

Critical temperatures of the three- and four-state Potts models on the kagome lattice

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The value of the internal energy per spin is independent of the strip width for a certain class of spin systems on two-dimensional infinite strips. It is verified that the Ising model on the kagome lattice belongs to this class through an exact transfer-matrix calculation of the internal energy for the two smallest widths. More generally, one can suggest an upper bound for the critical coupling strength $K_c(q)$ for the q -state Potts model from exact calculations of the internal energy for the two smallest strip widths. Combining this with the corresponding calculation for the dual lattice and using an exact duality relation enables us to conjecture the critical coupling strengths for the three- and four-state Potts models on the kagome lattice. The values are $K_c(q = 3) = 1.0565094269290$ and $K_c(q = 4) = 1.1493605872292$, and the values can, in principle, be obtained to an arbitrary precision. We discuss the fact that these values are in the middle of earlier approximate results and furthermore differ from earlier conjectures for the exact values.

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The finite-size scaling technique, known as phenomenological renormalization, has proven to be a very reliable method for obtaining critical properties of low-dimensional systems [1–3]. Since its beginning, this method has been used to extract thermodynamic quantities in the infinite-width limit from transfer-matrix calculations for infinite strips of finite width [1]. Since a transfer-matrix calculation gives exact results for an infinite strip with width L , it can give very precise information on the system in the thermodynamic limit, provided that the relevant thermodynamic functions have good convergences with respect to the width L . For this reason, corrections to the critical finite-size scaling have been a key issue in this phenomenological renormalization method [4,5]. The present investigation makes use of the recent progress in computing algorithms, which makes it possible to solve an eigenvalue problem for a transfer matrix with a considerable size in an exact or arbitrarily precise manner. This means that one may use symbolic algebra systems to solve a given transfer matrix in a closed form. Alternatively, if this is not possible, one can do numerical calculations with an arbitrary precision, which means that the numerical precision of every calculation is free from rounding errors but limited only by the computing memory. This makes it possible to take full advantage of the exactness of the transfer-matrix method. In the present work we use exact calculations of narrow infinite strips to locate the critical point of the q -state Potts models [6] on the kagome lattice with $q = 3$ and 4. The kagome lattice is one of the simplest two-dimensional (2D) structures belonging to the Archimedean lattices and has also drawn practical attention due to distinct structural properties [7,8]. The case of $q = 2$ on the kagome lattice was solved more than half a century ago [9], but the three- and four-state Potts models have been long-standing open questions in statistical physics, and have

given rise to, by now, classical conjectures [10,11], as well as a number of numerical and approximate determinations [12–15].

The zero-field q -state Potts model is defined by the following Hamiltonian:

$$H = -J \sum_{\langle ij \rangle} \delta(S_i, S_j),$$

where each spin S_k may take an integer value from 0 to $(q - 1)$, δ denotes the Kronecker delta function, and the sum is over all the nearest-neighbor pairs. We will set the interaction strength J as unity throughout this work and identify the inverse temperature β with the coupling strength $K \equiv \beta J$. According to the Fortuin-Kasteleyn representation [16], the partition function corresponding to this Potts Hamiltonian can be written as

$$Z = \sum_{\{S\}} e^{-\beta H} = \sum_{\{S\}} p^b (1 - p)^{B-b} q^{N_c} \quad (1)$$

with $p \equiv 1 - e^{-K}$, where the sum is over all the spin configurations with N_c clusters made of b connected bonds out of B total bonds inside the system. At the critical point K_c the partition function for the infinite system (= both length and width infinite) has singularities in its K derivatives. The conjecture in Ref. [10] states that the critical points can be located by solving the following sixth-order polynomial:

$$v^6 + 6v^5 + 9v^4 - 2qv^3 - 12qv^2 - 6q^2v - q^3 = 0 \quad (2)$$

with $v \equiv e^K - 1$. As will be described below, our estimates, based on the two thinnest infinite strips, are very close to the values predicted by this conjecture.

