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Low-temperature series for the square lattice Potts model using the improved finite-lattice method

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Abstract. The low-temperature series are calculated for the free energy, magnetization and susceptibility in the Q -state Potts model on the square lattice, using the improved algorithm of the finite lattice method. The series are obtained to the order of z^{41} for each of $Q = 5$ –50, and the result of their Padé-type analysis is compared with those of the large- Q expansion and the Monte Carlo simulations.

1. Introduction

The finite-lattice method is a very efficient technique for generating the expansion series in statistical models [1, 2] and in lattice gauge theory [3]. In this method the expansion series for the free energy density in the infinite-volume limit is given by an appropriate linear combination of the free energies on finite-size lattices. The partition function of the finite-size lattices, from which the free energy of the lattices is obtained, can be calculated using the transfer matrix formalism [4]. This method avoids the problem involved in the graphical method, in which it is rather difficult to give the algorithm that lists all the diagrams that contribute to the relevant order of the series. The maximum order of the expansion series is determined by the maximum size of the lattices whose partition function can be calculated exactly to the order.

In the case of the model whose spin variable at each site takes many discrete values, however, one can only calculate the partition function of the finite-size lattices whose sizes are relatively small and it is difficult to obtain the series to such high orders as in the Ising model, in which the spin variable takes only two values. Recently Arisue [5] proposed an improved algorithm of the finite-lattice method, which enables one to obtain higher-order terms than the standard finite-lattice method in the spin systems whose spin variables take a large or infinite number of discrete values. It was applied to the low-temperature expansion for the free energy of the solid-on-solid (SOS) model and it enabled him to extend the series to the order of u^{23} [5] from the order of u^{12} that was obtained by using the standard finite-lattice method [6].

In this paper we apply this improved finite lattice method to the calculation of the low-temperature series for the free energy, magnetization and susceptibility in the Q -state Potts model on the square lattice. This system has the first-order phase transition for $Q \geq 5$ [7]. The values of the free energy, latent heat, and the gap of the specific heat and magnetization

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at the critical point are known exactly [8], while the exact values of the specific heat itself and the magnetic susceptibility at the critical point are not known yet. We calculate the series to the order of z^{41} for each $Q = 5-50$. We can extend the series from the ones calculated previously by Bhanot *et al* [9] and Briggs *et al* [10] by using the standard finite-lattice method, to substantially higher orders for large values of $Q \leq 10$, and our series for $11 \leq Q \leq 50$ have an order that is about three times higher than the ones given by Kihara *et al* [11] for general Q and zero field or by Straley and Fisher [12] for general Q and general field. We analyse the obtained series using the inhomogeneous differential approximants and their integration. It serves to check the validity of the series obtained and of the method of the analysis used for the quantities whose values are known exactly. On the other hand, it makes a new prediction for the quantities whose exact values are not known.

In section 2, we describe the improved algorithm of the finite-lattice method for the low-temperature expansion of the Q -state Potts model on the square lattice. The series obtained by the improved algorithm of the finite-lattice method are given in section 3. We present the analysis of the series in section 4. The result of our analysis is compared with those of the large- Q expansion and the Monte Carlo simulations. Our results are summarized in section 5.

2. Algorithm

Here we give the improved algorithm of the finite-lattice method for the low-temperature expansion of the Q -state Potts model on the square lattice, which enables us to obtain longer series than the standard finite-lattice method. Let us consider the two-dimensional $L_x \times L_y$ rectangular lattice Λ_0 . The free energy density in the infinite-volume limit is given by

$$f = - \lim_{L_x, L_y \rightarrow \infty} \frac{1}{L_x L_y} \ln [Z(\Lambda_0; Q)] \quad (1)$$

with

$$Z(\Lambda_0; Q) = \sum_{\{0 \leq s_i \leq Q-1\}} \exp \left[-\beta \sum_{(i,j)} (1 - \delta_{s_i, s_j}) - h \sum_i (1 - \delta_{s_i, 0}) \right] \quad (2)$$

where the integer variable s_i at each site, i , of Λ_0 is restricted to $0 \leq s_i \leq Q-1$. The low-temperature series is calculated with respect to the expansion parameter $z = \exp(-\beta)$. We take the boundary condition that all the variables outside Λ_0 are fixed to be zero.

We consider the set $\{\Lambda\}$ of all two-dimensional rectangular sublattices of Λ_0 . The sublattice Λ is denoted by its size $l_x \times l_y$ and its position in Λ_0 . We define a set of integers ξ_q that consist of no and $(q-1)$ integers among the set of integers $\{1, 2, \dots, Q-1\}$. We define the H of Λ and ξ_q as

$$H(\Lambda; \xi_q) = -\ln [Z(\Lambda; \xi_q)]. \quad (3)$$

In the calculation of the partition function $Z(\Lambda; \xi_q)$, the variable s_i at each site i inside Λ is restricted to be one of the elements of ξ_q , and all the variables outside Λ are fixed to be zero. We define W of Λ and ξ_q recursively as

$$W(\Lambda; \xi_q) = H(\Lambda; \xi_q) - \sum_{\substack{\Lambda' \subset \Lambda \\ \xi_{q'} \subset \xi_q}} W(\Lambda'; \xi_{q'}). \quad (4)$$

Here the prime in the summation \sum' implies that the $W(\Lambda' = \Lambda; \xi_{q'} = \xi_q)$ should be excluded when taking the summation. We note that the $H(\Lambda; \xi_q)$ and $W(\Lambda; \xi_q)$ depend on

the size of Λ but not on its position and depend on the value of q but not on the details of the elements of the ξ_q . So we denote them as $H(l_x \times l_y; q)$ and $W(l_x \times l_y; q)$, then we can rewrite equation (4) as

$$W(l_x \times l_y; q) = H(l_x \times l_y; q) - \sum_{\substack{l'_x \leq l_x, l'_y \leq l_y \\ 2 \leq q' \leq q}} (l_x - l'_x + 1)(l_y - l'_y + 1) \binom{q-1}{q'-1} W(l'_x \times l'_y; q'). \quad (5)$$

We know

$$H(L_x \times L_y; Q) = \sum_{\substack{l_x \leq L_x, l_y \leq L_y \\ q \leq Q}} (L_x - l_x + 1)(L_y - l_y + 1) \binom{Q-1}{q-1} W(l_x \times l_y; q). \quad (6)$$

