i.e.

$$\bar{m}_n\sim\left(\frac{T_{c,n}}{T_c^*}\right)^{\dot\beta}n^{(\dot\beta-\beta)/\nu}. \tag{20}$$

Now, it is well known [11] that scaling (14) has as a necessary conclusion that the 'shift exponent' λ defined by

$$\Delta T_{c,n}\sim n^{-\lambda} \tag{21}$$

is equal to $1/\nu$, so that formulae (10) and (13) should apply.

But, apart from the estimation formula (11) used in CAM, finite-size scaling provides a further result which we shall find most useful. According to (14) and property (iii) of the sequence of approximations we may write.

$$m(n,T_c^*)\sim n^{-\beta/\nu}Q(0) \tag{22}$$

from which the equality $\lambda=1/\nu$ implies that

$$m(n,T_c^*)\sim(\Delta T_{c,n})^{\beta} \tag{23}$$

so defining successive estimates by

$$\beta_{m^*}(n+1,n)=\frac{\log[m(n+1,T_c^*)/m(n,T_c^*)]}{\log(\Delta T_{c,n+1}/\Delta T_{c,n})} \tag{24}$$

we should also expect that

$$\lim_{n\to\infty}\beta_m^*(n+1,n)=\beta. \tag{25}$$

Furthermore, from (22) and (20) we may write

$$\bar{m}_n\sim(m(n,T_c^*))^{(\beta-\dot\beta)/\beta} \tag{26}$$

and try to estimate β using the estimates

$$\beta_{\bar{m},m^*}(n+1,n)=\dot\beta\bigg/\left\{1+\frac{\log(\bar{m}_{n+1}/\bar{m}_n)}{\log[m(n,T_c^*)/m(n+1,T_c^*)]}\right\}. \tag{27}$$

Of course, from the definitions (27), (24) and (11) we find

$$\beta_{\bar{m},m^*}(n+1,n)=\dot\beta\beta_{m^*}(n+1,n)/\{\dot\beta+\beta_{m^*}(n+1,n)-\beta_{\bar{m}}(n+1,n)\} \tag{28}$$

and the sequence $\beta_{\bar{m},m^*}$ has as limit the critical exponent β if both sequences $\beta_{\bar{m}}$ and β_{m^*} have as limit the exponent β. However, in applications using the Baxter method it is much easier to calculate the terms of sequence (24).

The second formulation of finite-size scaling replaces $\varepsilon(T)$ by $\varepsilon_n(T)$ (see Barber [11]), i.e.

$$m(n,T)\sim n^{\omega}\bar{Q}(n^{1/\nu}\varepsilon_n(T))\qquad n\to\infty\qquad\varepsilon_n(T)\to 0 \tag{29}$$

and applying a similar reasoning one can obtain all previous formulae for the sequences $\beta_{\bar{m}}$, β_{m^*} and $\beta_{\bar{m},m^*}$, provided that one assumes again the equality $\lambda = 1/\nu$. But, unlike scaling (14), the equality $\lambda = 1/\nu$ is not now a necessary conclusion of scaling (29) (see Barber [11]). Therefore scaling (29) does not necessarily imply that the three sequences have as their common limit the critical exponent β.

To close this section we reformulate these scalings in a way that avoids the explicit use of the power law dependence (8) and (21) and permits exponential factors which appear for the sequence of Baxter variational approximations. We can do this by simply writing in place of (14) and (29).

$$m(n, T) \sim f(n) Q(g(n)\varepsilon(T)) \qquad n \to \infty \qquad \varepsilon(T) \sim 0 \tag{30}$$

and

$$m(n, T) \sim \bar{f}(n) \bar{Q}(\bar{g}(n)\varepsilon_n(T)) \qquad n \to \infty \qquad \varepsilon_n(T) \to 0 \tag{31}$$

respectively. The functions $f(n)$, $g(n)$ introduced here replace the power-law forms n^{ω} and $n^{1/\nu}$ (see (29)), respectively. In a straightforward way we may now repeat the steps of the previous reasoning and find that condition (16) is now replaced by $f(n)g^{\beta}(n) \to \alpha \in \Re^*$. Of course, this is a more general form and permits even exponential functions of n. For instance, we could take $f(n) \sim \exp(-\lambda n^{\theta})$ and $g(n) \sim \exp[(\lambda/\beta)n^{\theta}]$, with λ, $\theta > 0$.

Thus, from scaling ansatz (30) we may easily obtain, using a reasoning analogous to that used for scaling (14), that

$$\bar{m}_n \sim (g(n))^{\dot{\beta} - \beta} \tag{32}$$

and

$$m(n, T_c^*) \sim Q(0)(g(n))^{-\beta} \tag{33}$$

from which we may assume the validity of (26) and obtain sequence $\beta_{\bar{n},m^*}$ having β as limit. It is also a necessary conclusion of scaling (30) that

$$\lim_{n \to \infty} (g(n)\Delta T_{c,n}) = c \in \Re^* \tag{34}$$

and this is sufficient to establish that the three sequences $\beta_{\bar{m}}$, β_{m^*} and $\beta_{\bar{m},m^*}$ have a common limit, which is the true critical exponent β if scaling (30) is obeyed.