To illustrate the transfer-matrix method [17], we first consider a thin strip of spins with size $\infty \times L$ as shown in Fig. 1(a). Once the transfer matrix is obtained, the free energy per spin f_L is given in terms of the largest eigenvalue $\lambda_L^{(0)}$ of

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the matrix as

$$-\beta f_L = L^{-1} \log \lambda_L^{(0)} \quad (3)$$

and the internal energy per spin is therefore given as

$$u_L = \frac{\partial}{\partial \beta} (\beta f_L) = -\frac{1}{L \lambda_L^{(0)}} \frac{\partial \lambda_L^{(0)}}{\partial \beta}. \quad (4)$$

Furthermore, given the second largest eigenvalue $\lambda_L^{(1)}$, the inverse correlation length is obtained as $\xi_L^{-1} = \log \frac{\lambda_L^{(0)}}{|\lambda_L^{(1)}|}$. In the context of the arbitrary-precision arithmetic, the differentiation in Eq. (4) may need some care. The derivatives of the eigenvalues can be calculated by using the equation $\Lambda' = Y^* T' X$, where $T' = \partial T / \partial \beta$ is the first-order derivative of the matrix T and Λ is a diagonal matrix with the eigenvalues of T [18]. The matrices X and Y represent the right and left eigenvectors, respectively, which are constructed in such a way that $Y^* X = I$ is the identity matrix. Here the asterisk means the complex conjugate transpose. Suppose that the spins on the strips are described by the q -state Potts model with $q = 2$, which is equivalent to the Ising model with the temperature divided by 2. It has been shown in Ref. [1] that the correlation length is very well approximated by $\xi_L \propto L$ near the critical coupling strength $K_c = \beta_c J = \log(1 + \sqrt{2})$ [19,20]. This means that close enough to the critical coupling strength one may use the width L as a substitute for the correlation length and describe the system in terms of this length scale. The proportionality coefficient between ξ_L and L in the limit $L \rightarrow \infty$ is related to the correlation-decay exponent η by conformal invariance [21]. In fact, it has been furthermore found that $\frac{\partial}{\partial \beta} \xi_L^{-1} |_{\beta=\beta_c} = -\xi_L^{-2} (\partial \xi_L / \partial \beta) = \text{const.}$ for every finite L [22]. Assuming that $\xi_L \sim (\beta - \beta_c)^{-\nu}$ near β_c in the limit of $L \rightarrow \infty$, this yields the exact correlation-length exponent $\nu = 1$ [22]. Another interesting fact, crucial for the present investigation, is that the internal energy per spin [Eq. (4)] has at $\beta = \beta_c$ the same value for all the strips *irrespective* of their widths L [23]. This fact opens up a simple and practical way of locating the critical point of the 2D Ising model by calculating the internal energy for the two thinnest strips and then finding the coupling strength for which they have the same internal energy. For the square-lattice strip in the diagonal direction shown in Fig. 1(b), for example, equating the internal energy per spin for $L = 2$ to that of $L = 3$, we get

$$\frac{e^{2K}(e^{2K} - 1)(e^{4K} - 6e^{2K} + 1)}{(e^{2K} + 1)F(K) + (e^{2K} + 1)^2 \sqrt{F(K)}} = 0,$$

where $F(K) \equiv e^{8K} - 8e^{6K} + 30e^{4K} - 8e^{2K} + 1$. It is straightforward to see that the nonnegative solutions of the equation are $e^K = 0, 1, \infty$, and $\sqrt{2} \pm 1$. Only the latter two are nontrivial and give us the exact K_c for the 2D ferromagnetic and antiferromagnetic models, respectively. The largest eigenvalues for $L = 4$ and 5 are also available in closed forms and lead to the same conclusion. By using the geometry shown in Fig. 1(a), the exact results $e^K = 1 + \sqrt{q}$ have been obtained for $q \leq 5$ [23], but there are also cases where the method does not apply [23,24]. The invariance of the internal energy with respect to strip width has therefore been conjectured to be due to certain symmetries in the model [24,25].

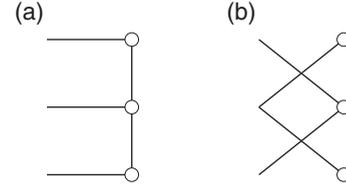


FIG. 1. Spin blocks to make spin strips of (a) the square-lattice type and (b) the double-square-lattice type. The periodic boundary condition is imposed in the vertical direction for all the cases, so the vertical lengths are regarded as $L = 3$. Note that the periodic boundary condition may introduce *double* connections in some pairs of spins if L is small.