Taking the infinite-volume limit we obtain

$$f = \lim_{L_x, L_y \rightarrow \infty} \frac{1}{L_x L_y} H(L_x \times L_y; Q) = \sum_{l_x, l_y, q \leq Q} \binom{Q-1}{q-1} W(l_x \times l_y; q). \quad (7)$$

The magnetization M and susceptibility χ are given from this free energy density, by

$$M = 1 - \frac{Q}{Q-1} \frac{\partial f}{\partial h} \quad (8)$$

and

$$\chi = \frac{\partial^2 f}{\partial h^2}. \quad (9)$$

In the practical calculation we introduce the variable $x \equiv \exp(h) - 1$ [13], then

$$\frac{\partial}{\partial h} \Big|_{h=0} = \frac{\partial}{\partial x} \Big|_{x=0} \quad (10)$$

and

$$\frac{\partial^2}{\partial h^2} \Big|_{h=0} = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial}{\partial x} \right) \Big|_{x=0} \quad (11)$$

and it is enough to evaluate the expansion series for the free energy density to second order in x in order to obtain the zero-field magnetization and susceptibility.

In the standard cluster expansion of free energy [14, 15] for this model, a cluster is composed of polymers and each of the polymers consists of the excited sites that are connected by nearest-neighbour bonds. An integer value $s_i \in \{1, 2, \dots, Q-1\}$ is put to each excited site i of the polymer. For each cluster we can define the subset of the set $\{1, 2, \dots, Q-1\}$ so that each element of this subset is found to be put on at least one of the excited sites of all the polymers the cluster is composed of. Then we can assign an integer \tilde{q} to the cluster so that $(\tilde{q}-1)$ is the number of the elements of the subset. We can prove [3] that the Taylor expansion of the $W(l_x \times l_y; q)$ with respect to z includes the contribution from all the clusters of polymers in the standard cluster expansion that have $\tilde{q} = q$ and that can be embedded into the $l_x \times l_y$ lattice but cannot be embedded into any of its rectangular sublattices.

So the series expansion of the $W(l_x \times l_y; q)$ starts from the order of $z^{n(l_x, l_y, q)}$ with $n(l_x, l_y, q)$ given as follows. It is enough to consider only $l_x \leq l_y$. We first define $k \equiv [(q-1)/(l_x l_y)]$, where we denote $[p]$ as the maximum integer that is less than p . In the case of $k = 0$ (namely $q-1 \leq l_x l_y$), the cluster that contributes to the lowest-order

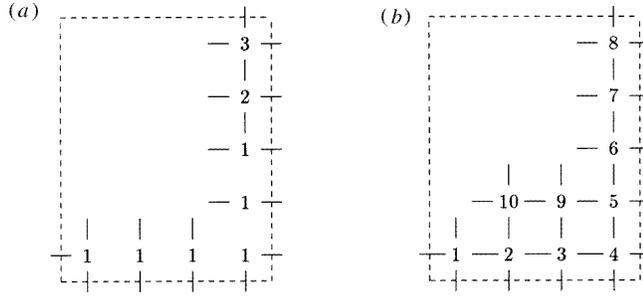


Figure 1. Examples of the cluster consisting of a single polymer ($k = 0$) that contributes to the lowest-order term of the expansion series for (a) $W(l_x = 4, l_y = 5; q = 4)$ and (b) $W(l_x = 4, l_y = 5; q = 11)$.

term of the expansion series of the $W(l_x \times l_y; q)$ consists of a single polymer. We know in this case that

$$n(l_x, l_y, q) = \begin{cases} 2(l_x + l_y) + q - 2 & \text{for } q \leq l_x + l_y \\ l_x + l_y + 2q - 2 & \text{for } q > l_x + l_y. \end{cases} \quad (12)$$

Examples of the clusters that correspond to these two cases in equations (12) and (13) are presented in figures 1(a) and (b), respectively. In the figures the integers denote the excited spin variables at the sites and the full lines represent the excited bonds. In the case of $k \geq 1$ (namely $q - 1 > l_x l_y$), the cluster that contributes to the lowest-order term is composed of $k + 1$ polymers, among which a polymer consists of $q' \equiv q - 1 - k l_x l_y$ sites and each of the other k polymers consists of the $l_x \times l_y$ sites. Then if $q' \leq l_x^2$

$$n(l_x, l_y, q) = \begin{cases} k\{l_x(l_y + 1) + (l_x + 1)l_y\} + 2q' + 2i + 1 & \text{for } q' \leq i(i + 1) \\ k\{l_x(l_y + 1) + (l_x + 1)l_y\} + 2q' + 2i + 2 & \text{for } q' > i(i + 1) \end{cases} \quad (14)$$

where $i \equiv [\sqrt{q'}]$. Examples of the clusters that correspond to these two cases in equations (14) and (15) are presented in figures 2(a) and (b), respectively. If $q' > l_x^2$

$$n(l_x, l_y, q) = k\{l_x(l_y + 1) + (l_x + 1)l_y\} + 2q' + 2l_x + j + 1 \quad (16)$$

where $j \equiv [(q' - l_x^2)/l_x]$. An example of the cluster that corresponds to equation (16) is presented in figure 2(c). To obtain the expansion series to the order of z^N , we should take into account all the combinations of l_x, l_y and q that satisfy $n(l_x, l_y, q) \leq N$ in the summation of equation (7) and should evaluate each of the W 's to the order of z^N .

We should stress that the improved algorithm described above enables us to calculate the series for large Q that is substantially longer than the case when one would apply the standard finite-lattice method naively [9, 10]. In the latter case one would define

$$\tilde{H}(\Lambda; \xi_Q) = -\ln[Z(\Lambda; \xi_Q)] \quad (17)$$

and

$$\tilde{W}(\Lambda; \xi_Q) = \tilde{H}(\Lambda; \xi_Q) - \sum_{\Lambda' \subset \Lambda} \tilde{W}(\Lambda'; \xi_Q) \quad (18)$$

for the rectangular $l_x \times l_y$ sublattice Λ . Here the variable s_i takes all integer values $0 \leq s_i \leq Q - 1$ for each site $i \in \Lambda$ in the calculation of the partition function $Z(\Lambda; \xi_Q)$. Then the free energy density in the infinite-volume limit would be given by

