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Critical point of the Kagomé Potts model: a Monte Carlo renormalization group and scaling determination

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Abstract. The determination of the critical point of the q-state Potts model on the Kagomé lattices has been an outstanding unsolved problem. Here we study this problem by regarding the Potts model as generating correlated bond percolations. By applying a combination of Monte Carlo renormalization group and finite-size scaling analyses to the percolation problem, numerical estimates with an accuracy of 0.01% are obtained for the Kagomé critical point for $q = 1, 2, 3, 4$. Our results for $q = 1$ are consistent with a recent highly accurate numerical estimate by Ziff and Suding, and results for $q = 2$ agree with the known exact result within the numerical accuracy. Compared with results obtained in a recent series analysis by Jensen *et al*, our numbers differ from theirs slightly for $q = 3$, and agree with theirs with a slightly better accuracy for $q = 4$. Our numbers also confirm that a conjecture due to Wu is extremely accurate.

1. Introduction

The q-state Potts model [1] is related to many interesting problems in mathematics and physics [2–6]. Particularly, Kasteleyn and Fortuin [2, 3] related the Potts model to a random cluster model which, in the limit of $q \to 1$, describes the problem of bond percolations. For general q, the random cluster model can also be interpreted as generating correlated bond percolations [6–8].

Consider a lattice, or more generally a graph, G consisting of N sites and B edges. Let the edges of G be covered by bonds in random, and associate weights p and $1 - p$, respectively, to the covered and open edges. We shall refer to p as the bond occupation (covering) probability. The bond coverings of G form subgraphs $G' \subseteq G$. Two sites belong to a cluster if they are connected via a sequence of covering bonds. Let $b(G')$ and $n(G')$ be, respectively, the numbers of bonds and clusters, including isolated points, in a subgraph G'. To each G' we associate a weight

$$\pi(G'; p, q) = p^{b(G')}(1 - p)^{B-b(G')}q^{n(G')}. \tag{1}$$

The Potts model partition function can then be written as

$$Z(G; p, q) = \sum_{G' \subseteq G} \pi(G'; p, q) \tag{2}$$

where $p = 1 - \mathrm{e}^{-K}$, $K = J/k_B T$, with J being the coupling between Potts spins.

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Writing the partition function of the Potts model in the form of (1) and (2), one can regard $Z^{-1}\pi(G'; p, q)$ as the probability of occurrence of the subgraph G', and the formulation can be interpreted as that of a correlated bond percolation [6]. The criticality in the Potts model reflects the fact that the thermodynamic limit of the per-site free energy

$$f(p, q) = \lim_{N\to\infty} \frac{1}{N} \ln Z(G; p, q) \tag{3}$$

becomes singular at a critical probability $p = p_c$. This formulation offers an alternate way of describing the critical point of the Potts model in terms of the critical probability p_c for the bond correlated percolation [6].

The exact critical probability p_c is known only for the square, triangular, and honeycomb lattices [9]; there has been no exact determination of the Potts critical point for other lattices. Particularly, the determination of the critical point for the Kagomé lattice has proven to be extremely elusive. Two conjectures have been proposed on the exact location of the critical point [10, 11], and an attempt has been made to test the two conjectures using simple Monte Carlo simulations [12]. A rigorous lower bound on p_c has also been established [13]. More recently, Ziff and Suding [14] determined the $q = 1$ critical point to an extremely high degree of accuracy by using highly precise Monte Carlo simulations, and Jensen *et al* [15] studied the $q = 3, 4$ cases by analysing exceptionally long series expansions. In view of the renewed interest on this yet unresolved problem, here we re-investigate the problem by using a combination of Monte Carlo renormalization group and finite-size scaling analyses, thus refining the simple Monte Carlo study of [12].

The outline of this paper is as follows. A summary of past works and the current status of the problem are described in section 2. The present approach is outlined in section 3, and the results of our findings are presented in section 4.