Again scaling ansatz (31) is more general and the sufficient condition (34) for the common limit β of the three sequences is not a necessary conclusion. The asymptotic behaviour of $\bar{m}_n$ and $m(n, T_c^*)$ is now given by

$$\bar{m}_n \sim (\bar{g}(n))^{\dot{\beta} - \beta} \tag{35}$$

and

$$m(n, T_c^*) \sim \bar{Q}(\bar{g}(n)\Delta T_{c,n})(\bar{g}(n))^{-\beta} \tag{36}$$

respectively. One should note here that the above relations do not necessarily imply the asymptotic forms (10) and (23) and therefore the validity of the limits (13) and (25) is not disclosed without further assumptions. The corresponding sequences may or may not tend to the true critical exponent β and this may now depend also on the way $\bar{c}_n = \bar{g}(n)\Delta T_{c,n}$ approaches its limit if this limit is not a constant $\neq 0$. However, if

$$\lim_{n \to \infty} \bar{c}_n = \infty$$

we may apply the $x\to\infty$ behaviour in (36) to obtain (23) so we expect (25) to be valid. In conclusion scaling (31) does not necessarily imply a common limit β for the three sequences $\beta_{\bar{m}}$, β_{m^*} and $\beta_{\bar{m},m^*}$ and it appears that the sequence β_{m^*} has more general applicability.

3. The Baxter–Tsang sequence of variational approximations

In 1968 Baxter [1] developed a sequence of variational approximations for the monomer–dimer problem on the square lattice. The method was generalized to the Potts model by Kelland [17] and to a square IRF (interaction-round-a-face) model with row and column reversal symmetry by Baxter [3]. This very important method and the related concept of 'corner transfer matrices' (chapter 13 in Baxter's book [18]) has several applications and it was soon used in various directions including series expansions on the square and other planar lattices [19–21], generalizations to problems with broken lattice symmetry [20, 22] and also to three-dimensional models [23]. It continues to give new results [24] not easily obtainable by other methods.

The finite-order variational approximations of Baxter exhibit classical critical behaviour as first noted by Baxter [3] but the direct application of these approximations for the estimation of the true critical behaviour has not been yet clarified, although Kelland [17] use the method for the estimation of β for the Potts model. Also we should note that Tsang [8] observed a crossover phenomenon and has pointed out that the data of the approximations support very well a scaling hypothesis.

In terms of the 'corner transfer matrices', $A(a)$, and the 'half-row transfer matrices', $F(a,b)$, Baxter's variational approximations for the square zero-field Ising model are described by the system [3, 8]

$$\sum_b F(a,b)A^2(b)F(b,a)=A^2(a) \tag{37a}$$

and

$$\sum_{b,b'} w(a,b,a',b')F(a,b)A(b)F(b,b')A(b')F(b',a')=\kappa A(a)F(a,a')A(a') \tag{37b}$$

where a, b, a' and b' take the spin values of $+1$ or -1 and the Boltzmann factor of a face for the zero field Ising model on the square lattice, with T the temperature and k_B the Boltzmann constant is given by

$$w(a,b,a',b')=z^{-(ab+a'b'+aa'+bb')/4} \tag{38a}$$

with

$$z=\exp(-2J/k_BT) \tag{38b}$$

where J is the nearest-neighbour interaction energy coefficient.

In (37b) κ is the partition function per site and the corresponding spontaneous magnetization is given by [3]

$$m(T)=\frac{\Sigma_a\, a \operatorname{Tr} A^4(a)}{\Sigma_a \operatorname{Tr} A^4(a)}. \tag{39}$$

In this form we may assume that the involved matrices are $2^m\times 2^m$ and for each value of $m(=0,1,2,\ldots)$ we obtain a system of a large ($\sim 2^{2m}$) number of equations representing the 'mth-order' variational approximation. It should be pointed out that since Baxter's approximations are derived from a variational principle [3], m defines the order of approximation. However, from the graphical representation of the 'corner transfer matrices' [3], m may also be interpreted as the system size of the scaling theory.

One may simplify the problem by using the symmetries of the model and a representation in which $A(a)$ are diagonal [3], but for the zero-field case Tsang [8] has reduced the number of equations to only $n=m+2$. Using Tsang representation the variational approximations in order $n(=2, 3, \ldots)$ are determined by the system [8]

$$2\sum_{l=1}^{n-1}\tan^{-1}\frac{C_l^{-1}+C_l}{C_j^{-1}-C_j}+\tan^{-1}\frac{h_1}{C_j^{-1}-C_j}+\tan^{-1}\frac{h_2}{C_j^{-1}-C_j}$$
$$=(n-j+1/2)\pi \qquad j=1,2,\ldots,n \tag{40a}$$

where

$$h_1=\{2+(C_n^2+C_n^{-2})(1+2z-z^2)/(1+z^2)\}^{1/2} \tag{40b}$$

and

$$h_2=\{2+(C_n^2+C_n^{-2})(1-2z-z^2)/(1+z^2)\}^{1/2}. \tag{40c}$$

The spontaneous magnetization is now given by [8]

$$m(T)=\prod_{j=1}^{n-1}\frac{1-C_j^4}{1+C_j^4}. \tag{41}$$

Using a Newton–Raphson method Tsang [8] has solved system (40) for a range of values z below the critical point ($z_c=0.414\,213\,562\,373\ldots$) and has also calculated the approximate critical temperatures for $n=2$–20. It was found that the estimates of spontaneous magnetization converge rapidly to the exact ones for $z<z_c$ and that also the approximate $T_{c,n}$ approaches the exact T_c^* with an exponential law and not a power law!

In the next section we solve again system (40) for $n=2$–20 but now we focus upon the estimation of $m(n, T_c^*)$ and by analysing the data of the classical behaviour near $T_{c,n}$ we also obtain the amplitudes $\bar{m}_n$ so that all sequences of β-estimates mentioned earlier can be calculated.