$$f = \sum_{l_x, l_y} \tilde{W}(l_x \times l_y; \xi_Q). \quad (19)$$

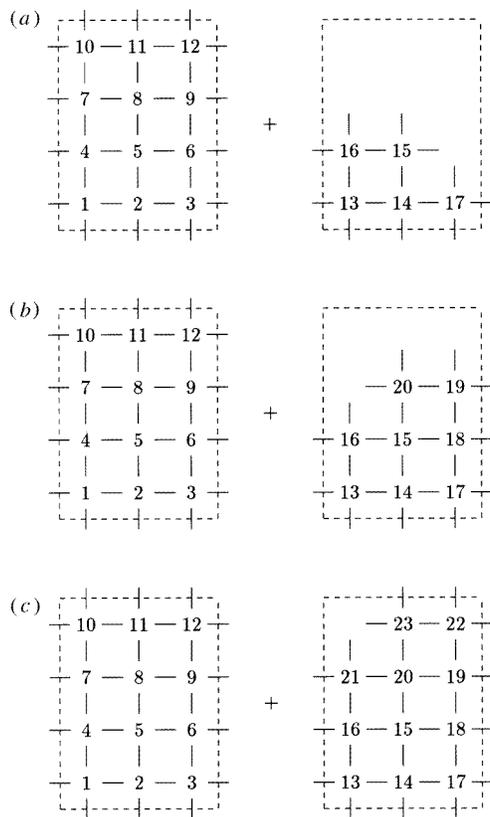


Figure 2. Examples of the cluster consisting of two polymers ($k = 1$) that contributes to the lowest-order term of the expansion series for (a) $W(l_x = 3, l_y = 4; q = 18)$, (b) $W(l_x = 3, l_y = 4; q = 21)$ and (c) $W(l_x = 3, l_y = 4; q = 24)$.

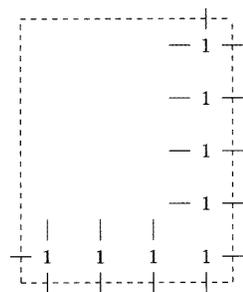


Figure 3. Examples of the cluster consisting of a single polymer that contributes to the lowest-order term of the expansion series for $\tilde{W}(l_x = 4, l_y = 5; \xi_Q)$.

The series expansion of this $\tilde{W}(l_x \times l_y; \xi_Q)$ starts from the order of $z^{2(l_x+l_y)}$. The clusters that give the contribution to this order are the clusters consisting of a single polymer, an example of which is depicted in figure 3. So for the series expansion to the order of z^N , one should take into account all the rectangular lattices that satisfy $2(l_x + l_y) \leq N$ in the summation of equation (19). The improved algorithm might appear to be more complicated

than this standard algorithm, since the former involves the summation with respect to q as well as the summation with respect to $l_x \times l_y$. The CPU time and memory for evaluating the partition functions of the finite-size lattices needed to obtain the series to the same order are, however, much smaller in the improved algorithm. In order to obtain the series to the order of z^{41} , for instance, we should calculate the partition functions up to the lattice-size of 10×10 either in the standard algorithm or in the improved algorithm. In the standard algorithm, the partition function with $q = Q$ is needed for this maximum size of the lattice. On the other hand, in the improved algorithm the partition function with $q = 2$ is enough for this size of the lattice.

3. Series

Using the improved algorithm of the finite-lattice method described in the previous section we have calculated the low-temperature series for the free energy density f , magnetization M and susceptibility χ in the zero field for the Potts model on the square lattice to the order of z^{41} for $Q = 5-50$. The coefficients obtained are listed in tables 1 and 2 only for $Q = 20$ and 50 , where we give the series for $z = \exp(f)$ instead of the free energy density f , as well as the series for the magnetization and susceptibility. If the reader would like to know the coefficients for the other values of Q , they can be obtained from the authors by E-mail or from the authors' web-site. The calculation was performed by FACOM-VPP500 at KEK (Tsukuba) and FACOM-VP2600 at Kyoto University Data Processing Center. The maximum size of the used main memory was about 500 Mbytes. We have checked that each of the $W(l_x \times l_y; q)$'s in equation (7) starts from the correct order of $z^{n(l_x, l_y, q)}$ described in the previous section.

The series were obtained previously by using the standard finite-lattice method by Bhanot *et al* [9] to the order of z^{25} for $Q = 8$ and by Briggs *et al* [10] to the order of z^{39} , z^{39} , z^{39} , z^{35} , z^{31} and z^{31} for $Q = 5-10$, respectively. The series were also calculated by Kihara *et al* [11] to the order of z^{16} for general Q and zero field and by Straley and Fisher [12] for general Q and general field to the order of z^{13} using the graphical method. The series coefficients we obtained here are consistent with the coefficients previously obtained by the authors cited.

We note that in the standard finite-lattice method the maximum order of the obtainable expansion series reduces when one increases the value of Q , while the improved algorithm enables us to calculate the series to the same order for all Q that are larger than or equal to some value. In fact, we can calculate the series to the order of z^{41} for an arbitrarily large $Q (> 17)$ using the $W(l_x, l_y; q)$'s that have been evaluated here to obtain the series to the order of z^{41} for $Q = 17$, although we have stopped it at $Q = 50$. This can be understood by noticing from equations (12)–(16) that the series expansion of the $W(l_x, l_y; q)$ for arbitrary l_x, l_y and q with $q > 17$ starts from an order that is higher than z^{41} and does not contribute to the expansion series to the order of z^{41} .

4. Analysis of the series

The Q -state Potts model with $Q > 4$ has a first-order phase transition. For the first-order phase transition, some important quantities, such as the susceptibility and specific heat, have finite values at the critical point, in contrast with the fact that these values are infinite for the second-order phase transition.

The infiniteness of the critical value for the second-order phase transition sometimes

Table 1. The low-temperature expansion coefficients for the free energy, magnetization and susceptibility for the $Q = 20$ square lattice Potts model.