2. Results to this date

In 1979, on the basis of a reasonable extension of known results for the triangular lattice, one of us [10] proposed a conjecture on the critical condition for the Kagomé Potts model. The expression, which we shall refer to as the Wu conjecture, reads

$$w^6 + 6w^5 + 9w^4 - 2qw^2 - 6q^2w - q^3 = 0 \qquad \text{(Wu)} \tag{4}$$

where $w = p/(1-p) = \mathrm{e}^K - 1$. The Wu conjecture is actually more general and applies to the triangular Potts model with both pair and triplet interactions which can be ferromagnetic and/or antiferromagnetic. While it has subsequently been shown by Enting and Wu [16] that the conjecture cannot hold in a regime where the pair interaction is highly antiferromagnetic, it still needs to be tested, however, whether the Wu conjecture holds in the ferromagnetic regime.

An alternate conjecture of the Kagomé Potts critical point was proposed in 1982 by Tsallis [11]†. Tsallis conjectured the critical condition in the ferromagnetic regime to be

$$\frac{1 + (q-1)u^3}{u + u^2 + (q-2)u^3} = 2\cos\left[\frac{1}{3}\cos^{-1}\left(\frac{q}{2} - 1\right)\right] \qquad q \leqslant 4 \qquad \text{(Tsallis)} \tag{5}$$

where $u = p/[1 + (q-1)(1-p)]$. Since both the Wu and Tsallis conjectures yield the exact critical p_c for $q = 2$, the relative merit of the two conjectures can be judged only by comparing with results for other values of q.

† [11] contains a misprint. The exponent $\frac{1}{2}$ in the first line of (6′) should be deleted.

In 1994, using the method of a histogram Monte Carlo renormalization group proposed by CKH [17, 18], we have evaluated the critical point for the Kagomé Potts model numerically [12]. The method of analysis used in [17, 18] is a simple sampling Monte Carlo approach. While the results suggested that the Wu conjecture works better than the Tsallis conjecture, the standard deviations incurred were too large to draw a definitive conclusion. Very recently, Ziff and Suding [14] carried out a highly accurate Monte Carlo simulation of bond percolation for the Kagomé lattice, the $q = 1$ version of the correlated percolation problem, and obtained a highly accurate percolation threshold $p_c = 0.524\,4053(3)$. Subsequently, Jensen *et al* [15] analysed extremely long series expansions for the $q = 3, 4$ Kagomé lattice obtained in a *tour de force* application of the finite-lattice method and its extension, leading to a determination of p_c within an accuracy of 0.01%. These studies confirm that the Wu conjecture works better than the Tsallis conjecture, in addition to providing highly accurate determinations of the critical point. The purpose of this paper is to provide an independent assessment of the accuracy of the Wu conjecture.

3. A renormalization group and scaling analysis

Our numerical determination of the Potts critical point p_c is a combination of the Swendsen–Wang cluster Monte Carlo method [19], the cell-to-cell renormalization group [17, 18, 20], and the finite-size scaling analysis [21]. Due to the nature of our procedure which is most suitable for investigating second-order transitions, we confine our studies to $q \leqslant 4$.

The cluster Monte Carlo method developed by Swendsen and Wang is an importance-sampling Monte Carlo method which is effective for improving standard deviations. As in all prior investigations, the determination of the critical p_c is effected by considering a lattice G of linear dimension L, and a numerical determination of the existence probability

$$E(L, p, q) = Z^{-1} \sum_{G' \subseteq G}{}' \pi(G'; p, q) \tag{6}$$

where the prime over the summation denotes that it is taken over subgraphs in which there is at least one cluster spanning the lattice vertically. For this reason, the existence probability has also been termed the crossing probability by Kesten [22] and the spanning probability by Ziff [23].