4. Numerical estimates and asymptotic analysis

A suitable temperature parameter may be defined by

$$t=\operatorname{cosech}^4(2J/k_BT)-1. \tag{42}$$

Following Tsang [8] we now express t with the help of (40c) as

$$t=r(z)(1-h_2^2/2)/(C_n^2+C_n^{-2}) \tag{43a}$$

where

$$r(z)=2(1+2z-z^2)(1+z^2)^3/(1-z^2)^4. \tag{43b}$$

From the numerical solutions it is verified (see also [8]) that for all finite values of n, h_2 vanishes at the approximate critical point, i.e. at $T_{c,n}$ (or $t_{c,n}$). Thus the parametric critical temperature $t_{c,n}$ is related to C_n by

$$t_{c,n}=r(z_{c,n})/(C_n^2+C_n^{-2}). \tag{44a}$$

It is also verified that as $n\to\infty$, $C_n\to 0$ and $z_{c,n}\to z_c^*=\sqrt{2}-1$. Therefore the asymptotic behaviour of $t_{c,n}$ is determined from that of C_n, i.e.

$$t_{c,n}\sim r(z_{c,n})C_n^2\sim r(z_c^*)C_n^2=8\sqrt{2}C_n^2. \tag{44b}$$

In the limit $n\to\infty$ we obtain the exact critical temperature

$$t_c^*=0 \quad \text{or } k_BT_c^*/J=2.269\,185\,314\,21\ldots . \tag{44c}$$

Furthermore, we can easily show that

$$(T_2-T_1)/T_2=R(T_2)(t_2-t_1) \qquad T_1\to T_2 \tag{45a}$$

with

$$R(T)=\frac{k_BT\sinh^5(2J/k_BT)}{8J\cosh(2J/k_BT)}. \tag{45b}$$

We may now transform the classical behaviour (2) in t-representation, i.e.

$$m(n,T)\sim\bar{m}_n[R(T_{c,n})t_{c,n}]^{\beta}[\tau_n(t)]^{\beta}=\bar{m}'_n[\tau_n(t)]^{\beta} \qquad t\to t_{c,n} \tag{46a}$$

where

$$\tau_n(t)=(t_{c,n}-t)/t_{c,n}. \tag{46b}$$

It follows that the classical amplitudes $\bar{m}_n$ and $\bar{m}'_n$ in the two representations should satisfy

$$\bar{m}'_n=[R(T_{c,n})t_{c,n}]^{\beta}\bar{m}_n. \tag{47}$$

Assuming that (10) is obeyed and since $\beta<\dot{\beta}$ the above transformation shows (because of the term $t_{c,n}^{\beta}$ in (47)), that $\bar{m}_n\to\infty$ whereas $\bar{m}'_n\to 0$ as $n\to\infty$. Furthermore assuming that (23) is also obeyed we may write

$$\bar{m}'_n\sim m(n,T_c^*)\sim t_{c,n}^{\beta}. \tag{48}$$

Thus in a fashion analogous to (11) and (24) we may define the sequences $\beta'_{\bar{m}'}(n+1,n)$ and $\beta'_{m^*}(n+1,n)$ by

$$\beta'_{\bar{m}'}(n+1,n)=\log(\bar{m}'_{n+1}/\bar{m}'_n)/\log(t_{c,n+1}/t_{c,n}) \tag{49}$$

$$\beta'_{m^*}(n+1,n)=\log[m(n+1,T_c^*)/m(n,T_c^*)]/\log(t_{c,n+1}/t_{c,n}) \tag{50}$$

respectively.

Table 1. The critical temperatures $t_{c,n}$, $T_{c,n}$ and C_n at the critical point for $n=2$–20.

n	$t_{c,n}$	$k_BT_{c,n}/J$	C_n
2	0.388 836 182 8857E+00	2.425 665 733 9651	0.170 341 669 9163E+00
3	0.557 083 519 7377E−01	2.294 044 370 7466	0.692 216 201 1541E−01
4	0.135 336 061 0379E−01	2.275 314 918 4824	0.344 701 279 8683E−01
5	0.413 977 213 7161E−02	2.271 066 630 1302	0.191 089 581 9001E−01
6	0.145 897 425 8379E−02	2.269 848 986 0314	0.113 517 550 1645E−01
7	0.568 044 548 1742E−03	2.269 443 794 8837	0.708 479 103 2891E−02
8	0.238 469 714 4168E−03	2.269 293 839 4380	0.459 079 853 5011E−02
9	0.106 265 118 8318E−03	2.269 233 676 7387	0.306 465 320 1948E−02
10	0.497 207 596 4870E−04	2.269 207 943 1881	0.209 633 645 6279E−02
11	0.242 348 677 4489E−04	2.269 196 344 1184	0.146 357 574 4315E−02
12	0.122 322 305 3447E−04	2.269 190 881 4368	0.103 979 807 2890E−02
13	0.636 378 960 7495E−05	2.269 188 210 5545	0.749 988 705 5335E−03
14	0.339 989 576 9465E−05	2.269 186 861 6038	0.548 188 524 4944E−03
15	0.185 973 940 4011E−05	2.269 186 160 6346	0.405 436 974 2955E−03
16	0.103 896 420 3303E−05	2.269 185 787 0761	0.303 038 415 8659E−03
17	0.591 578 323 9215E−06	2.269 185 583 4577	0.228 667 039 7971E−03
18	0.342 709 619 9946E−06	2.269 185 470 1902	0.174 044 626 0127E−03
19	0.201 693 527 2402E−06	2.269 185 406 0097	0.133 519 121 5006E−03
20	0.120 433 544 6552E−06	2.269 185 369 0259	0.103 174 228 2380E−03

In table 1, the critical temperatures $t_{c,n}$ and $T_{c,n}$ are given together with the values of C_n at the critical point for $n=2$–20. The results given in this table are accurate to 13 significant figures and agree completely with the 11 significant figures given by Tsang [8]. Since $t_{c,n}$ and C_n were obtained by independent extrapolations the equation (44*a*) served as a good test of our accuracy.

