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Internal Energy Density of the Critical Three-state Potts Model on the Kagome Lattice

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The internal energy density of the Potts model on a semi-infinite strip with a width L has been conjectured to have no finite-size corrections at the critical point $K = K_c$. By factorizing the transfer matrix for the kagome lattice with larger widths, we have found that this conjecture is not correct in that the internal energy density varies slightly with L at the critical point. From this size dependence of the internal energy density, we obtain an upper bound as $K_c < 1.0565615$, which is close to a recent estimate $K_c^{\rm JS} = 1.0565600(7)$ by Jacobsen and Scullard [J. Phys. A **45**, 494003 (2012)]. We also obtain a lower bound as $K_c > 1.0560$ by calculating the correlation length along the strips.

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I. INTRODUCTION

The q-state Potts model has served as a paradigm in classical statistical physics because it allows exact and nontrivial analytic results to be obtained. The model is defined by the following Hamiltonian:

$$H = -J \sum_{\langle ij \rangle} \delta(S_i, S_j), \tag{1}$$

where J is an interaction constant, the summation runs over the nearest neighbors, δ is the Kronecker delta function, and spin S_i at site i can take a value $0, \cdots, q-1$. For $q \leq 4$, the Potts model on a two-dimensional (2D) lattice undergoes a continuous phase transition at a certain inverse temperature $\beta = \beta_c(q)$, which is not a universal value, but depends on the underlying lattice structure. One might say that locating β_c is, therefore, of somewhat less importance than understanding the universal behavior independent of lattice structures, but it can be understood as a question of which factors characterize the critical point when the lattice symmetry is not high enough, a question whose answer is still under debate. In a classical review article [1], the critical point of the Potts model on the kagome lattice is actually listed as the second unsolved problem involving the Potts model. Wu's conjecture [1] suggests that by solving the polynomial,

$$v^6 + 6v^5 + 9v^4 - 2qv^3 - 12qv^2 - 6q^2v - q^3 = 0, \tag{2}$$

where $v \equiv e^K - 1$ with coupling strength $K \equiv \beta J$, one can get the critical point $K_c \equiv \beta_c J$. For $q = 3$, the prediction is $K_c \approx 1.056494$, for example. Equation (2) is undoubtedly a good prediction, but differs slightly from Monte Carlo calculations [2] and series expansion results [3].

In a recent article [4], this problem was tackled by using an idea that certain spin models on an infinite strip with a finite width L do not show finite-size corrections in the internal energy density u_L [5]. By solving transfer matrices for two smallest widths $L = 1$ and 2 [see Figs. 1(a) and (b)] and comparing the resulting internal energy densities, we conjectured $K_c^{\rm conj}(q = 3) = 1.0565094269290\ldots$ and $K_c^{\rm conj}(q = 4) = 1.1493605872292\ldots$ by using finite-size scaling arguments. We also suggested that one could directly check these conjectured values by calculating the internal energy density for a strip with $L = 3$ as shown in Fig. 1(c): If the calculated value for $q = 3$ deviates from $u_{L=3}^{\rm conj}(q = 3) = -1.6295437063996$ given in Ref. [4], our determination based on the assumption of L-independent $u_L(K_c)$ must be incorrect. In this work, we carry out this calculation by using the factorization technique [6–8] and

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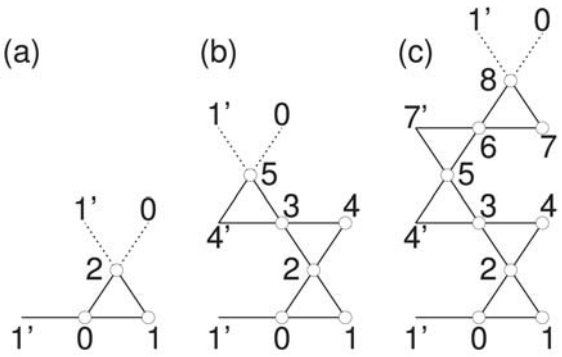

Fig. 1. Unit cells of the kagome lattice with different widths: (a) $L = 1$, (b) $L = 2$, and (c) $L = 3$. The dotted lines mean the periodic boundary condition so that $1'$ and 0 on the top are connected to $1'$ and 0 on the bottom, respectively.