| n | z | M | χ |
|-----|------------------------------------|--------------------------------------|---------------------------------------|
| 0 | 1 | 1 | 0 |
| 1 | 0 | 0 | 0 |
| 2 | 0 | 0 | 0 |
| 3 | 0 | 0 | 0 |
| 4 | 19 | -20 | 19 |
| 5 | 0 | 0 | 0 |
| 6 | 38 | -80 | 152 |
| 7 | 684 | -1 440 | 2 736 |
| 8 | -589 | 1 460 | -2 280 |
| 9 | 4 104 | -12 960 | 36 936 |
| 10 | 34 466 | -109 520 | 323 912 |
| 11 | -46 512 | 138 240 | -199 728 |
| 12 | 483 398 | -2 040 420 | 7 678 261 |
| 13 | 1 614 240 | -7 086 240 | 30 536 496 |
| 14 | -2 010 808 | 4 671 200 | -19 059 128 |
| 15 | 48 638 556 | -259 282 080 | 1 242 232 920 |
| 16 | 66 750 002 | -417 704 060 | 2 800 285 550 |
| 17 | 94 851 648 | -1 155 653 280 | 11 160 075 600 |
| 18 | 4 264 583 402 | -27 837 269 920 | 166 147 691 080 |
| 19 | 2 711 283 660 | -28 967 068 800 | 314 891 078 616 |
| 20 | 36 660 260 676 | -326 575 493 500 | 2 700 423 490 565 |
| 21 | 350 530 337 736 | -2 773 117 509 120 | 20 580 457 476 816 |
| 22 | 226 902 725 452 | -3 504 413 044 080 | 47 276 982 916 744 |
| 23 | 5 653 101 156 048 | -54 127 038 428 640 | 481 746 412 796 832 |
| 24 | 28 469 510 466 547 | -273 739 383 621 540 | 2 536 124 771 313 858 |
| 25 | 42 704 598 074 544 | -626 534 197 990 560 | 8 388 189 200 399 472 |
| 26 | 700 159 265 957 050 | -7 500 005 076 811 440 | 75 083 308 577 493 088 |
| 27 | 2 423 368 661 949 468 | -28 449 325 073 826 720 | 325 937 254 907 403 792 |
| 28 | 7 731 033 540 174 246 | -110 572 911 429 835 580 | 1 480 698 106 281 593 115 |
| 29 | 78 953 345 947 533 348 | -956 758 345 892 651 520 | 10 938 227 296 679 669 016 |
| 30 | 233 171 802 367 220 678 | -3 290 695 663 943 877 920 | 45 003 875 885 372 649 120 |
| 31 | 1 207 925 854 600 942 620 | -17 857 155 839 057 961 120 | 248 795 624 942 616 383 064 |
| 32 | 8 578 891 752 427 054 593 | -118 198 071 379 878 114 580 | 1 550 417 616 117 914 081 584 |
| 33 | 26 279 052 771 743 353 332 | -427 018 427 440 815 394 080 | 6 633 731 834 136 735 494 256 |
| 34 | 169 448 419 303 276 320 478 | -2 669 246 990 084 147 723 840 | 39 743 309 408 406 296 543 112 |
| 35 | 934 014 456 459 287 376 408 | -14 635 750 107 536 528 768 640 | 219 466 703 191 297 256 269 272 |
| 36 | 3 342 530 604 057 094 050 901 | -59 864 493 412 976 212 314 860 | 1 016 877 625 830 611 545 531 997 |
| 37 | 22 227 466 452 797 269 128 528 | -378 821 839 108 831 184 988 000 | 6 119 224 442 354 906 298 876 816 |
| 38 | 105 216 422 923 458 425 776 276 | -1 862 780 050 724 742 025 689 040 | 31 557 668 972 616 720 906 032 400 |
| 39 | 449 173 545 929 305 443 593 316 | -8 659 232 479 851 255 144 790 560 | 157 936 029 967 724 328 819 066 816 |
| 40 | 2 809 270 008 061 904 464 069 897 | -52 184 954 811 154 800 744 150 940 | 921 011 351 332 383 770 376 427 924 |
| 41 | 12 477 877 823 064 242 776 774 212 | -246 220 110 417 995 423 090 111 520 | 4 633 614 244 759 932 587 057 525 712 |

makes the analysis easier; if the physical quantity had a strong singularity, we would be able to determine the critical exponent with a satisfactory accuracy by the differential approximations such as the Padé analysis.

On the other hand, in the case of the first-order phase transition, we have to integrate the differential approximants to determine the critical amplitude. This integration, however, has a subtle problem discussed below, and as a result, we must choose the approximants carefully.

When analysing the expansion series, we use homogeneous or inhomogeneous first-order differential approximants [16], in which the approximants to a function $f(z)$ satisfy

$$Q_1(z)f'(z) + Q_2(z)f(z) = R(z). \tag{20}$$

Table 2. The low-temperature expansion coefficients for the free energy, magnetization and susceptibility for the $Q = 50$ square lattice Potts model.

| n | z | M | χ |
|-----|---------------------------------|------------------------------------|------------------------------------|
| 0 | 1 | 1 | 0 |
| 1 | 0 | 0 | 0 |
| 2 | 0 | 0 | 0 |
| 3 | 0 | 0 | 0 |
| 4 | 49 | -50 | 49 |
| 5 | 0 | 0 | 0 |
| 6 | 98 | -200 | 392 |
| 7 | 4704 | -9600 | 18816 |
| 8 | -4459 | 11150 | -20580 |
| 9 | 28224 | -86400 | 254016 |
| 10 | 659246 | -2019800 | 6003872 |
| 11 | -1025472 | 3225600 | -7018368 |
| 12 | 12281948 | -50077050 | 193485271 |
| 13 | 89987520 | -370953600 | 1510567296 |
| 14 | -162228808 | 567974000 | -886343752 |
| 15 | 3720812256 | -19045411200 | 92683335360 |
| 16 | 12381176822 | -67093148150 | 376836950000 |
| 17 | 4469044608 | -89631139200 | 1066326898560 |
| 18 | 895089855002 | -548225826800 | 3292683018720 |
| 19 | 1892364280800 | -13708568736000 | 107149526869056 |
| 20 | 13423422398316 | -111911089584250 | 924768638863685 |
| 21 | 206844895493376 | -1536698755564800 | 11106335245654656 |
| 22 | 478049132085952 | -4409226660382200 | 42663913301510704 |
| 23 | 5667428458933248 | -51068413852233600 | 452593396732200192 |
| 24 | 49346646734282527 | -435539546923202850 | 3808046989807658388 |
| 25 | 172491504405475584 | -1825893233439542400 | 19671214965561745152 |
| 26 | 1938967535168345710 | -19591446789689634600 | 194639282941507768168 |
| 27 | 13089424692665334048 | -135834659906560636800 | 1410212431991986624512 |
| 28 | 63921872954358377616 | -750734284293452018450 | 8836405252541575381155 |
| 29 | 628985731889425518048 | -7147786492756957612800 | 80157906305935393997376 |
| 30 | 3839485035589391850158 | -45982543354085211648800 | 55176352039729755084960 |
| 31 | 23463259463706802592160 | -302788074318283787164800 | 3888163728504881482313664 |
| 32 | 203694326578125205781552 | -2595462149212992934427950 | 32749085439406082880398944 |
| 33 | 1225877434229949054953952 | -1660699340819591568259200 | 224791274766846749241618696 |
| 34 | 8555010161977020587142598 | -120783311584253799401189600 | 1691607730655033745533673792 |
| 35 | 66800901314888122476718848 | -948877081581250695129561600 | 13374510959732980701033577152 |
| 36 | 41735480596924273677903151 | -6276444566058217793336109650 | 93992501752971816579399237857 |
| 37 | 3081300147534452125687872768 | -47482109079734479233388368000 | 725062658320307588405549126016 |
| 38 | 22520630415621757023630981256 | -353898756249751908192492010600 | 5251526378626835675327811477000 |
| 39 | 148545447485043078418570354656 | -2445977768521719097911967382400 | 39997172375744231349328962685056 |
| 40 | 1106109615352046378739786168307 | -1855945185458259101244861914850 | 308483818208942470837183549866604 |
| 41 | 7848119276197068664163827052832 | -135219203614185545984625196732800 | 2311827629935984338141853691434752 |