In table 2, the spontaneous magnetizations at the exact critical temperature $m(n, T_c^*)$ and the amplitude $\bar{m}_n$ (in T-representation) and $\bar{m}_n'$ (in t-representation) are

Table 2. Spontaneous magnetizations $m(n, T_c^*)$ at the exact critical temperature and the classical amplitudes $\bar{m}_n$ and $\bar{m}_n'$ for $n=2$–20.

n	$m(n, T_c^*)$	$\bar{m}_n$	$\bar{m}_n'$
2	0.751 099 850 4534	0.434 820 2730E+01	0.104 279 5749E+01
3	0.614 379 008 1302	0.100 262 9783E+02	0.103 358 3871E+01
4	0.522 183 883 3766	0.186 527 7951E+02	0.965 792 9102E+00
5	0.453 864 995 7972	0.311 515 1085E+02	0.895 922 6185E+00
6	0.400 483 776 7501	0.486 378 1389E+02	0.831 452 9716E+00
7	0.357 313 812 3122	0.724 583 0610E+02	0.773 210 7238E+00
8	0.321 539 653 0038	0.104 229 4466E+03	0.720 761 6538E+00
9	0.291 345 945 2471	0.145 880 4197E+03	0.673 447 1660E+00
10	0.265 493 897 4786	0.199 701 4567E+03	0.630 627 0850E+00
11	0.243 101 260 4967	0.268 398 3029E+03	0.591 735 6262E+00
12	0.223 518 350 9501	0.355 153 5258E+03	0.556 287 1057E+00
13	0.206 253 696 6728	0.463 695 4047E+03	0.523 868 0482E+00
14	0.190 927 179 7873	0.598 375 2085E+03	0.494 126 5624E+00
15	0.177 239 294 1010	0.764 253 7426E+03	0.466 762 2633E+00
16	0.164 950 288 1579	0.967 198 1236E+03	0.441 517 5984E+00
17	0.153 865 609 0666	0.121 398 9831E+04	0.418 170 6482E+00
18	0.143 825 494 4958	0.151 244 5175E+04	0.396 529 2324E+00
19	0.134 697 372 7837	0.187 154 9431E+04	0.376 426 1031E+00
20	0.126 370 210 5853	0.230 160 5985E+04	0.357 715 0218E+00

Table 3. Three sequences of estimates for the critical exponent β (see definitions (24), (11) and (27)). The extrapolations below correspond to three assignments of the parameter a_m of the algorithm (51).

$n+1$	$\beta_{m^*}(n+1, n)$	$\beta_{\bar{m}}(n+1, n)$	$\beta_{\bar{m},m^*}(n+1, n)$
3	0.109 216 518 263 688	0.045 879 842 373 226	0.096 937 162 923 974
4	0.116 129 674 759 230	0.056 612 157 129 964	0.103 776 621 017 411
5	0.118 713 941 405 179	0.065 792 831 585 284	0.107 351 608 843 302
6	0.120 090 073 267 272	0.072 394 784 823 732	0.109 632 194 945 979
7	0.120 957 417 577 197	0.077 280 992 115 565	0.111 240 263 429 201
8	0.121 558 993 689 614	0.081 047 084 848 797	0.112 448 025 382 373
9	0.122 002 593 699 642	0.084 052 600 461 788	0.113 395 850 202 845
10	0.122 343 969 455 855	0.086 519 107 354 216	0.114 164 140 290 161
11	0.122 615 119 982 613	0.088 588 999 426 468	0.114 802 549 222 611
12	0.122 835 833 312 747	0.090 357 689 848 638	0.115 343 544 913 996
13	0.123 019 049 972 836	0.091 891 534 490 371	0.115 809 336 163 923
14	0.123 173 609 102 463	0.093 238 185 562 961	0.116 215 678 015 797
15	0.123 305 762 877 845	0.094 432 819 604 937	0.116 574 088 773 357
16	0.123 420 062 500 901	0.095 502 025 046 360	0.116 893 204 763 371
17	0.123 519 902 971 903	0.096 466 310 141 064	0.117 179 642 309 684
18	0.123 607 865 432 535	0.097 341 790 115 782	0.117 438 565 043 487
19	0.123 685 956 921 875	0.098 141 294 459 135	0.117 674 068 215 510
20	0.123 755 742 818 376	0.098 875 243 870 353	0.117 889 446 327 698
$a_m=0$	0.124 697 527 579 979	0.111 663 526 924 864	0.122 368 316 209 902
	0.124 697 897 973 314	0.110 324 950 746 364	0.122 372 136 153 307
$a_m=1$	0.124 593 813 476 846	0.111 906 961 614 679	0.121 610 165 887 981
	0.124 617 215 062 186	0.112 132 258 605 121	0.121 691 398 595 983
a_m from (52)	0.124 998 573 727 193	0.125 409 370 433 708	0.124 958 116 126 477
	0.124 998 518 109 150	0.125 413 962 122 192	0.124 950 966 885 229

given, also for $n=2$–20. The amplitudes $\bar{m}_n$ and $\bar{m}_n'$ were obtained using the formulae (2) and (46), respectively. These values are related by (47) and they agree to 10 significant figures which is also the accuracy we required for the amplitudes. It may be noted here that to obtain the required accuracy in the amplitudes we had to work very close *to the critical temperatures* $t_{c,n}$, *and also use two independent extrapolation techniques* in each case. The values of $m(n, T_c^*)$ are also accurate to 13 significant figures, as tested by increasing the accuracy of our solutions.