We use the Swendsen–Wang cluster Monte Carlo method to simulate the existence probability (6) for various linear sizes L. This is followed by an application of the cell-to-cell renormalization group transformation [17, 18, 20]

$$E(L', p', q) = E(L, p, q) \tag{7}$$

connecting two cells of linear sizes L' and L, where we take $L' = L/2$. The transformation (7) yields a renormalized bond occupied probability p' as a function of p. An estimate of the critical probability $p_c(L)$ for a given L is then made by determining the fixed point of this transformation, namely, the solution of the equation

$$E[L/2, p_c(L), q] = E[L, p_c(L), q]. \tag{8}$$

Finally, the critical probability $p_c(\infty)$ for an infinite lattice is extracted by using the finite-size scaling relation [21]

$$p_c(\infty) - p_c(L) \propto L^{-1/\nu} \tag{9}$$

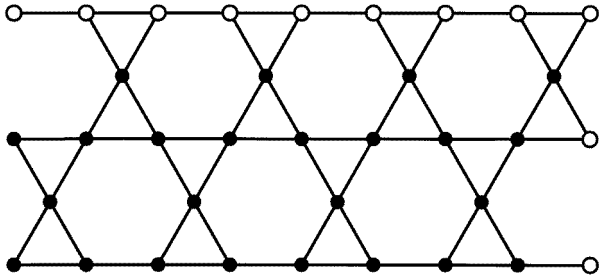


Figure 1. An 8×4 Kagomé lattice with periodic boundary conditions. Full circles denote lattice sites; open circles denote repeated sites.

Table 1. Numerical estimates of the critical points $p_c(L)$. Numbers in parentheses denote uncertainties attached to the last digits.

q	$p_c(16)$	$p_c(32)$	$p_c(64)$	$p_c(128)$
1	0.524 13(1)	0.524 38(2)	0.524 40(2)	0.524 41(2)
2	0.607 07(2)	0.606 86(5)	0.606 71(4)	0.606 69(2)
3	0.652 74(2)	0.652 48(4)	0.652 41(2)	0.652 35(1)
4	0.683 45(6)	0.683 27(2)	0.683 20(2)	0.683 18(1)

Table 2. Numerical estimates of the critical probability. The Tsallis [11] and Wu [10] conjectures; the King–Wu lower bound p_b [13]; Ziff–Suding [14]; Jensen [15]; this work.

q	p_b	Tsallis	Wu	Ziff–Suding	Jensen *et al*	This work
1	0.517	0.522 372 07	0.524 429 71	0.524 405 3(3)		0.524 41(1)
2	0.597	0.606 680 11	0.606 680 11			0.606 62(8)
3	0.641	0.653 932 82	0.652 327 40		0.652 12(5)	0.652 32(7)
4	0.672	0.685 967 83	0.683 127 34		0.683 15(5)	0.683 17(2)

where ν is the correlation exponent 1, $\frac{5}{6}$, and $\frac{2}{3}$ for, respectively, $q = 2, 3, 4$ [4]. For $q = 1$, we adopted the Aharony–Hovi scaling relation [24]

$$p_c(\infty) - p_c(L) \propto L^{-0.85-1/\nu} \tag{10}$$

where $\nu = \frac{4}{3}$.

4. Numerical results

We evaluate the existence probability $E(L, p, q)$ by carrying out Monte Carlo simulations on a Kagomé lattice G of linear size L with periodic boundary conditions. The example of an 8×4 lattice is shown in figure 1.

We choose a set of n bond occupied probabilities, p_i, $i = 1, 2, \ldots, n$, in the neighbourhood of the expected critical point p_c, and for each p_i carry out 16 independent Swendsen–Wang cluster Monte Carlo simulations. The existence probability is evaluated in each simulation after 10^5–10^7 Swendsen–Wang iterations, and using the 16 sets of data we calculate the existence probability $E^{(i)}$ and the corresponding standard deviation $\delta E^{(i)}$. The n discrete values of $E^{(i)}$ and the associated standard deviations are next fitted to a quadratic