Here, $Q_1(z)$, $Q_2(z)$ and $R(z)$ are polynomials of the order of M_1 , M_2 , and M , respectively, which are determined so that equation (20) is satisfied to the order of z^N with N being the maximum order of the expansion series of the $f(z)$. If $R(z)$ is identically zero, the approximant is just the D-log Padé approximant.

To obtain the value of $f(z)$ at the critical point $z = z_c$, we must integrate the function $f'(z) = \{-Q_2(z)f(z) + R(z)\}/Q_1(z)$ from 0 to z_c . For the first order phase transition, the denominator $Q_1(z)$ of $f'(z)$ has in most cases a zero close to the critical point. The zero point is usually slightly above the critical point on the real axis of z . It is sometimes, however, below the critical point, in which case the integral of $f'(z)$ will diverge and we should abandon such an approximant. Even if the zero point is above the critical point, it is so close to the critical point that its subtle fluctuation makes the fluctuation of the critical value $f(z_c)$ rather large.

First, in order to examine the accuracy of the analysis of the series described above, we apply it to the free energy density f_c at the critical point ($z_c = 1/(1 + \sqrt{Q})$), the latent heat ΔU and the magnetization gap ΔM , whose exact values were obtained by Baxter [8]. In table 3 the estimates of the free energy density, latent heat and magnetization gap from the longest series ($N = 41$) are presented for $Q \geq 7$, and their exact values are in parentheses. These estimates obtained by the analysis of the series may contain errors due to two reasons: one of them is the statistical fluctuation among the approximants with the different orders M_1 , M_2 and M of the polynomials $Q_1(z)$ and $Q_2(z)$ in equation (20) but with the same order N of the original series. About these statistical errors we find two common tendencies. (i) If the order M is too large, the convergence of the approximants

Table 3. Estimates of the free energy density f_c , the latent heat ΔU and the magnetization gap ΔM .

| Q | f_c | ΔU | ΔM |
|-----|--|---|---|
| 7 | $-0.043\,0048 \pm 0.000\,0024$ ($-0.043\,1119$) | $0.357\,20 \pm 0.008\,83$ ($0.353\,28$) | 0.7681 ± 0.0060 ($0.749\,565$) |
| 8 | $-0.039\,2927 \pm 0.000\,0055$ ($-0.039\,3533$) | $0.490\,58 \pm 0.001\,93$ ($0.486\,36$) | 0.8080 ± 0.0056 ($0.799\,837$) |
| 9 | $-0.036\,0255 \pm 0.000\,0044$ ($-0.036\,0805$) | $0.603\,75 \pm 0.002\,19$ ($0.599\,67$) | 0.8394 ± 0.0020 ($0.833\,261$) |
| 10 | $-0.033\,2047 \pm 0.000\,0035$ ($-0.033\,2365$) | $0.698\,32 \pm 0.001\,82$ ($0.696\,05$) | 0.8605 ± 0.0020 ($0.857\,107$) |
| 11 | $-0.030\,7291 \pm 0.000\,0024$ ($-0.030\,7586$) | $0.780\,47 \pm 0.000\,57$ ($0.778\,60$) | $0.877\,46 \pm 0.000\,72$ ($0.875\,107$) |
| 12 | $-0.028\,5722 \pm 0.000\,0025$ ($-0.028\,5900$) | $0.851\,22 \pm 0.000\,27$ ($0.849\,94$) | $0.890\,53 \pm 0.000\,47$ ($0.888\,878$) |
| 13 | $-0.026\,6652 \pm 0.000\,0023$ ($-0.026\,6817$) | $0.913\,16 \pm 0.000\,29$ ($0.912\,16$) | $0.901\,14 \pm 0.000\,32$ ($0.899\,999$) |
| 14 | $-0.024\,9831 \pm 0.000\,0021$ ($-0.024\,9931$) | $0.967\,56 \pm 0.000\,12$ ($0.966\,89$) | $0.909\,89 \pm 0.000\,25$ ($0.909\,086$) |
| 15 | $-0.023\,4812 \pm 0.000\,0018$ ($-0.023\,4908$) | $1.015\,966 \pm 0.000\,090$ ($1.015\,414$) | $0.920\,94 \pm 0.001\,24$ ($0.916\,664$) |
| 16 | $-0.022\,1416 \pm 0.000\,0018$ ($-0.022\,1471$) | $1.059\,128 \pm 0.000\,067$ ($1.058\,749$) | $0.923\,51 \pm 0.000\,18$ ($0.923\,075$) |
| 17 | $-0.020\,9338 \pm 0.000\,0015$ ($-0.020\,9393$) | $1.098\,023 \pm 0.000\,054$ ($1.097\,700$) | $0.928\,88 \pm 0.000\,012$ ($0.928\,570$) |
| 18 | $-0.019\,8439 \pm 0.000\,0013$ ($-0.019\,8486$) | $1.133\,140 \pm 0.000\,041$ ($1.132\,916$) | $0.933\,58 \pm 0.000\,12$ ($0.933\,332$) |
| 19 | $-0.018\,8560 \pm 0.000\,0011$ ($-0.018\,8594$) | $1.165\,129 \pm 0.000\,038$ ($1.164\,923$) | $0.937\,683 \pm 0.000\,094$ ($0.937\,499$) |
| 20 | $-0.017\,9567 \pm 0.000\,0010$ ($-0.017\,9586$) | $1.194\,298 \pm 0.000\,036$ ($1.194\,155$) | $0.941\,318 \pm 0.000\,008$ ($0.941\,176$) |
| 30 | $-0.012\,0422 \pm 0.000\,0004$ ($-0.012\,0425$) | $1.390\,466 \pm 0.000\,011$ ($1.390\,442$) | $0.962\,987 \pm 0.000\,006$ ($0.962\,963$) |
| 40 | $-0.008\,9727 \pm 0.000\,0002$ ($-0.008\,9727$) | $1.498\,232 \pm 0.000\,008$ ($1.498\,224$) | $0.972\,980 \pm 0.000\,004$ ($0.972\,930$) |
| 50 | $-0.007\,1096 \pm 0.000\,0001$ ($-0.007\,1096$) | $1.567\,525 \pm 0.000\,003$ ($1.567\,522$) | $0.978\,726 \pm 0.000\,001$ ($0.978\,723$) |