Table 3 shows the three sequences $\beta_{m^*}(n+1, n)$, $\beta_{\bar{m}}(n+1, n)$ and $\beta_{\bar{m},m^*}(n+1, n)$ defined in (24), (11) and (27), respectively. The convergence of these sequences, and in particular of the last two, to the true critical exponent $\beta(=0.125)$ is rather slow.

To accelerate the convergence of the sequences we have applied the so-called alternating ε-algorithm defined in [11]

$$P_l^{(m+1)}=P_l^{(m)}+1/[Q_l^{(m)}-Q_{l-1}^{(m)}] \tag{51a}$$

$$Q_l^{(m)}=\alpha_m Q_l^{(m-1)}+1/[P_{l+1}^{(m)}-P_l^{(m)}] \tag{51b}$$

where $Q_l^{(-1)}=0$ and $P_l^{(0)}=P$ $(l=1, \ldots, N)$ are the first N available terms of the original sequence. The algorithm was applied for three assignments of the parameter α_m, namely,

$\alpha_m = 0$ (Shank's transform), $\alpha_m = 1$ (Wynn's ε-algorithm) and finally (alternating ε-algorithm).

$$\alpha_m = -[1-(-1)^m]/2. \tag{52}$$

In almost all cases considered in this paper assignment (52) seems to have produced the best estimates. We have therefore given in our tables, below each sequence, the last column ($m = \max$) of extrapolation according to (51*a*), (51*b*) and (52), and only in cases where we have remarkable differences we give also the extrapolations for the other two assignments.

One may be inclined from table 3 to conclude that the three sequences of estimates have as their common limit the true critical exponent $\beta = 0.125$. However, two of the assignments for α_m give for the sequence $\beta_{\bar{m}}(n+1, n)$ extrapolates not very close to 0.125.

We now turn to a different asymptotic analysis of our results. According to Tsang [8] the values of C_n fit extremely accurately to the formula:

$$C_n = 1.681\,792\,8304 \exp[-(4.934\,802\,2005n - 4.626\,377\,0635)^{1/2}]. \tag{53}$$

We therefore assume that similar asymptotic laws are followed not only for $t_{c,n}$ (because of (44*b*)), but also for $m(n, T_c^*)$ and m_n^t, i.e., we assume

$$t_{c,n} \sim r(z_{c,n}) C_n^2 \sim A_t \exp[-(B_t n + \Gamma_t)^{1/2}] \tag{54a}$$

$$m(n, t=0) \sim A_{m^*} \exp[-(B_{m^*} n + \Gamma_{m^*})^{1/2}] \tag{54b}$$

$$\bar{m}_n^t \sim A_{\bar{m}^t} \exp[-(B_{\bar{m}^t} n + \Gamma_{\bar{m}^t})^{1/2}]. \tag{54c}$$

The asymptotic behaviour of $\bar{m}_n$ should then follow from the combination of (54*a*), (54*c*) and (47). Alternatively, we may assume that

$$\bar{m}_n \sim A_{\bar{m}} \exp[+(B_{\bar{m}} n + \Gamma_{\bar{m}})^{1/2}] \tag{54d}$$

and obtain m_n^t from (54*d*), (54*a*) and (47). We can now see that if (23) is valid, then the coefficients B_{m^*} and B_t should satisfy

$$\beta = (B_{m^*}/B_t)^{1/2} \tag{55}$$

from which β may be obtained if B_{m^*} and B_t are known. An analogous relationship should give β from $B_{\bar{m}^t}$ and B_t, and from (10) we should also have

$$\beta = \dot{\beta} - (B_{\bar{m}}/B_t)^{1/2}. \tag{56}$$

In order to apply these relationships we should calculate the coefficients in (54). We can do this by fitting exactly the functions (54) for every three values of n. For instance we may define the sequences $A_{m^*}(n)$, $B_{m^*}(n)$ and $\Gamma_{m^*}(n)$ ($n = 3, \ldots, 19$) as the values that fit exactly three successive estimates of m^*, i.e. $m(n-1, T_c^*)$, $m(n, T_c^*)$ and $m(n+1, T_c^*)$ to (54*b*). The resulting sequences for m^* (54*b*) and for $\bar{m}$ (54*d*) are given in tables (4) and (5), respectively.

Table 4. Fitting of the values $m(n, T_c^*)$ for $n=2$–20 to the asymptotic formula (54*b*). Extrapolations given correspond to the assignment (52) for the parameter a_{m^*}.

