Delta expansion at low temperatures

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In the low-temperature phase of a square Ising model, we describe the inverse temperature β as a function of the squared mass M and study the critical behavior of $\beta(M)$ via the large M expansion. Using the δ expansion by which the large mass expansion is transformed into a series exhibiting expected scaling behavior, we estimate the critical inverse temperature β_c with the help of a linear differential equation to be satisfied by the ansatz of $\beta(M)$. To improve the estimation accuracy, we independently estimate the leading correction exponent ν from $\beta^{(2)}/\beta^{(1)}$ and then use it to estimate β_c, which significantly improves the accuracy.

I. INTRODUCTION

The δ expansion introduced in [1] has been applied to various models and developed to the level that it is now effective in the estimation of critical exponents in the cubic Ising model [2]. Due to space-time discretization, the field theoretic and condensed matter models share a similar form of action and allow us to use similar method of calculations. The Boltzmann distribution usually takes the form of $\exp(-\beta H)$, where H means the energy function in a Euclidean lattice and β stands for inverse bare coupling for field theory models or inverse temperature in condensed matter models.

In models featuring separated phases, the playing field of the δ expansion has so far been limited to regions of small $\beta < \beta_c$, where β_c denotes the critical inverse temperature (or critical inverse coupling). In this study, we apply the δ expansion method to a system in the low-temperature phase for the first time. As an explicit example, we take up a 2D square Ising model. The square Ising model has a long history in the works of Ising, Onsager, Yang, and Lee, as well as many successors [3]. Making use of exact results, we explore the δ expansion applied to a new arena of the low-temperature phase. In this paper, we confine ourselves to the very basic points of δ expansion, such as the estimation of ν and β_c from low-temperature expansion. Specifically, we place emphasis on how to independently estimate ν to improve the β_c estimate.

This paper is organized as follows.: In section II, we introduce the estimation task by explaining low-temperature expansion and the basic strategy of our approach. In section III, we turn to the explicit estimation of β_c and the exponent ν, where we make an effort to improve the accuracy of the β_c estimation. We conclude in section IV with a brief summary.

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II. LOW-TEMPERATURE EXPANSION AND BASIC STRATEGY FOR ESTIMATION

The square Ising model is controlled by the Boltzmann distribution:

$$\exp(-\beta \sum_{<i,j>} s_i s_j), \qquad (2.1)$$

where the spin variable $s_n \in \{+1, -1\}$ is on the site n that composes the square lattice system. Here, $<i,j>$ means that sites i and j are the nearest neighbor pair and the summation should be taken over all nearest neighbor pairs.

As in the high-temperature phase, the squared mass is extracted from the two-point function at a large enough separation. At low temperature, there is non-vanishing magnetization per site, $\mathcal{M} = <s_0>$, and the two point function fluctuates around $\mathcal{M}^2$. At present, the large separation limit of the fluctuation is explicitly known for cases in which the two sites are on diagonal or parallel lines to axes [3, 4]. Here, we employ the latter case, the same as was considered in [5]. The correlation length ξ of the fluctuation is then known as [3, 4]

$$\xi^{-1} = \log(\tanh\beta) + 2\beta. \qquad (2.2)$$

At low enough temperatures, $\xi^{-1} = 2\beta - 2e^{-2\beta} - 2e^{-6\beta}/3 + \cdots$. Since for the application of δ expansion the corresponding mass squared M proves to be more convenient than ξ, we use M defined by [6]

$$M = 2(\cosh \xi^{-1} - 1). \qquad (2.3)$$

From (2.2) and (2.3), the squared mass M can be expanded as $M = e^{2\beta} - 4 + 3e^{-2\beta} + 4e^{-6\beta} + 4e^{-10\beta} + \cdots$. Then, inversion gives

$$\beta = \frac{1}{2}\log M + \frac{2}{M} - \frac{11}{2M^2} + \frac{68}{3M^3} - \frac{451}{4M^4} + \cdots. \qquad (2.4)$$

This is large mass expansion at low temperature. It differs compared to the high temperature case in that a logarithmic term of the mass squared exists as the leading contribution.