We apply the transfer-matrix method to the Potts models on the kagome lattice. First, we verify that the known exact solution for the two-state Potts model is reproduced by assuming that the internal energy per spin is invariant also in this case. We construct two spin blocks for generating the kagome lattice, as illustrated in Figs. 2(a) and 2(b). Writing down the corresponding transfer matrices and denoting their largest eigenvalues as $\lambda_a^{(0)}$ and $\lambda_b^{(0)}$, respectively, we compute the internal energies per spin as $u_a = -(3\lambda_a^{(0)})^{-1} (\partial \lambda_a^{(0)} / \partial \beta)$ for Fig. 2(a) and $u_b = -(6\lambda_b^{(0)})^{-1} (\partial \lambda_b^{(0)} / \partial \beta)$ for Fig. 2(b). Indeed, it is readily found that $u_a = u_b = -(7 + 2\sqrt{3})/6$ at $\beta = \frac{1}{2} \log(3 + 2\sqrt{3})$, which is the exact critical point of this system [9]. This verifies that the correct critical K_c can be obtained from the two thinnest strips also for the two-state Potts model on the kagome lattice. Or, in other words, this shows that the internal energy per spin is invariant also for the two-state Potts model on the kagome lattice.

In case of the three- and four-state Potts models on the kagome lattice, neither the critical values K_c are exactly known, nor is it *a priori* known if the internal energy is invariant. In order to generalize the method, we study pairs of strips, one with finite length M and width L and the other with $2M$ and $2L$. The two strips in such a pair have the same aspect ratio $r = M/L$ where M and L are chosen such that r is a positive number. When r is suitably chosen, each such pair will have a single $K_{\text{cross}}(L)$ for which the internal energy per spin is the same. Figures 3(a) and 3(b) show that the crossing point $K_{\text{cross}}(L)$ monotonically decreases with increasing L . In the limit of $L \rightarrow \infty$, the crossing point approaches the true critical K_c , that is, $[K_{\text{cross}}(L) - K_c] \rightarrow 0^+$. This implies that

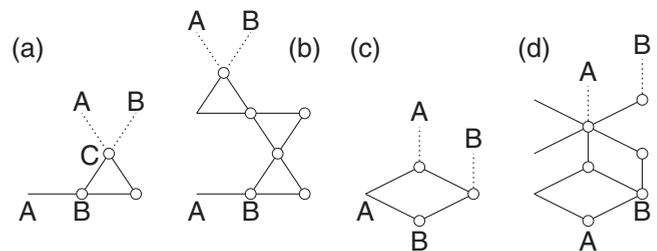


FIG. 2. Spin blocks to make spin strips of the kagome type with (a) $L = 1$ and (b) $L = 2$, and those of the dice type with (c) $L = 1$ and (d) $L = 2$. The dotted lines show the periodic boundary condition in the vertical direction. Note that B and C are *doubly* connected in (a), and such double connections are also found in (c).

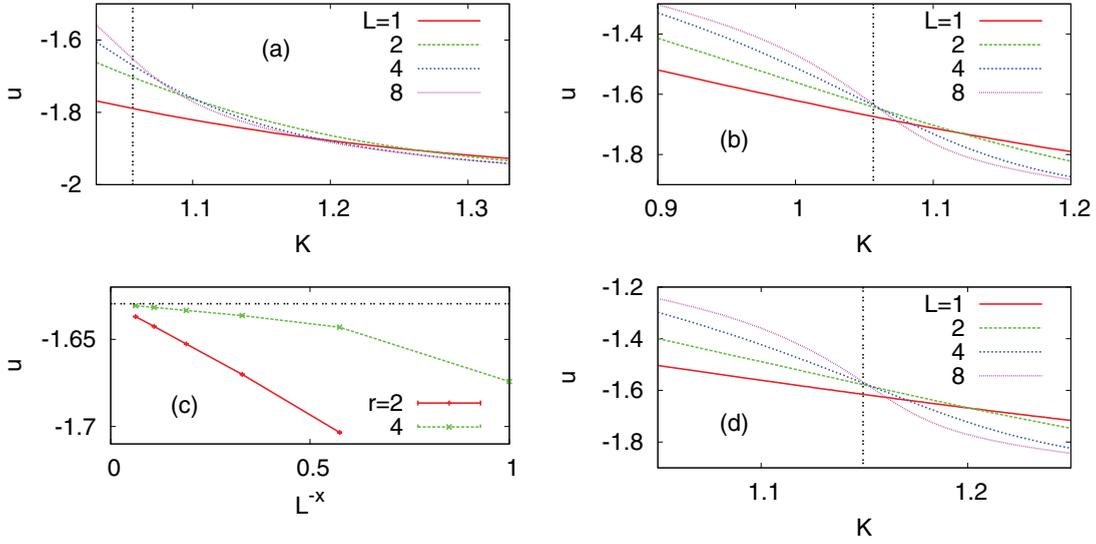


FIG. 3. (Color online) Monte Carlo data of the internal energy per spin for $q = 3$, with aspect ratios (a) $r = 2$ and (b) $r = 4$, respectively. The vertical dotted lines show the critical coupling strength obtained in this work. (c) Sectional view at this particular point, where the horizontal dotted line indicates the value obtained in this work, $u = -1.6295437063996$. The scaling dimension x is expressed as $(1 - \alpha)/\nu$ with the specific-heat exponent α , and therefore $x = 4/5$ for $q = 3$. (d) Qualitatively the same behavior is observed for $q = 4$. Here we plot it with $r = 4$.