Order	A_{m^*}	B_{m^*}	Γ_{m^*}
3	1.468 495 514 410 883	0.309 795 998 073 952	−0.170 081 959 714 988
4	1.463 034 785 386 955	0.308 584 517 377 469	−0.172 926 335 472 207
5	1.462 328 620 143 789	0.308 449 124 289 896	−0.173 379 313 268 722
6	1.462 213 635 881 570	0.308 429 445 884 962	−0.173 464 916 411 396
7	1.462 191 683 275 632	0.308 426 021 067 377	−0.173 483 252 943 640
8	1.462 186 954 284 099	0.308 425 338 695 964	−0.173 487 590 768 238
9	1.462 185 832 702 361	0.308 425 187 417 561	−0.173 488 704 062 798
10	1.462 185 544 762 219	0.308 425 150 821 306	−0.173 489 010 044 268
11	1.462 185 465 732 823	0.308 425 141 296 414	−0.173 489 099 220 250
12	1.462 185 442 762 806	0.308 425 138 657 725	−0.173 489 126 566 479
13	1.462 185 435 738 473	0.308 425 137 885 371	−0.173 489 135 343 910
14	1.462 185 433 499 323	0.308 425 137 648 882	−0.173 489 138 268 179
15	1.462 185 432 755 854	0.308 425 137 573 231	−0.173 489 139 279 328
16	1.462 185 432 496 575	0.308 425 137 547 748	−0.173 489 139 645 443
17	1.462 185 432 403 406	0.308 425 137 538 882	−0.173 489 139 781 675
18	1.462 185 432 360 009	0.308 425 137 534 877	−0.173 489 139 847 235
19	1.462 185 432 377 661	0.308 425 137 536 460	−0.173 489 139 819 738
	1.462 185 432 348 565	0.308 425 137 533 816	−0.173 489 139 865 874

Table 4 shows that (54*b*) is very well satisfied even for small values of n and that the corresponding coefficients converge very fast to their limits. The same is true for the sequence C_n (not shown) for which, in almost complete agreement with (53), we obtain

$$C_n = 1.681\,792\,830\,508 \exp[-(4.934\,802\,200\,545n - 4.626\,377\,063\,01)^{1/2}]. \tag{53'}$$

We may now apply (55) to obtain an estimate of β. From (54*a*) and (53′) we have $B_t = 4 \times 4.934802200545$ and from table 4 we take as the best value of $B_{m^*} = 0.308425137534$, so the resulting estimate for β is according to (55)

$$\beta = 0.124\,999\,999\,999\,987. \tag{57}$$

This excellent estimate outlaws any reservations that the values of spontaneous magnetization at the exact critical point obeys the law (23) with β the true critical exponent. Furthermore, an inspection of table 4 shows that an estimate with several significant figures of B_{m^*} could be obtained using only, say, the first five variational approximations. Since this is also true for B_t (not shown) one could obtain several significant figures of β using only the first 5 or 6 variational approximations. This point may be of great interest since the method could be applied to several unsolved problems where the critical exponent is not exactly known.

Table 5 shows that the situation for the amplitudes $\bar{m}_n$ is unconvincing. If the assumed behaviour (54*d*) is true then it is at least surprising that even for $n=20$ the asymptotic behaviour has not settled. This effect is related to the fact that the parameter

$$\bar{c}_n = (\bar{m}_n)^{1/(\bar{\beta}-\beta)}(\Delta T_{c,n}) \tag{58}$$

continues to increase even for $n=20$. This parameter may be identified with $\bar{c}_n$ used in section 2 if (35) is written as an equality, so that $\bar{g}(n)$ is specified if the functional dependence of $\bar{m}_n$ is known. Since $\bar{c}_n$ seems to tend to infinity one could recall the

Table 5. Fitting of the classical amplitudes $\bar{m}_n$ for $n=2$–20 to the formula (54*d*).

Order	$A_{\bar{m}}$	$B_{\bar{m}}$	$\Gamma_{\bar{m}}$
3	0.804 019 7650	3.518 272 9157	−4.187 559 6051
4	0.924 766 0162	3.344 556 6436	−4.352 950 6585
5	1.011 448 2616	3.252 653 0767	−4.515 649 5226
6	1.079 546 7553	3.194 592 2258	−4.667 755 5001
7	1.136 380 0502	3.153 6896 295	−4.810 443 7563
8	1.185 670 5567	3.122 813 6421	−4.945 370 9846
9	1.229 510 5210	3.098 400 9156	−5.073 797 8338
10	1.269 187 1638	3.078 452 9992	−5.196 645 2802
11	1.305 552 7919	3.061 748 9276	−5.314 607 5359
12	1.339 205 8875	3.047 492 8017	−5.428 230 8549
13	1.370 585 5768	3.035 139 6179	−5.537 957 7909
14	1.400 025 9948	3.024 301 1471	−5.644 157 3273
15	1.427 788 3021	3.014 692 0985	−5.747 141 7316
16	1.454 081 5354	3.006 097 2338	−5.847 179 9733
17	1.479 076 0860	2.998 350 6266	−5.944 506 0171
18	1.502 912 3047	2.991 322 1911	−6.039 322 3775
19	1.525 708 7644	2.984 907 8837	−6.131 811 4731

discussion at the end of section 2 and observe that our results support scaling (31) and not scaling (30). Thus sequences based on classical amplitudes $\bar{m}_n$, such as (11) or (49), could, but not necessarily, approach in the limit the true critical exponent β. The situation seems worse if we apply (54*c*) to our data for $\bar{m}'_n$. In this case the sequence for $B_{\bar{m}'}$ (not shown) exhibits an erratic behaviour around a value 0.26 with a very slow tendency to increase for $n>14$. However, the estimates for $B_{\bar{m}'}$ do not seem to tend to the value 0.3084 . . . which will be in accord with (48) and give the true critical exponent. To clarify completely this situation and its consequences for the scaling laws (30) and (31) further study would be required, but a convincing explanation will be given below.