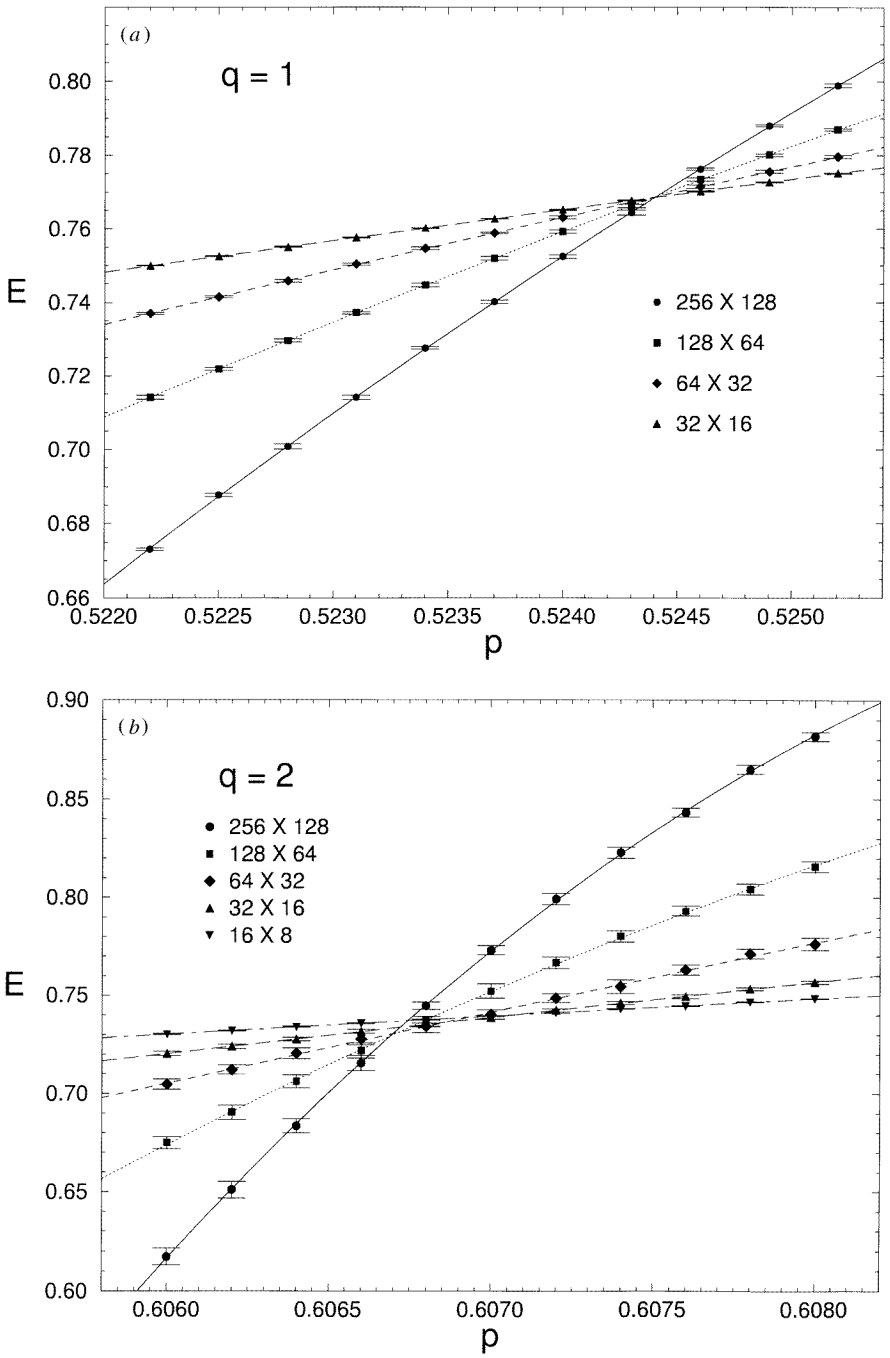
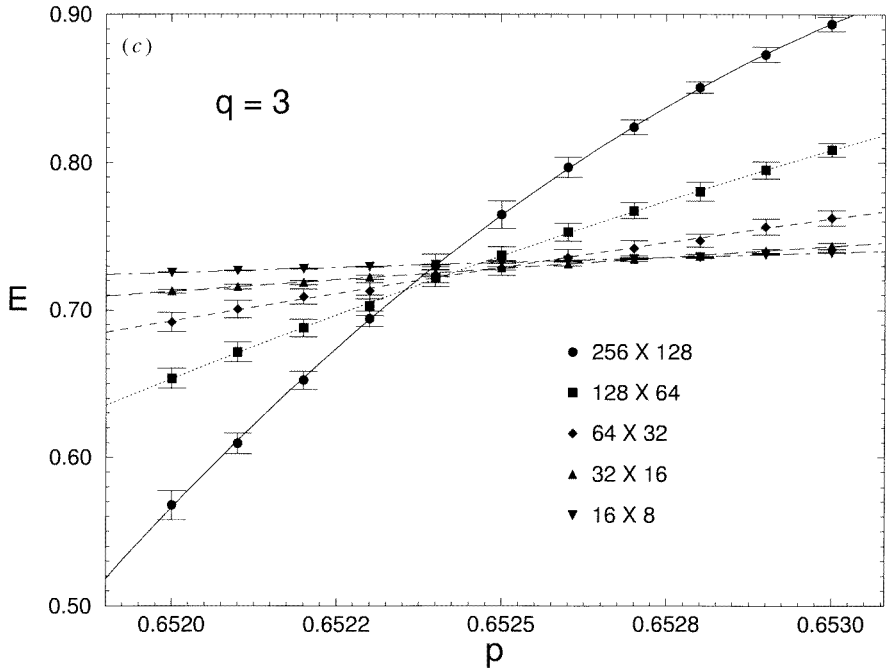