The behavior of $\beta(M)$ near the critical point $\beta_c = \log(1 + \sqrt{2})/2$, given from (2.2) by solving $\xi^{-1} = 0$, is easily derived

from (2.2) and (2.3). The result of expansion provides

$$\beta = \beta_c + \frac{M^{1/2}}{4}(1 - \frac{M}{24} + \frac{3M^2}{640} - \cdots) + R, \qquad (2.5)$$

where R denotes the analytic background given by

$$R = \frac{M}{16\sqrt{2}}(1 - \frac{3M}{32} + \frac{19M^2}{1536} - \cdots). \qquad (2.6)$$

From the definition of critical exponent ν, $\xi \sim (\beta - \beta_c)^\nu$ and $\beta - \beta_c \sim M^{1/2\nu}$. Then, we find from (2.5) that $\nu = 1$.

The motivation behind our recent series of works is to pave the way for a new quantitative computational method of critical behaviors from simply accessible series expansions, such as high- and low-temperature expansions. The δ-expansion [1, 5] provides us with a new way of handling the series and enables the estimation of critical quantities. Suppose a given truncated expansion of $f(M)$ to the order N, $f(M) = \sum_{n=0}^{N} a_n (1/M)^n$. The minimal result of δ-expansion needed in this study is that it induces transformation summarized as

$$D_N[M^{-\lambda}] = C_{N,\lambda} t^\lambda, \qquad (2.7)$$

where

$$C_{N,\lambda} = \frac{\Gamma(N+1)}{\Gamma(\lambda+1)\Gamma(N-\lambda+1)}. \qquad (2.8)$$

Here, D_N means the transformation that is N dependent. Note that $D_N[1] = 1$ and $D_N[M^\ell] = 0$ for positive integer ℓ. Then, we have

$$D_N[f] =: \bar{f}(t) = \sum_{n=0}^{N} C_{N,n} a_n t^n. \qquad (2.9)$$

The coefficients are dependent on the truncation order N. In the examples investigated so far, it is numerically verified that $\bar{f}(t)$ recovers in its effective region the small M behavior of $f(M)$ [7].

In the low-temperature phase, $\beta(M)$ at large M involves $\log M$ as manifested in (2.4). The transformation rule of the logarithmic function can also be drawn from (2.7). For instance, putting $\lambda = \varepsilon$ and expanding in ε and the comparison of coefficients of ε in the result, we find

$$D_N[\log M] = -\log t - \sum_{n=1}^{N} \frac{1}{n}. \qquad (2.10)$$

In what follows, we use notation $f_>$ for the series expansion of f at large M. Expansion at small M is denoted as $f_<$. The transformed series follows the same notation. For example, we obtain

$$D_N[\beta >] =: \bar{\beta}_>(t) = \frac{1}{2}(-\log t - \sum_{k=1}^{N} \frac{1}{k})$$
$$+ C_{N,1} 2t - C_{N,2} \frac{11}{2} t^2 + C_{N,3} \frac{68}{3} t^3 - \cdots, (2.11)$$

where the last term is $const \times t^N$. We now see the behaviors of $\bar{\beta}_>$ and its derivatives with respect to $\log t$ in Fig. 1. From the
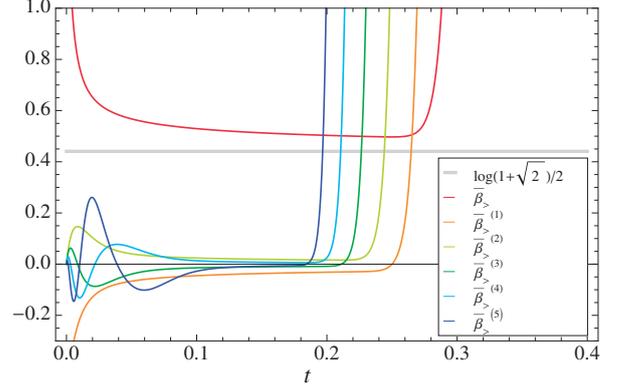

FIG. 1. The plots of $\bar{\beta}_>$ at $N = 25$ and its derivatives with respect to $d/d\log t$ to the 5th order. The gray line indicates $\beta_c = \log(1 + \sqrt{2})/2 = 0.4406867935\cdots$.

plots, we find that $\bar{\beta}_>$ gradually approaches β_c but the speed of convergence is too slow. This is because $M^{1/2\nu}$ exists in the second place of the expansion (2.5). If we could effectively subtract the correction terms, an accurate estimation of β_c would be possible. This strategy is conveniently carried out by setting up the differential equation approximately satisfied by $\beta_<$ [2, 5].