is not so good, and if the orders M_1 and M_2 are too small, the integral of $f'(z)$ diverges frequently, therefore we restrict the order M to be $M = -1$ (D-log Padé approximant) or $M = 0-6$ (inhomogeneous differential approximants) and the orders M_1 and M_2 to satisfy $|M_1 - M_2| \leq 10$. (ii) For smaller Q , some approximants are finite at the critical point but apparently far from the exact value, then we must exclude them. We present only the statistical errors in table 3. The other error is from the finiteness of the series. If there is a discrepancy between an estimate for the finite series and the corresponding exact value beyond the statistical error for each N , we may say that the discrepancy is caused by the finiteness of the series and the error arising from the finiteness of the series has the order of magnitude of this discrepancy.

Now, we present the result of the individual analysis for the free energy density, the latent heat and the magnetization gap.

For the free energy density f_c , both the inhomogeneous and homogeneous differential approximants give well converged results, the latter converging more excellently. The data

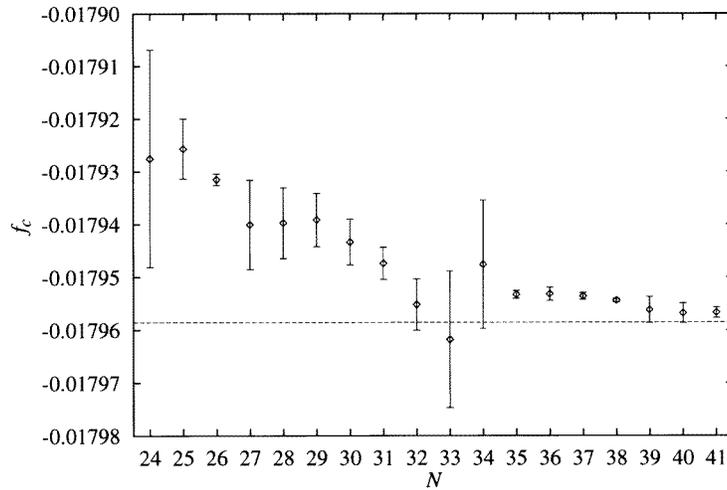


Figure 4. The estimates of the free energy density f_c for $Q = 20$ versus the number of terms of the series. The broken line shows the exact value.

in table 3 are from the latter. For $Q \gtrsim 30$, the estimates from the D-log Padé approximants agree with the exact value within one standard deviation. On the other hand, for $Q \lesssim 20$, the estimates are larger than the exact value, and do not agree with it within one standard deviation. As an example, in figure 4, we present a plot of the estimates for $Q = 20$ versus the number, N , of terms of the truncated series. The difference between the estimates and the exact value is about 0.01% while the fluctuation of the approximants is about 0.005%, the former is about two times larger than the latter. The ratio of the difference between the estimate and the exact value to the statistical fluctuation becomes larger for smaller Q . Nevertheless, the figure also exhibits the tendency that the difference between the estimates and the exact value decreases when the number of terms increases. (We should mention that the errorbars for $35 \leq N \leq 38$ are relatively small. It is because, for these N , some approximants have divergent integral of $f'(z)$ and the remaining fewer approximants happen to be very close.) Therefore, this difference can be expected to shrink for longer series. It would, however, be difficult to extrapolate the data to $N \rightarrow \infty$ to estimate the exact value, if it were not known, since we do not know what asymptotic behaviour the approximants should follow with respect to N .

For latent heat, the inhomogeneous differential approximants give more convergent results than the D-log Padé approximants, in contrast with the case of the free energy density. Then, by using the inhomogeneous differential approximants, we can obtain about 60 estimates of the latent heat for each model with $Q \geq 7$. For $Q \gtrsim 40$, the estimates coincide with the exact value within one standard deviation. For $Q \lesssim 30$, although the estimates do not agree with the exact value within one standard deviation, we find that their difference becomes smaller as the number of terms of the expansion series gets larger and so we can say that the difference would disappear for long enough series, as in the previous case of the free energy density.

For the magnetization gap, about 10 estimates obtained by the D-log Padé approximants converge well for each Q , while those obtained by the inhomogeneous differential approximants do not. Although it does not agree with the exact value within one standard deviation, except for $Q \simeq 50$, the estimates themselves are very close to the exact value;

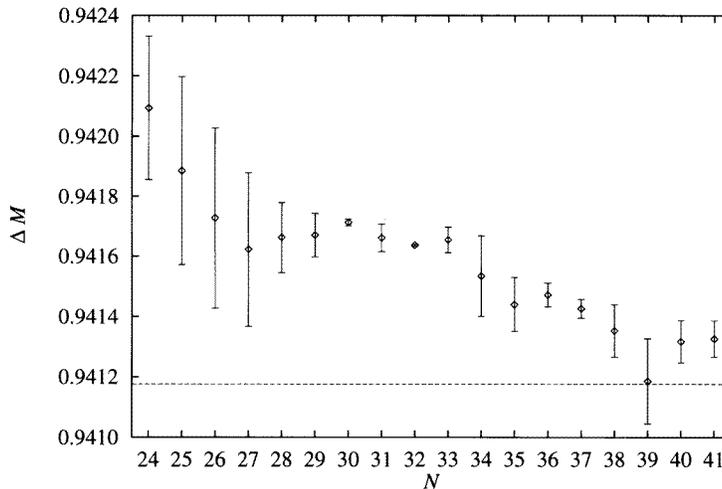


Figure 5. The estimates of the magnetization gap ΔM for $Q = 20$ versus the number of terms of the series. The broken line shows the exact value.

for example, in the case of $Q = 20$, the difference between the estimates and the exact value is about 0.015%. Further, figure 5 shows that the differences would disappear for a larger number of terms as well as in the case of the free energy density and the latent heat.