Figure 2. Monte Carlo data and the linear regression fit of the existence probability for five different lattice sizes as indicated. (*a*) $q = 1$, (*b*) $q = 2$, (*c*) $q = 3$, (*d*) $q = 4$.

polynomial

$$a_0 + a_1 p + a_2 p^2 \tag{11}$$



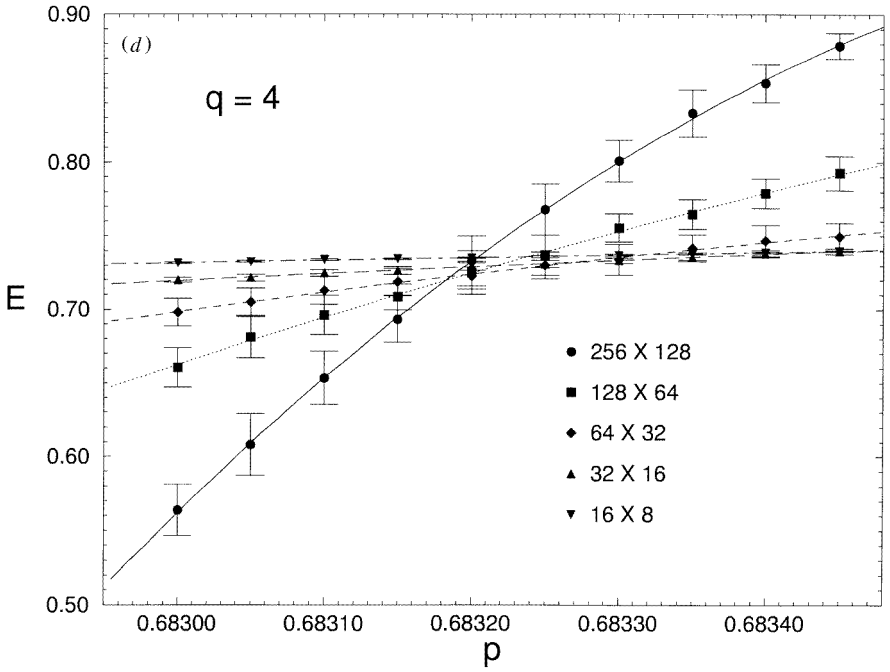


Figure 2. (Continued)

using the Linear Regression package in Mathematica 3.0. This determines the parameters a_0, a_1 and a_2, and the associated uncertainties δa_0, δa_1 and δa_2. Using these numbers the critical probability $p_c(L)$ and the associated uncertainty are determined from (8) for each L.