Suppose we have no information on the exponents and let $\beta_< = \beta_c + \sum_{n=1} A_n M^{\lambda_n}$. Then, the δ-expansion to order N is given by

$$\bar{\beta}_< = \beta_c + \sum_{n=1} C_{N,-p_n} A_n t^{-p_n}. \qquad (2.12)$$

Here, the set of exponents $\{p_n\}$ is the subset of $\{\lambda_n\}$ obtained from removing the integer ones (Note that $D_N[M^\ell] = 0$, $(\ell = 1, 2, 3, \cdots)$. The analytic part R thus becomes negligible.). Truncating the summation at order K in (2.12), the resulting series $\bar{\beta}_< = \beta_c + \sum_{n=1}^{K} C_{N,p_n} A_n t^{-p_n}$ is considered ansatz to the Kth order. It satisfies

$$\prod_{k=1}^{K}[1 + p_k^{-1} \frac{d}{d\log t}]\bar{\beta}_< = \beta_c. \qquad (2.13)$$

In this linear differential equation (LDE), the highest derivative order is K. If the transformed function $\bar{\beta}_>^{(K)}$ shows expected scaling, it is allowed to substitute $\bar{\beta}_>^{(n)}$ ($n = 0, 1, 2, \cdots, K$) into $\bar{\beta}_<^{(n)}$ included in the above LDE.

Now, in reality, LDE is only valid locally at a certain t due to the truncation of expansion. Then, at te^ε in the neighborhood of t, we have the following expansion:

$$\prod_{k=1}^{K}[1 + p_k^{-1} \frac{d}{d\log t}]\bar{\beta}(te^\varepsilon) = \prod_{k=1}^{K}[1 + p_k^{-1} \frac{d}{d\log t}]\beta(t)$$
$$+ \prod_{k=1}^{K}[1 + p_k^{-1} \frac{d}{d\log t}]\beta^{(1)}(t)\varepsilon$$
$$+ O(\varepsilon^2). \qquad (2.14)$$

A good adjustment of the values of unknown exponents $p_1, p_2, \cdots$ should make LDE approximately valid over a wide

region of a plateau indicating β_c. Thus, we employ the extended version of the principle of minimum sensitivity [8] (PMS) to fix the exponents and t at which β_c is estimated. The extended PMS reads

$$\prod_{k=1}^{K}[1+p_k^{-1}\frac{d}{d\log t}]\bar{\beta}_<^{(n)}=0 \qquad (2.15)$$

for various sets of n. In the above LDE, unknown variables are $(t;p_1,p_2,\cdots,p_K)$. Hence, we need $K+1$ equations to estimate all values. Then, the last LDE includes a $2K+1$th order derivative. At low orders, fewer derivatives exhibit scaling, and at large orders, derivatives to several orders are available. When the solution of the set $(t^*;p_1^*,\cdots,p_K^*)$ is obtained in the scaling region, we estimate β_c by

$$\prod_{k=1}^{K}[1+p_k^{-1}\frac{d}{d\log t}]\bar{\beta}_<\Big|_{(t^*;p_1^*,\cdots,p_K^*)}=\beta_c. \qquad (2.16)$$

This is the basic strategy utilized in our approach. A similar approach is taken for the estimation of ν and the improved estimation of β_c.

III. ESTIMATION

A. Naive estimation of β_c

In this subsection, we present our estimation study in the manner detailed in the previous section. In the protocol, we treat introduced exponents as adjustable ones to satisfy the extended PMS condition, which was adopted in [9]. Here, we call this protocol the naive protocol.