To overcome the 'erratic' behaviour of the classical amplitudes we suggest an improvement of the asymptotic relation (48), i.e. we assume that

$$\bar{m}'_n \sim n^{\mu} m(n, T^*_c). \tag{59}$$

In fact our data support (59) with $\mu=0.25$. The asymptotic relations (54*a*), (54*b*) and (59) may now be used in order to accelerate the convergence of sequences (50) and (49). Details of the necessary modifications are given in appendix 1. It is shown there, that sequence (50) can be replaced by an equivalent sequence (A.1*a*) which shows a very fast convergence (see table A1) to the true critical exponent. Now, in connection with sequence (49), based on the classical amplitudes, there is also defined in appendix 1 a modified sequence (A.2*b*) which is included in table (A2) together with sequence (49).

A major improvement is observed for the new sequence (A.2*b*) and the three extrapolations seem now to point to the same value, namely, the true critical exponent β. Thus we may conclude that all sequences of β-estimates defined in this paper tend to the true value of the critical exponent and the apparently 'erratic' behaviour of the sequences based on the classical amplitudes is an effect of the combination of the power law in (59) with the exponential laws in (54).

We close this section by pointing out that the asymptotic formulae (59) and (54*b*) with the help of (47), (54*a*) and (55) determine the functional dependence of $\bar{m}_n$ on n.

From (35) one can specify the asymptotic behaviour of an arbitrarily introduced function $\bar{g}(n)$

$$\bar{g}(n) \sim n^{2/3} \exp[B_t^{1/2} n^{1/2}]. \tag{60}$$

The function $\bar{f}(n)$ is specified by requirement $\bar{f}(n) \sim \bar{g}(g)^{-\beta}$ which produces the true critical exponent from scaling (31).

5. Conclusions

In the present paper we have reformulated the 'mean-field scaling theory' in a way that seems very well directed to Baxter's variational approximations.

It has been shown that the approximate critical temperatures, $T_{c,n}$, and spontaneous magnetization at the exact critical point, $m(n, T_c^*)$, both obey, in an almost perfect way, similar exponential laws from which the true critical exponent β can be obtained with impressive accuracy. The situation is more complex for the classical amplitudes and the corresponding estimates are slowly converging. However, our analysis conclusively supports the coherent-anomaly method of Suzuki [4–7].

Thus the present paper adds a surprising and unexpected element of generality in the mean-field finite-size scaling theory of Suzuki [4] by showing that 'exponential-law' scaling is possible when the 'canonical approximations' approach the critical point faster than any power law. It is not known whether this novel feature is a peculiar characteristic of Baxter's variational approximations, but one should now suspect that other sequences of mean-field approximations (obtained self-consistently) may as well show up similar novel features. The resulting behaviour seems to be in contradiction with finite-size scaling, and until a well founded explanation is given, one should be careful in interpreting the 'order of approximation' simply as the size of a 'finite system'. One should always have in mind that mean-field theories may crucially depend on the way self-consistency is applied.

However, if the occurrence of these 'perfect exponential laws' is not a coincidence but a general feature of Baxter's series, then the proposed method may prove to be the most efficient tool for calculating non-classical exponents. This hope is supported by our earlier observation that several significant figures of β could be obtained using only the first 5 or 6 variational approximations. It is well known that several variational approximations can be generated for a variety of unsolved problems [3] for which, of course, Tsang's reduction of the number of equations does not apply. We are currently applying the idea of this paper to the Ising model with second-neighbour interaction where the critical exponent β is known by universality. This may well be a necessary step in order to establish the generality of the exponential laws observed in Baxter's variational sequence and may also provide guidance to additional difficulties that may be encountered in other problems in which a convenient t-representation is not available.

Finally, we mentioned that Tsang [8] used log–log plots of $\log m(n, t)$ versus $\log \tau_n(t)$ in order to estimate the critical exponent β. This method shows very well a crossover phenomenon but it has not been clarified whether and how one could obtain from these plots a systematic series of estimates converging to the true value of the critical exponent.

Table A1. Sequences of estimates for the critical exponent β as defined in (50) and (A.1). Note the fast convergence of the modified sequence $\tilde{\beta}'_{m^*}$. Three cases of the extrapolation algorithm (51) are given.

Order	β'_{m^*}	$\tilde{\beta}'_{m^*}$
3	0.103 408 998 550 813	0.116 183 827 099 838
4	0.114 909 887 467 937	0.123 215 401 892 822
5	0.118 375 550 811 812	0.124 512 880 719 431
6	0.119 978 593 514 722	0.124 840 926 297 178
7	0.120 916 102 334 786	0.124 941 369 226 117
8	0.121 542 293 165 194	0.124 976 389 784 199
9	0.121 995 372 547 265	0.124 989 819 619 462
10	0.122 340 673 097 077	0.124 995 362 803 963
11	0.122 613 546 184 953	0.124 997 789 838 923
12	0.122 835 052 858 757	0.124 998 905 532 819
13	0.123 018 650 101 289	0.124 999 439 919 981
14	0.123 173 398 293 576	0.124 999 705 063 426
15	0.123 305 648 952 527	0.124 999 840 718 481
16	0.123 419 999 766 907	0.124 999 912 025 329
17	0.123 519 867 138 467	0.124 999 950 419 803
18	0.123 607 845 757 691	0.124 999 971 543 662
19	0.123 685 943 193 266	0.124 999 983 394 271
20	0.123 755 737 868 767	0.124 999 990 161 384
$a_m=0$	0.124 736 379 476 796	0.124 999 997 205 088
	0.124 745 293 861 349	0.125 000 000 001 709
$a_m=1$	0.124 700 654 383 830	0.124 999 999 974 519
	0.124 703 207 263 248	0.124 999 999 888 064
a_m from (52)	0.124 861 315 447 512	0.124 999 999 960 884
	0.124 858 373 496 780	0.125 000 000 000 927