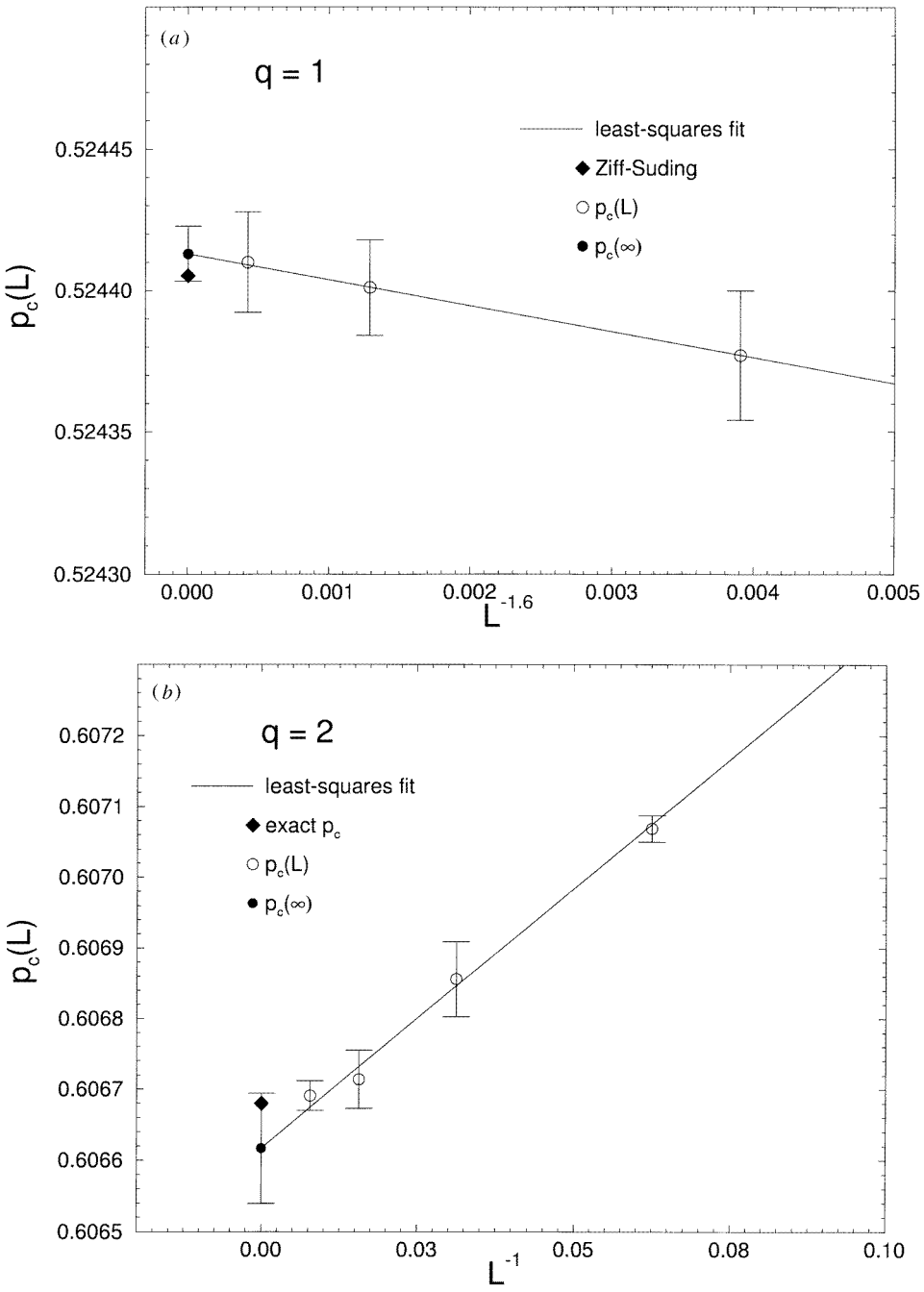


Figure 3. Results of finite-size scaling analyses for (*a*) $q = 1$ (*b*) $q = 2$ (*c*) $q = 3$ and (*d*) $q = 4$. Data points are denoted by open circles, and the extrapolated critical point $p_c(\infty)$, is denoted by the full circle.