The number of exponents in ansatz (2.12) agrees with the order K of LDE (kLDE) to be imposed. At 1LDE, we use ansatz $\bar{\beta}_<=\beta_c+A_1M^{p_1}$ and impose $[1+p_1^{-1}(d/d\log t)]\bar{\beta}_<=\beta_c$. Then, we first consider

$$[1+p_1^{-1}(d/d\log t)]\bar{\beta}_<^{(k)}=0, \quad k=1,2. \qquad (3.1)$$

This set of LDEs includes derivatives to the 3rd order. By substituting $\bar{\beta}_>(t)$ into $\bar{\beta}_<(t)$, we obtain the solution of the set $(t^*;p_1^*)$. For details on the estimation process, see [5, 9]. Then, by substituting set $(t^*;p_1^*)$ into the left-hand-side of $[1+p_1^{-1}(d/d\log t)]\bar{\beta}_<=\beta_c$, we obtain the estimation of β_c, as suggested in (2.16). We also performed for 2- and 3-parameter ansatz the same estimation protocol to the 50th order. The result is given in Fig. 2 and summarized in Table I.

The scaling behavior of the left-hand side of LDE sets in at orders depending on the number of exponent parameters of ansatz (in this context, see [5, 9]). At $K=1$, it is no sharp transition for odd orders. For even orders, rough scaling behavior begins to appear from the 6th order. At $K=2$, the onset orders are 11th for odd orders and 14th for even orders. At $K=3$, the orders are 19th for odd N and 22nd for even N.

As expected, increasing the number of terms in the ansatz improves the accuracy. However, the reliability of estimates for each K actually depends on the order N of large mass expansion, as suggested just before by the concerned function's
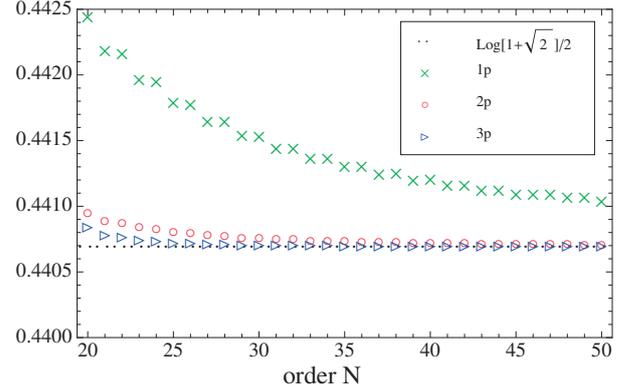

FIG. 2. Plots of naive estimation results with K-parameter ansatz where $K=1,2,3$.

behaviors. Although the convergence to the exact value of β_c is strongly indicated, at least with 2- and 3-parameters, we would still like to improve the accuracy. As in the high-temperature case demonstrated in [5], we turn to the estimation of ν and then revisit the estimation of β_c under the bias of the estimated ν.

B. Estimation of ν

As long as the order N of a large mass expansion is big enough, the estimation of $\nu=(2p_1)^{-1}$ is effective in the naive estimation discussed above. However, a precise value cannot be obtained at moderate orders. It seems that obtaining a precise value of p_1 would help to estimate β_c since the leading correction t^{-p_1} is effectively subtracted in LDE. To solve this problem, we consider the function $\beta^{(2)}/\beta^{(1)}=:f_\beta$, where $\beta^{(\ell)}(M)=(d/d\log M)^\ell\beta(M)$. From (2.5), we find the critical behavior

$$f_{\beta<}(M)=\frac{1}{2\nu}+\frac{M^{1/2}}{4\sqrt{2}}-\frac{3M}{16}+\cdots. \qquad (3.2)$$

The exponent p_1 appears as the leading term of the constant and its estimation may become accurate. Writing ansatz as $f_{\beta<}(M)=p_1+\sum_{k=1}B_kM^{q_k}$, we obtain its δ expansion, giving

$$\bar{f}_{\beta<}(t)=p_1+\sum_k C_{N,q_k}B_kt^{-q_k}. \qquad (3.3)$$

The truncated series at t^{-q_K} satisfies the following LDE:

$$\prod_{k=1}^{K}[1+q_k^{-1}\frac{d}{d\log t}]\bar{f}_{\beta<}=p_1. \qquad (3.4)$$

As in the previous section, the above LDE should be valid at certain t and the estimation of p_1 requires the optimal set $(t^*;q_1^*,\cdots,q_K^*)$. The set is determined by the extended PMS.