Appendix 1. On the convergence of β-estimates

As mentioned in section 4, the convergence of the sequences estimating the critical exponent β (such as (11), (24), (49) and (50)) is rather slow. We present here modifications of these sequences which have the effect of accelerating their convergence. These modifications are inspired from the asymptotic forms (54) and (59). First we replace sequence (50) by

$$\tilde{\beta}'_{m^*}(n+1,n)=\frac{\log[m(n+1,T_c^*)/m(n,T_c^*)]}{\delta_{n+1}\log\tilde{t}_{c,n+1}-\delta_n\log\tilde{t}_{c,n}} \qquad (A.1a)$$

where

$$\tilde{t}_{c,n}=t_{c,n}/A_t \qquad (A.1b)$$

and the correction factors δ_n will be chosen to depend on $\tilde{t}_{c,n}$ in such a way that the new sequence (A.1) will have the same limit as sequence (50). A general condition for this requirement is, of course

$$\lim_{n\to\infty}\frac{\delta_{n+1}\log\tilde{t}_{c,n+1}-\delta_n\log\tilde{t}_{c,n}}{\log(t_{c,n+1}/t_{c,n})}=1. \qquad (A.1c)$$

Table A2. Sequences of estimates for the critical exponent β as defined in (49) and (A.2*b*). Note the major improvement achieved by the assumption (59) which implies the modification of (49) to (A.2). The three extrapolations point now to the true value.

Order	$\beta'_{\bar{m}'}$	$\hat{\beta}'_{\bar{m}'}$
3	0.004 566 623 209 540	0.046 718 103 996 983
4	0.047 943 670 620 345	0.093 684 547 901 027
5	0.063 396 501 393 298	0.107 157 95 1266 711
6	0.071 606 863 104 235	0.112 958 557 893 882
7	0.076 989 254 944 916	0.116 120 166 18 5780
8	0.080 929 203 457 131	0.118 099 687 738 533
9	0.084 001 633 682 103	0.119 450 225 367 539
10	0.086 495 839 637 807	0.120 425 546 023 690
11	0.088 577 888 284 282	0.121 158 780 506 393
12	0.090 352 178 564 940	0.121 726 826 232 027
13	0.091 888 710 065 085	0.122 177 347 854 357
14	0.093 236 696 393 774	0.122 541 504 800 205
15	0.094 432 014 339 612	0.122 840 525 946 662
16	0.095 501 579 06 1906	0.123 089 359 928 759
17	0.096 466 060 107 108	0.123 298 821 744 673
18	0.097 341 643 394 724	0.123 476 915 130 654
19	0.098 141 216 076 960	0.123 629 679 0 38 094
20	0.098 875 187 040 355	0.123 761 746 806 221
$a_m=0$	0.114 620 395 141 755	0.124 967 509 770 696
	0.114 631 724 475 007	0.124 967 547 328 187
$a_m=1$	0.112 868 157 807 973	0.124 921 171 906 689
	0.113 522 674 167 067	0.124 973 923 856 405
a_m from (52)	0.118 923 154 945 770	0.125 039 0170 00132
	0.125 115 263 333 392	0.125 039 157 855 336

The choices for these factors can be derived from the assumed asymptotic forms (54*a*) and (54*b*) and are

$$A_t \sim 32 \tag{A.1d}$$

$$\delta_n = (1 + C \log^{-2} \tilde{t}_{c,n})^{1/2} \tag{A.1e}$$

with

$$C = \frac{\Gamma_{m^*}}{\beta^2} - \Gamma_t \sim 7.402\,2033\ldots. \tag{A.1f}$$

Table A.1 contains sequence (50) and sequence (A.1). Since the asymptotic forms (54*a*) and (54*b*) are very well obeyed the new sequence (A.1) shows, as expected, as very fast convergence to the true critical exponent.

Finally, we modify sequence (49) introducing, as above, correction factors δ_n and taking (59) into account, i.e.

$$\beta_{\bar{m}'}(n+1, n) = \frac{\log[\bar{m}'(n+1)/\bar{m}'(n)]}{\delta_{n+1} \log \tilde{t}_{c,n+1} - \delta_n \log \tilde{t}_{c,n}} \tag{A.2a}$$

and

$$\hat{\beta}_{m'}(n+1, n) = \tilde{\beta}_{m'}(n+1, n) + \frac{0.25 \log(n/n+1)}{\delta_{n+1} \log \tilde{t}_{c,n+1} - \delta_n \log \tilde{t}_{c,n}}. \qquad (A.2b)$$

One can easily show that the correction term in (A.2b) will vanish as $n^{-1/2}$ and therefore the new sequence (A.2b) tends to the same limit as sequence (49).

Table A.2 contains sequence (49) and sequence (A.2) with the same assignments for the factors δ_n given in (A.1d–f). The improved sequence strongly suggests that the coherent-anomaly method of Suzuki [4–7], in spite of its slow convergence, also applies to the Baxter variational sequence.

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