$K_{\text{cross}}(L)$ will give an upper bound for K_c for each of the fixed aspect ratios. As long as the aspect ratio does not change any essential physics but only the convergence rate toward the bulk criticality [Fig. 3(c)], we can suggest that the crossing point $K_{\text{cross}}(L = 1)$ for $r = \infty$ will either give an upper bound or alternatively the exact results: that is, for the case of $q = 2$ it gives the exact result, whereas it gives at least an upper bound for $q = 3$ and $q = 4$. An argument can be given in the following way: the crossing point would fail to be an upper bound if crossing could be found on both sides of the true critical point K_c . This actually means that the internal energy per spin u_L would not be a monotonic function of L at $K = K_c$. We note that the classical Potts model on the $L \times M$ strip can be mapped to the one-dimensional quantum Potts model of size L by putting the strip length M in the imaginary-time direction [26]. One can describe the finite-size scaling around the critical point as $u_L - u_\infty = L^{-x} a[(K - K_c)L^{1/\nu}, ML^{-z}]$ to the leading order with a two-parameter function a [27], the dynamic critical exponent $z = 1$ [26], and the scaling dimension x of the energy-density operator [28]. At $K = K_c$, the scaling function reduces to $a(ML^{-1}) = a(r)$, so we find that $u_L \sim u_\infty + a(r)L^{-x}$. The geometric factor r is absorbed

by the coefficient a which determines the convergence rate. It would be plausible to say that $a(r)$ is continuous and nonvanishing for any finite r and hence cannot change the sign. The theory of the finite-size scaling therefore tells us that u_L is a monotonic function of L so that the crossing point for a fixed aspect ratio will exist only on one side, which is $K \geq K_c$ in this case.

In the present investigation we are for practical reasons restricted to $q \leq 4$ and $L \leq 2$ since the transfer-matrix size increases as $q^{3L} \times q^{3L}$. It is straightforward to write the transfer matrices for $q = 3$ and 4 and solve the eigenvalue problem. By equating u_a to u_b as above, we obtain the two values $K_{\text{cross}}(L = 1)$, which are 1.0565094269290 and 1.1493605872292 for $q = 3$ and $q = 4$, respectively. These values are shown in Table I together with other existing estimates. Note that the arbitrary-precision arithmetic can make our values as precise as we want, in principle. As seen in Table I, our values are somewhere in the middle of the earlier existing estimates and conjectures, suggesting that they may be the exact values. In order to further examine the obtained values, we make use of the fact that there exists an exact relation between the critical coupling strengths of the kagome

TABLE I. Critical thresholds of the q -state Potts models on the kagome lattice in terms of $p = 1 - e^{-K}$.

Reference	$q = 1$	$q = 2$	$q = 3$	$q = 4$
Exact [9]		$1 - 1/\sqrt{3 + 2\sqrt{3}}$		
Conjecture [10]	0.52442971	$1 - 1/\sqrt{3 + 2\sqrt{3}}$	0.65232740	0.68312734
Conjecture [11]	0.52237207	$1 - 1/\sqrt{3 + 2\sqrt{3}}$	0.65393282	0.68596783
Series [12]			0.652350(5)	0.68315(5)
Monte Carlo [30]	0.5244053(3)			
Monte Carlo [13]		0.60662(8)	0.65232(7)	0.68317(2)
Subnet [15]	0.524404978(5)	0.60668010683(15)	0.6523502(4)	0.683163(5)
This work		$1 - 1/\sqrt{3 + 2\sqrt{3}}$	0.65233274726401	0.68316070428484

lattice and its dual [called a dice lattice, compare Figs. 2(c) and 2(d)] [10,29],

$$(e^{K_c} - 1)(e^{\tilde{K}_c} - 1) = q, \quad (5)$$

where \tilde{K}_c means the critical coupling strength of the dice lattice. This means that the upper bound $\tilde{K}_{\text{cross}}(L=1)$ obtained for the dual lattice can be turned into a *lower* bound for K_c of the kagome lattice. Repeating the calculation for $\tilde{K}_{\text{cross}}(L=1)$ with the two thinnest strips, given in Figs. 2(c) and 2(d), gives $\tilde{K}_{\text{cross}}(L=1) = 0.9550805683974$ as an upper bound for \tilde{K}_c , which through Eq. (5) gives the *lower* bound $K_c = 1.0565094269290$. This is, to all 14 decimal places, identical to the *upper* bound obtained directly for the kagome lattice. The most reasonable conclusion is that the calculation gives the exact value and that, just as for the two-state Potts model on the kagome lattice, the internal energy is independent of the strip width at the critical temperature and that, furthermore, the same is true for the $q=4$ case [Fig. 3(d)]. A complete analytic argument is called for, and a simple way to test this conjecture would be to solve the transfer matrix with $L=3$.