Now, we attempt to estimate p_1 from the large mass expansion obtained from (2.4)

$$f_{\beta>}(x)=\frac{4}{M}-\frac{28}{M^2}+\frac{208}{M^3}-\frac{1616}{M^4}+\cdots. \qquad (3.5)$$
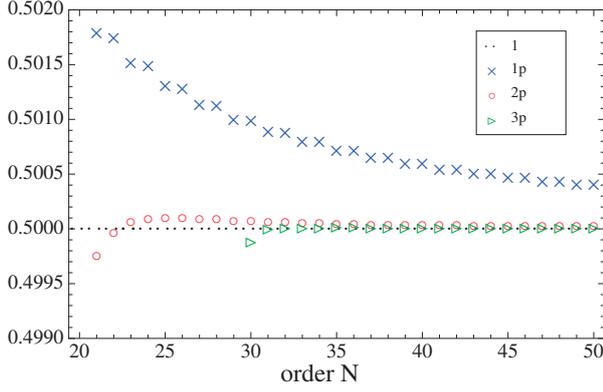
FIG. 3. Plots of $p_1 = 1/(2\nu) = 0.5$ estimate. 1p (2p, 3p) denotes the result in the 1 (2, 3)-parameter ansatz.

We substitute $\bar{f}_{\beta>}$ into $\bar{f}_{\beta<}$ in the derivatives of (3.4), $\prod_{k=1}^{K}[1 + q_k^{-1}(d/d\log t)]\bar{f}_{\beta<}^{(\ell)} = 0$ ($\ell = 1 \sim K + 1$). The solution determines the optimal set $(t^*; q_1^*, \cdots, q_K^*)$ and the substitution into (3.4) provides the p_1 estimate. The result is shown in Fig. 3 and summarized in Table II.

The quality of the series of $\bar{f}_\beta$ is lower than that of $\bar{\beta}$. In the 1-parameter ansatz, the orders at which the solution $(t^*; q_1^*)$ is found at the rough scaling region (we call such solutions gproperh) are 17th for odd order and 20th for even order. In the 2-parameter ansatz, the behavior characteristic to 2-parameter ansatz appears at the 19th (for odd) and the 20th (for even) orders and proper solution sets in from the 27th (for odd) and the 30th (for even) in the 3-parameter ansatz.

This quality difference affects the estimation accuracy at low orders. For the same given orders, the estimate from $\bar{f}_\beta$ is slightly more accurate than the estimate from $\bar{\beta}$. As the order grows, the estimate from $\bar{f}_\beta$ improves more and more. As for the relation between the accuracy and the number of parameters, a positive correlation is clearly confirmed. The main finding of this experiment is that the estimation of critical exponent ν is better in f_β.

C. Improved estimation of β_c

In this subsection, we experimentally investigate the best way to estimate β_c. In addition to the naive way presented in the subsection A, we here examine two ways: (i) using p_1 estimated from $\bar{f}_\beta$, with the rest of the exponents adjusted under the extended PMS as usual, and (ii) using exactly known values of exponents p_i for all exponents included in the ansatz. For example, at $K = 2$, we simply substitute $p_1 = 1/2$, $p_2 = 3/2$, and at $K = 3$, we substitute in addition $p_3 = 5/2$. This prescription supplies us the standard reference of estimation accuracy.

As shown in Fig. 4, in the 1-parameter cases, both prescriptions (i) and (ii) provide better estimates than the naive one, with (i) yielding the best estimates among the three. In the 2-parameter cases, we first note that the used p_1 value is the
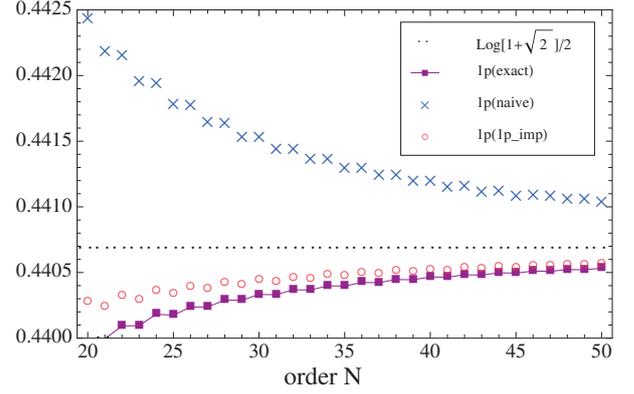