Our computer program is capable of studying the q-state Potts model for any positive integer q, including $q = 1$, which corresponds to the bond percolation model. We

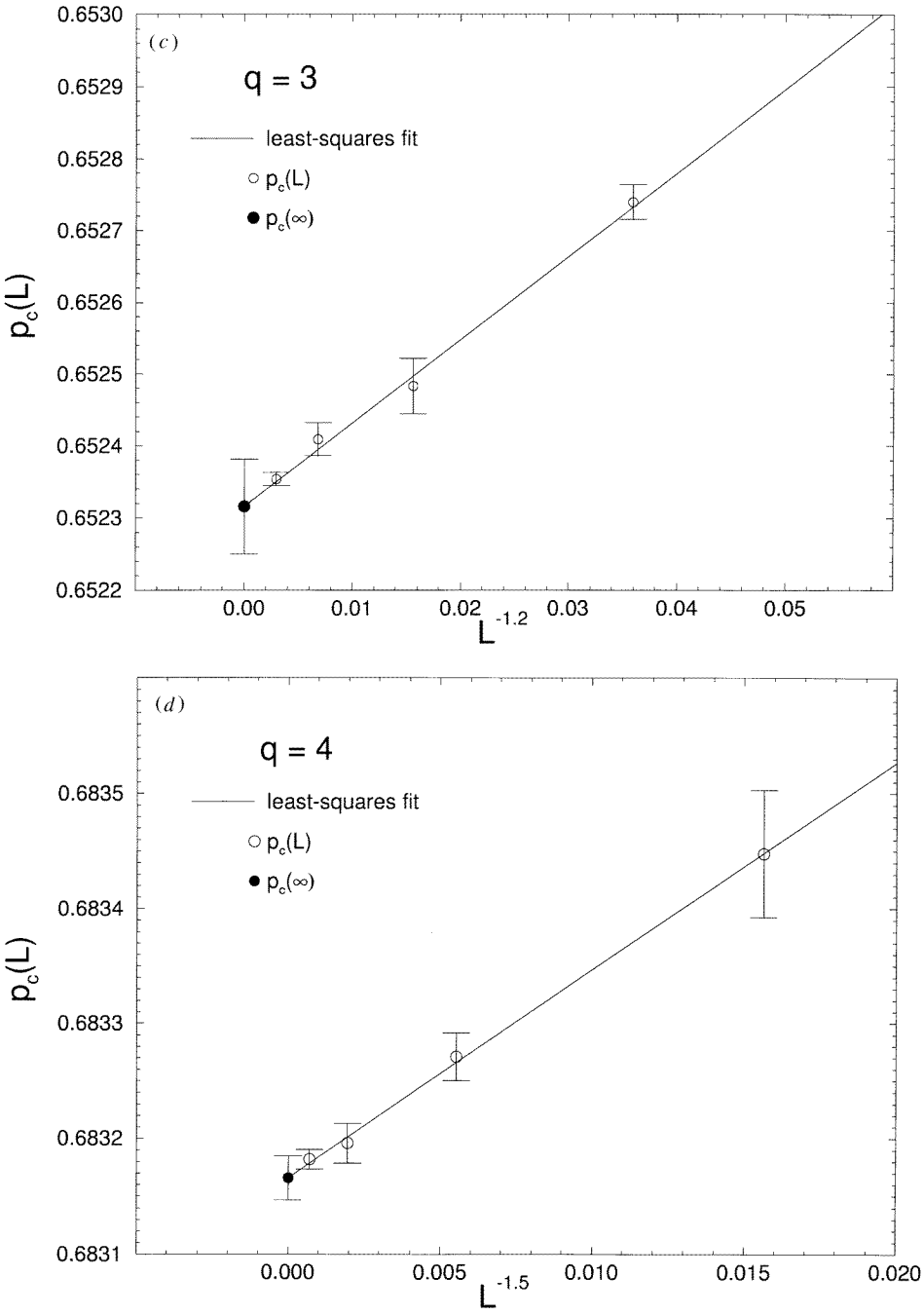


Figure 3. (Continued)

have carried out Monte Carlo simulations for systems of sizes $L \times L/2$ for $L = 16, 32, 64, 128, 256$ for $q = 1, 2, 3, 4$. The critical point, which is the solution of the renormalization group equation transforming a $2L \times L$ system to a $L \times L/2$ system as