Now using the same method as above, we estimate the values of the susceptibility and specific heat at the critical point, whose exact values are not known.

The behaviour of the differential approximants for the susceptibility is like that for the magnetization gap. The D-log Padé approximants for the susceptibility show better convergence than the inhomogeneous approximants, although the errors of the estimates for the susceptibility are larger than those for the magnetization gap. The estimates from the longest series ($N = 41$) are listed in table 4, and our estimates for $7 \leq Q \leq 10$ are consistent with the estimates obtained by Briggs *et al* [10].

For $Q = 10, 15, 20$, Monte Carlo estimates are given by Janke and Kappler [22]. As their definition of the susceptibility is different from ours in the normalization factor, the results in [22] should be multiplied by a factor of $\{q/(q - 1)\}^2$ to fit into our definition. The estimates obtained in [22] are 3.777 ± 0.035 ($Q = 10$), 0.7052 ± 0.0033 ($Q = 15$) and 0.30242 ± 0.00050 ($Q = 20$). Our corresponding estimates are 2.78 ± 0.14 ($Q = 10$), 0.657 ± 0.017 ($Q = 15$) and 0.2938 ± 0.0036 ($Q = 20$). Although there are differences of more than one standard deviation, which are especially large for $Q = 10$, we may expect that the differences would disappear for larger Q .

For the specific heat, the estimates obtained by the D-log Padé approximants give good converging results, while the inhomogeneous differential approximants do not. We list the estimates from the longest series ($N = 41$) by the D-log Padé approximants in table 5. The errors of the estimates for the specific heat are smaller than those for the susceptibility. Nevertheless, our estimates for $7 \leq Q \leq 10$ are inconsistent with the estimates obtained by Briggs *et al* [10]. Therefore we should check the validity of our approximants in some way.

Fortunately, due to the duality relation [8], we can obtain the exact value of the gap of the specific heat as follows [8];

$$C_v^+ - C_v^- = \frac{\beta^2 \Delta U}{\sqrt{Q}}. \tag{21}$$

Table 4. Estimates of the susceptibility χ_c .

| Q | $\chi(z_c)$ |
|-----|----------------------|
| 5 | 154 ± 19 |
| 6 | 49.5 ± 4.1 |
| 7 | 19.0 ± 1.3 |
| 8 | 8.09 ± 0.29 |
| 9 | 4.55 ± 0.20 |
| 10 | 2.78 ± 0.14 |
| 11 | 1.900 ± 0.047 |
| 12 | 1.372 ± 0.026 |
| 13 | 1.036 ± 0.027 |
| 14 | 0.815 ± 0.019 |
| 15 | 0.657 ± 0.017 |
| 16 | 0.539 ± 0.016 |
| 17 | 0.4490 ± 0.0080 |
| 18 | 0.3844 ± 0.0061 |
| 19 | 0.3347 ± 0.0047 |
| 20 | 0.2938 ± 0.0036 |
| 30 | 0.1195 ± 0.0002 |
| 40 | 0.0697 ± 0.0002 |
| 50 | 0.0478 ± 0.00004 |

Table 5. Estimates of the specific heat.

| Q | C_v^- | C_v^+ | ΔC_v (series) | ΔC_v (exact) |
|-----|---------------------|---------------------|-----------------------|----------------------|
| 7 | 52.98 ± 0.61 | 68.01 ± 0.47 | 15.0 ± 0.76 | 0.2234 |
| 8 | 28.47 ± 0.47 | 30.17 ± 0.06 | 1.70 ± 0.48 | 0.3099 |
| 9 | 20.03 ± 0.27 | 20.87 ± 0.05 | 0.84 ± 0.27 | 0.3841 |
| 10 | 15.579 ± 0.083 | 16.294 ± 0.034 | 0.715 ± 0.090 | 0.4476 |
| 11 | 12.856 ± 0.061 | 13.493 ± 0.034 | 0.637 ± 0.070 | 0.5021 |
| 12 | 10.985 ± 0.050 | 11.622 ± 0.055 | 0.636 ± 0.074 | 0.5492 |
| 13 | 9.598 ± 0.032 | 10.258 ± 0.062 | 0.659 ± 0.070 | 0.5901 |
| 14 | 8.548 ± 0.027 | 9.204 ± 0.020 | 0.656 ± 0.034 | 0.6260 |
| 15 | 7.721 ± 0.028 | 8.388 ± 0.004 | 0.666 ± 0.029 | 0.6576 |
| 16 | 7.044 ± 0.011 | 7.739 ± 0.002 | 0.695 ± 0.011 | 0.6856 |
| 17 | 6.4908 ± 0.0086 | 7.2061 ± 0.0041 | 0.715 ± 0.010 | 0.7106 |
| 18 | 6.0251 ± 0.0074 | 6.7637 ± 0.0095 | 0.739 ± 0.012 | 0.7330 |
| 19 | 5.6317 ± 0.0061 | 6.3859 ± 0.0098 | 0.754 ± 0.012 | 0.7532 |
| 20 | 5.2913 ± 0.0053 | 6.0645 ± 0.0069 | 0.773 ± 0.009 | 0.7714 |
| 30 | 3.4012 ± 0.0010 | 4.2919 ± 0.0051 | 0.8906 ± 0.0052 | 0.8861 |
| 40 | 2.5864 ± 0.0006 | 3.5303 ± 0.0019 | 0.9439 ± 0.0020 | 0.9393 |
| 50 | 2.1218 ± 0.0004 | 3.0936 ± 0.0007 | 0.9717 ± 0.0008 | 0.9668 |

In table 5, we also list the estimates of the gap of the specific heat, where the specific heat C_v^+ is calculated using the high-temperature expansion series obtained from the low-temperature series by duality. It is clear that for $Q \geq 11$ there exists a gap of the specific heat and moreover almost all the estimated values of the gap of the specific heat coincide with the exact values given by equation (21) within the standard deviation. Therefore, we are convinced of the validity of our estimates for the specific heat.