FIG. 4. Plots of β_c estimates. 1p (exact) means the result under the substitution $p_1 = 1/2$ (prescription (ii)). 1p (naive) means the result under the naive prescription. 1p (1p-imp) means the result under the substitution $p_1 = p_1^*$, where p_1^* is estimated in 1-parameter ansatz of $\bar{f}_{\beta<}$ (prescription (i)).
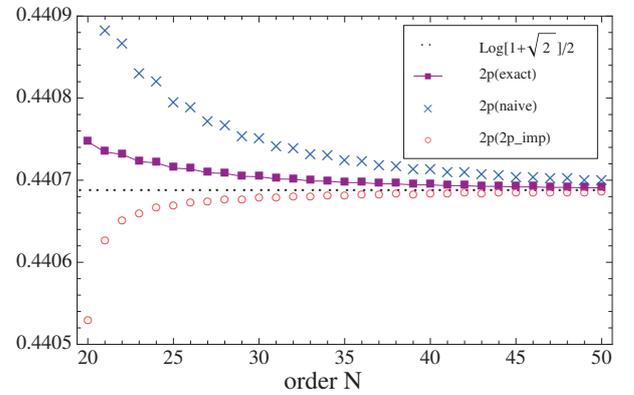

FIG. 5. Plots of β_c estimates. 2p (exact) means the result under substitution $p_1 = 1/2$ (prescription (ii)). 2p (naive) means the result under the naive prescription. 2p (2p-imp) means the result under the substitution $p_1 = p_1^*$, where p_1^* is estimated in the 2-parameter ansatz of $\bar{f}_{\beta<}$ (prescription (i)).

one from the 2-parameter ansatz of $\bar{f}_<$ (see Fig. 5). The result is that the whole trend is the same as that of the 1-parameter ansatz. Still, we note that prescription (i) becomes the best one from the 22nd order. In the 3-parameter cases, we examined two versions of prescription (i): one, using p_1 from the 2-parameter ansatz of $\bar{f}_<$, and two, using p_1 from the 3-parameter ansatz of $\bar{f}_<$. In the latter case, stable estimation sets in from the 30th order (see Fig. 6). In 2- and 3- parameter ansatz, prescriptions (i) and (ii) resulted in competing estimates, and numerical Table III is necessary for discussion.

From Table III, we find in the 2-parameter case that from moderate orders, or as the order grows higher, the best estimation is realized in prescription (i), where p_1^* at $K\nu = 2$ is substituted and p_2 is adjusted to satisfy extended PMS. A similar trend is observed in the 3-parameter case, though the 50th order is exceptional. Though the exact reason is not known,
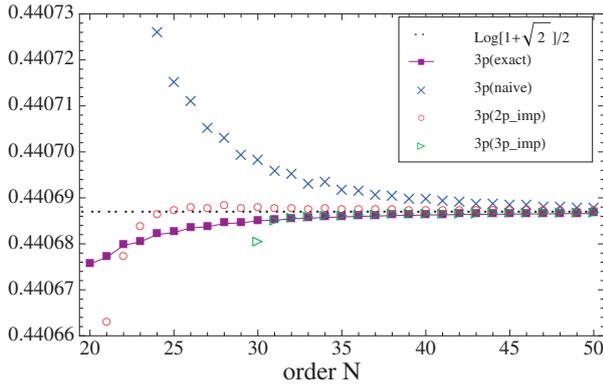
FIG. 6. Plots of β_c estimates. 3p (exact) means the result under substitution $p_1 = 1/2$ (prescription (ii)). 3p (naive) means the result under the naive prescription. 3p (kp-imp, $k = 1, 2$) means the result under substitution $p_1 = p_1^*$, where p_1^* is estimated in the k-parameter ansatz of $\bar{f}_{\beta<}$ (prescription (i)).

we can conclude that the best estimation does not come from the substitution of exact exponents in the ansatz; rather, the use of the leading exponent value obtained from $\bar{f}_\beta$ with ex-tended PMS provided the best results.