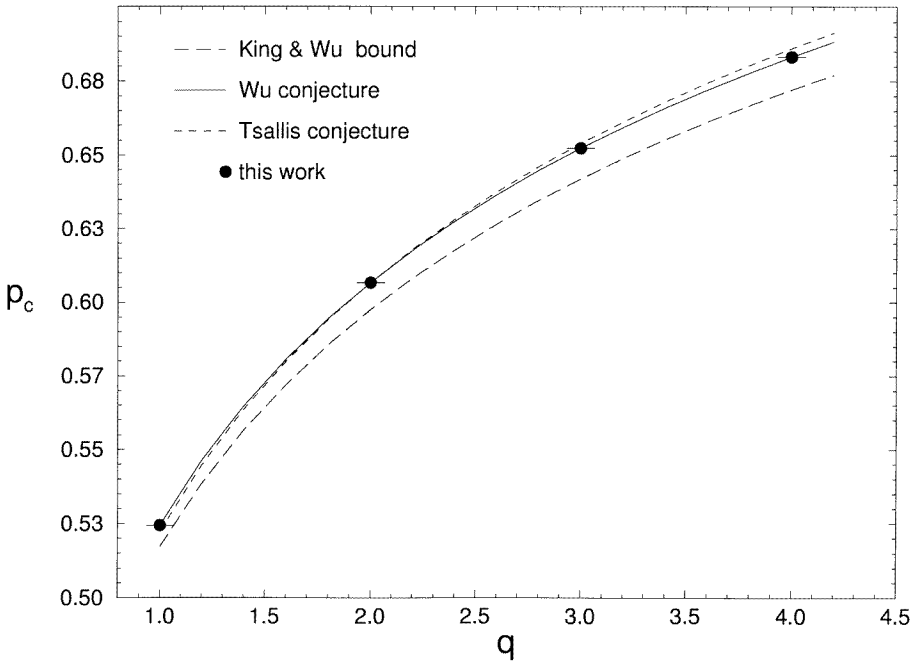


Figure 4. Critical point p_c as a function of q. Present results are compared with the Wu and Tsallis conjectures and the King–Wu lower bound.

indicated in (8), is $p_c(L)$. Results obtained in this way are given in table 1 and shown graphically in figures 2(*a*)–(*d*).

We next extract the critical point $p_c(\infty)$ using the finite-size scaling relation (9) and the least-squares method of [25] for fitting the scaling relation (9). The results are shown in figures 3(*a*)–(*d*), and the extrapolated values of $p_c(\infty)$ and the associated uncertainties are given in table 2 and shown in figure 4. Since for $q = 1$ the scaling behaviour manefits itself only for larger L, we have used only last three data point in the first row of table 2 in the fitting. The statistical analysis of [25] dictates that the probability that the *exact* critical point lies within the uncertainty ranges of table 2 is 0.683.

In table 2 and figure 4 we also show results of p_c deduced from the Wu and Tsallis conjectures as well as the King–Wu rigorous lower bound p_b [13] given by

$$q[n^3 + 3(q + 2w)n^2 + (q^2 + 3qw + wn)(3n + q)] = wn^4 \tag{12}$$

where $n = w(w + 3)$ and $w = p_b/(1 - p_b)$.

It is clear that the Wu conjecture is extremely accurate, confirming earlier findings [12, 15]. In fact, it appears that the consideration of our results alone does not rule out the possibility that the Wu conjecture is actually exact. Comparison with the results of Jensen *et al* [15], our determination of p_c for $q = 4$ is consistent with theirs with a slightly better accuracy. But our value of p_c for $q = 3$ does not coincide with theirs within the limits of respective deviations. Further clarification of this discrepancy, albeit slight, is needed.

5. Summary

In summary, we have used a combination of Monte Carlo simulations, cell-to-cell renormalization groups, finite-size scalings and a linear regression analysis to determine the critical point for the Kagomé Potts model. Other than a slight discrepancy with the finding of Jensen *et al* [15] for $q = 3$, our results agree well with prior highly accurate determinations of p_c. Our numbers also support the conclusion that the Wu conjecture (4) is extremely accurate as an approximation to the exact Kagomé Potts critical point.

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