Finally, we compare our estimates of the specific heat at the critical point with the estimates obtained from the large- Q expansion series that was recently obtained by

Table 6. Estimates of the specific heat: low-temperature series, large Q series and Monte Carlo simulations.

| Q | Low-temperature series | Large Q series | Monte Carlo simulations |
|-----|------------------------|-------------------------|--|
| 7 | 52.98 ± 0.61 | 69.6 ± 0.5 | 50 ± 10 [18] 47.5 ± 2.4 [20] 44.4 ± 2.2 [21] |
| 8 | 28.47 ± 0.47 | 36.9 ± 0.2 | |
| 9 | 20.03 ± 0.27 | 24.1 ± 0.2 | |
| 10 | 15.579 ± 0.083 | 17.98 ± 0.02 | 12.7 ± 0.3 [18] 17.81 ± 0.10 [22] |
| 11 | 12.856 ± 0.061 | 14.24 ± 0.05 | |
| 12 | 10.985 ± 0.050 | 11.84 ± 0.02 | |
| 13 | 9.598 ± 0.032 | 10.17 ± 0.01 | |
| 14 | 8.548 ± 0.027 | 8.939 ± 0.009 | |
| 15 | 7.721 ± 0.028 | 7.999 ± 0.003 | 8.004 ± 0.019 [22] |
| 16 | 7.044 ± 0.011 | 7.248 ± 0.004 | |
| 17 | 6.4908 ± 0.0086 | 6.643 ± 0.003 | |
| 18 | 6.0251 ± 0.0074 | 6.142 ± 0.002 | |
| 19 | 5.6317 ± 0.0061 | 5.720 ± 0.001 | |
| 20 | 5.2913 ± 0.0053 | 5.3612 ± 0.0004 | 5.2 ± 0.2 [18] 5.3612 ± 0.0055 [22] |
| 30 | 3.4012 ± 0.0010 | 3.41294 ± 0.00005 | |
| 40 | 2.5864 ± 0.0006 | 2.58986 ± 0.00002 | |
| 50 | 2.1218 ± 0.0004 | 2.123198 ± 0.000006 | |

Bhattacharya *et al* [17], and with the ones obtained from Monte Carlo simulations [18–22]. In table 6, we show our estimates of the specific heat again and the estimates obtained from the large- Q expansion series and the Monte Carlo simulations. For $Q = 7, 8, 10, 15, 20, 30$, the values of the estimates from the large- Q expansion are in [17], the others are calculated by using the regularized logarithmic Padé approximants given in [17]. Among the Monte Carlo results those of [22] have small statistical errors and they are consistent with the results of the large- Q expansion for $Q = 10, 15, 20$. Our estimates from the low-temperature series are systematically smaller than the estimates from the large- Q expansion. In figures 6 and 7, we present a plot of the estimates of the specific heat C_v^- for $Q = 20$ and $Q = 50$, respectively, versus the number N of the terms of the truncated series. We can see that the estimates are approaching the result of the large- Q expansion from below for each Q and that they approach faster for larger Q . Thus we can expect that, if we extrapolate the estimates in some way to $N \rightarrow \infty$ for each Q , we would obtain the estimates that may be more consistent with the result of the large- Q expansion, although we do not know how to make the extrapolation correctly, as mentioned above.

5. Summary

We obtained the low-temperature series for the free energy, magnetization and susceptibility of the Potts model on the square lattice.

Using an improved algorithm of the finite lattice method, we extended the series from those given by the standard algorithm of the finite lattice method. Our improved algorithm is more efficient for the higher-state Potts models.

Using the new series, we calculated the critical values of the free energy density, latent heat, magnetization gap, susceptibility and specific heat.

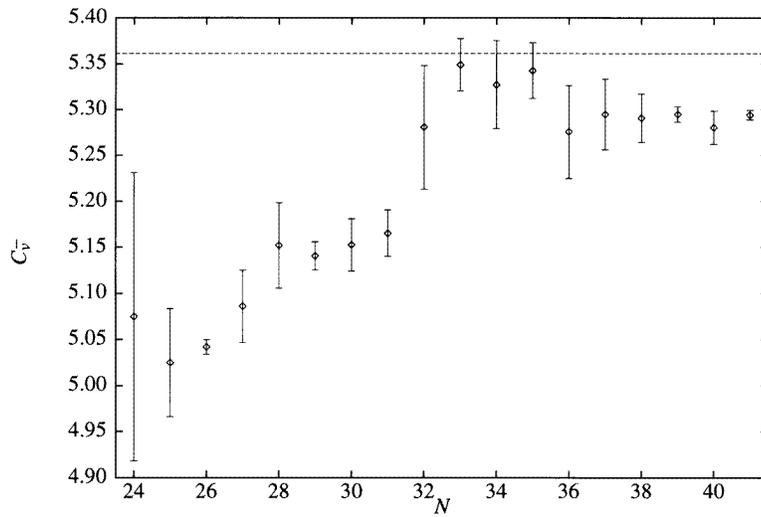


Figure 6. The estimates of the specific heat C_v^- for $Q = 20$ versus the number of terms of the series. The broken line shows the estimates obtained from the large- Q expansion series by using the regularized logarithmic Padé approximants.

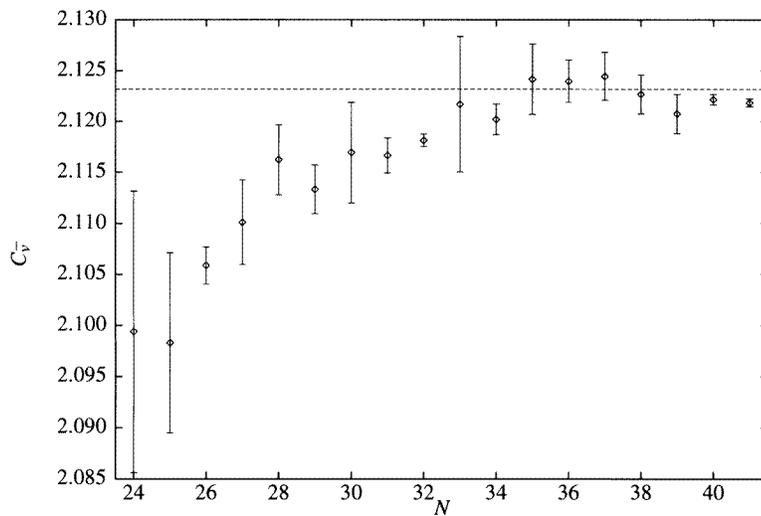


Figure 7. The estimates of the specific heat C_v^- for $Q = 50$ versus the number of terms of the series. The broken line shows the estimates obtained from the large- Q expansion series by using the regularized logarithmic Padé approximants.

The estimated values of the former three are very close to the known exact values. The values of the latter two, which are not known exactly, are obtained for various Q with high precision. Especially, the estimates of the specific heat are very close to the estimates from the large Q expansion series.

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