IV. SUMMARY

We performed the basic task of estimating critical quantities ν and β_c and demonstrated that the large mass expansion with δ expansion also works at the low-temperature phase. We also found that prescription (i), the substitution of leading correction exponent $p_1 = 1/(2\nu)$ estimated with $\bar{f}_\beta$ under extended PMS, provided better β_c value than naive estimation of β_c with extended PMS. Moreover, the (i)-prescription delivered better estimates than the prescription in which exact exponents in the ansatz are used. This sheds light on the accurate estimation of β_c in the cubic model presented in citeyam2.

Encouraged with the results thus far, we intend to attempt computation of the exponent of spontaneous magnetization $\mathcal{M}$ in the present approach and additional estimation of other critical quantities from the low-temperature phase. By these further studies on the method of large mass expansion with δ-expansion, its full aspects and power will be grasped. Such a thorough examination may stimulate the improvement of the method and help us to apply the method to more complicated and interesting physics models.

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	20	25	30	35	40	45	50
$K = 1$	0.44243483	0.44178017	0.44152678	0.44129454	0.44119466	0.44108312	0.44103340
$K = 2$	0.44093637	0.44079480	0.44075068	0.44072337	0.44071252	0.44070368	0.44069980
$K = 3$	0.44083163	0.44071513	0.44069812	0.44069176	0.44068964	0.44068834	0.44068783

TABLE II. K_ν- and K- parameter estimation results of $p_1 = 0.5$ via $\bar{f}_\beta$ and $\bar{\beta}$, respectively. At $K_\nu = 1$, a proper estimate appears from the 17th for odd orders and the 20th for even orders. At $K_\nu = 2$, a proper estimate appears from the 27th for odd orders and the 30th for even orders. At $K_\nu = 3$, a proper estimate appears from the 37th for odd orders and the 42nd for odd orders.

	20	25	30	35	40	45	50
$K_\nu = 1$	0.50208109	0.50129729	0.50098433	0.50071069	0.50058813	0.50045795	0.50039751
$K = 1$	0.51821317	0.51317267	0.51100350	0.50882559	0.50781555	0.50660710	0.50603627
$K_\nu = 2$	0.49843886	0.50008775	0.50006051	0.50003490	0.50002454	0.50001621	0.50001244
$K = 2$	0.50380104	0.50199096	0.50132581	0.50085852	0.50065241	0.50046897	0.50038216
$K_\nu = 3$			0.50058851	0.50000241	0.50000213	0.50000098	0.50000066
$K = 3$	0.50243597	0.50064853	0.50030467	0.50015361	0.50009665	0.50005811	0.50004131

TABLE III. Relative error $(\beta_{c,estimated}/\beta_c - 1)$ in 2- parameter estimation results of $\beta_c = 0.4406867935 \cdots$ via three prescriptions.

	20	25	30	35	40	45	50
Naive	0.00056634	0.00024509	0.00014498	0.00008301	0.00005839	0.00003832	0.00002952
Exact	0.00013657	0.00006330	0.00003965	0.00002339	0.00001698	0.00001135	0.00000893
$p_1(K_\nu = 2)$	-0.00035963	-0.00004278	-0.00002146	-0.00001539	-0.00000959	-0.00000751	-0.00000517

TABLE IV. Relative error $(\beta_{c,estimated}/\beta_c - 1)$ in 3- parameter estimation results of $\beta_c = 0.4406867935 \cdots$ via three prescriptions.

	20	25	30	35	40	45	50
Naive	0.000328649	0.000064305	0.000025697	0.000011261	0.000006458	0.000003519	0.000002342
Exact	?0.000025312	?0.000009856	?0.000003990	?0.000002217	?0.000001156	?0.000000759	?0.000000455
$p_1(K_\nu = 2)$	-0.000216960	0.000000710	0.000002244	0.000001161	0.000000944	0.000000567	0.000000464
$p_1(K_\nu = 3)$			-0.000014723	-0.000001518	-0.000000711	-0.000000483	-0.000000282