As seen from Table I, the situation for the three-state Potts model is as follows: both the two earlier conjectured exact values can be ruled out, although the conjecture by Wu in Ref. [10] is very close to the value in this work. Our conjectured exact value is somewhat surprisingly outside the bounds of the value estimated from series expansion in Ref. [12] and the subnet estimate in Ref. [15]. It agrees well with and is inside the bounds of the Monte Carlo estimate in Ref. [13]. For the four-state Potts model, the situation is somewhat different: again, the earlier conjectured exact values can be ruled out. However, our conjectured exact value is inside the bounds of all the other estimates.

The conjecture by Wu in Ref. [10] gives the critical coupling strengths as solutions of the sixth-order polynomial given in Eq. (2). It is important to note that we have also given our values as solutions of certain polynomial equations since we are dealing with transfer matrices. Although we have not factorized the full polynomials yet, one may ask if such sixth-order polynomials as Wu has derived can be eventually factored out. To answer this, we follow Ref. [30] and try to determine polynomials in the variable $v = e^K - 1$ which have roots at the exact critical values. Even if we work with numeric values, instead of symbolic manipulations, this method makes it possible to find such a polynomial. For example, in case of $q=2$, one recovers the compact analytic expression $v = \sqrt{3 + 2\sqrt{3}} - 1$ by solving the obtained polynomial equation. Based on the conjecture by Wu, we try to find the value for the $q=3$ case as the solution of the sixth-order polynomial $\sum_{i=0}^6 c_n v_n^i = 0$ with integer-valued coefficients. We furthermore assume that $c_6 = 1$, and let c_5 and c_4 vary from -25 to 25 , while the other four coefficients may take values

from -10^2 to 10^2 . Substituting our value $v = 1.876313463895$ for $q=3$, the best polynomial is found to be

$$v^6 - 6v^5 + 22v^4 - 79v^3 + 99v^2 + 28v - 56 = 0,$$

yielding a solution $v^{\text{poly}} = 1.876313463898$. Even if the discrepancy between our conjectured exact value and the solution of the polynomial is tiny, it is still significant, which means that there is no such polynomial within the range of coefficients tested. This might suggest that the solution cannot be obtained from a simple sixth-order polynomial as was assumed in the conjecture by Wu.

We conclude this work with a brief sideline: the Fortuin-Kasteleyn representation [Eq. (1)] for $q=1$ recovers the bond-percolation problem on the kagome lattice. The method in the present paper cannot be directly used in this case, since the internal energy becomes a constant independent of the coupling strength. Without the knowledge of the exact q dependence of K_c , one can only interpolate it from the other estimates. For the case of the square lattice, which has coordination number 4, as does the kagome lattice, we have a general expression of the critical point as $v^{\text{sq}} = \sqrt{q}$ [6]. We assume that $v(q)$ of the kagome lattice can be expanded in series of this variable: $v(q) = a(\sqrt{q})^3 + b(\sqrt{q})^2 + c\sqrt{q}$, where we further note that $v(0) = 0$ is an exact limit. Finding the three parameters a , b , and c by substituting the conjectured values for $v(2)$, $v(3)$, and $v(4)$, we can interpolate the value at $q=1$ and obtain $p \approx 0.52433$. Compared to the numerical estimate shown in Table I, the fractional error amounts to be about 140 parts per million.

In summary, we have conjectured the exact values of critical temperatures for the three-state and four-state Potts models on the kagome lattice by using exact transfer-matrix calculations on thin infinite strips. This suggests that the internal energy can provide a sharper condition for criticality than lattice symmetries considered in the earlier conjecture by Wu. It has also been noted that, for the three-state Potts model on the kagome lattice, the series expansion in Ref. [12] does not contain our result within its bounds. The method devised to obtain the results is based on exact solutions of the two thinnest infinite strips. These solutions have been obtained by taking full advantage of computational symbolic algebra systems. Since the method itself appears to be quite general, it may possibly be used to solve other problems.

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