report that u_L at $K_c^{\rm conj}(q = 3)$ is different from the conjectured value $u_L^{\rm conj}(q = 3)$ given above, which means that in general, the absence of finite-size corrections assumed in Ref. [4] is not true except for $q = 2$. This was recently pointed out by Jacobsen and Scullard [9]: They mentioned the existence of finite-size corrections for $q \neq 2$, and our conjectured values are not compatible with their results obtained by improving the polynomial in Eq. (2) systematically with larger subgraphs of the kagome lattice. Thus, the conjecture in Ref. [4] is disproved, which is the main result of this work. Nevertheless, it is possible to find bounds for K_c by using the size dependence of the numerical results. Our upper bound in this work is $K_c < 1.0565615$, and a lower bound is obtained as $K_c > 1.0560$, which are consistent with the value $K_c^{\rm JS} = 1.0565600(7)$ estimated by Jacobsen and Scullard [9].

II. METHOD AND RESULT

It is straightforward, in principle, to construct a transfer matrix T describing the three-state Potts model on an infinite strip with a width L. The problem is that it gets too large as L grows. Therefore, we need to factorize T into sparse matrices [6–8] and then use the power iteration method to get the largest eigenvalue and the corresponding left and right eigenvectors. Factorization means that a transfer matrix for a unit cell of width L as in Fig. 1 is equivalent to a product of $3L$ sparse matrices each of which describes adding a single spin. The advantage of factorization lies in the fact that multiplying a vector by sparse matrices one after another is much faster than dealing with the original dense matrix all at once, because only a few elements of the vector are affected by a sparse matrix. Note that we have to be careful about the order of adding spins under the periodic boundary condition along the vertical direction because each spin addition amounts to replacing a spin value in a layer by a new one. For example, in Fig. 1(a), adding spin 1 replaces the old value of spin $1'$, eliminating its information. For that reason, one possible correct order for $L = 1$ is $0 \to 2 \to 1$, where spin 1 is added after spin 2 because spin 2 should have a link to spin $1'$ before spin 1 replaces it, according to the periodic boundary condition [see the dotted line between spin 2 and spin $1'$ in Fig. 1(a)]. For the same reason, one correct order for $L = 2$ is $0 \to 2 \to 3 \to 5 \to 4 \to 1$, and Table 1 shows a possible order for $L = 3$ in detail. This approach can be extended to larger L's in a straightforward manner. For direct comparison, we have chosen the same transfer direction as in Ref. [4]. Notably transfer matrix calculations were also carried out in Ref. [9] to assess the approximation, but in a different transfer direction.

Table 1. One possible correct order of adding spins for $L = 3$ [Fig. 1(c)]. A link between spins i and j is denoted by (i, j).

spins added	links added
0	(0,1')
2	(2,0)
3	(3,4'), (3,2)
5	(5,4'), (5,7'), (5,3)
4	(4,3), (4,2)
6	(6,7'), (6,5)
7	(7,6)
8	(8,1'), (8,0), (8,6), (8,7)
1	(1,0), (1,2)

As we multiply an arbitrary vector by the transfer matrix T over and over again, it almost surely converges to the eigenvector with the largest eigenvalue λ_1 of T. Once we have obtained the left eigenvector $\mathbf{v}_L$ and the right eigenvector $\mathbf{v}_R$ corresponding to λ_1, we are able to get $u_L = -(3L\lambda_1)^{-1}\partial\lambda_1/\partial\beta = -(3L\lambda_1)^{-1}\mathbf{v}_L^* \cdot (\partial T/\partial\beta) \cdot \mathbf{v}_R$, where $*$ means the complex conjugate transpose. The factor of $3L$ appears because it is the number of spins for constructing L layers, as depicted in Fig. 1. The numerical error δu_L in the internal energy density increases with L, and it is estimated as $\delta u_L \sim O(10^{-11})$ for $L = 5$ and $O(10^{-9})$ for $L = 6$. For $L = 3$, the internal energy density at $K_c^{\rm conj}(q = 3)$ obtained by using this method reads $u_{L=3}^{\rm power} = -1.62949\ldots$, which clearly deviates from the value of $u_{L=3}^{\rm conj} = -1.62954\ldots$ conjectured in Ref. [4], disproving the conjecture on the lack of finite-size corrections in $u_L(K_c)$.

Our results up to $L = 6$ are depicted in Fig. 2(a). The line of $L = 1$ behaves differently from the others because the size is too small and should, therefore, be discarded from consideration. The crossing points of lines for $L \geq 2$

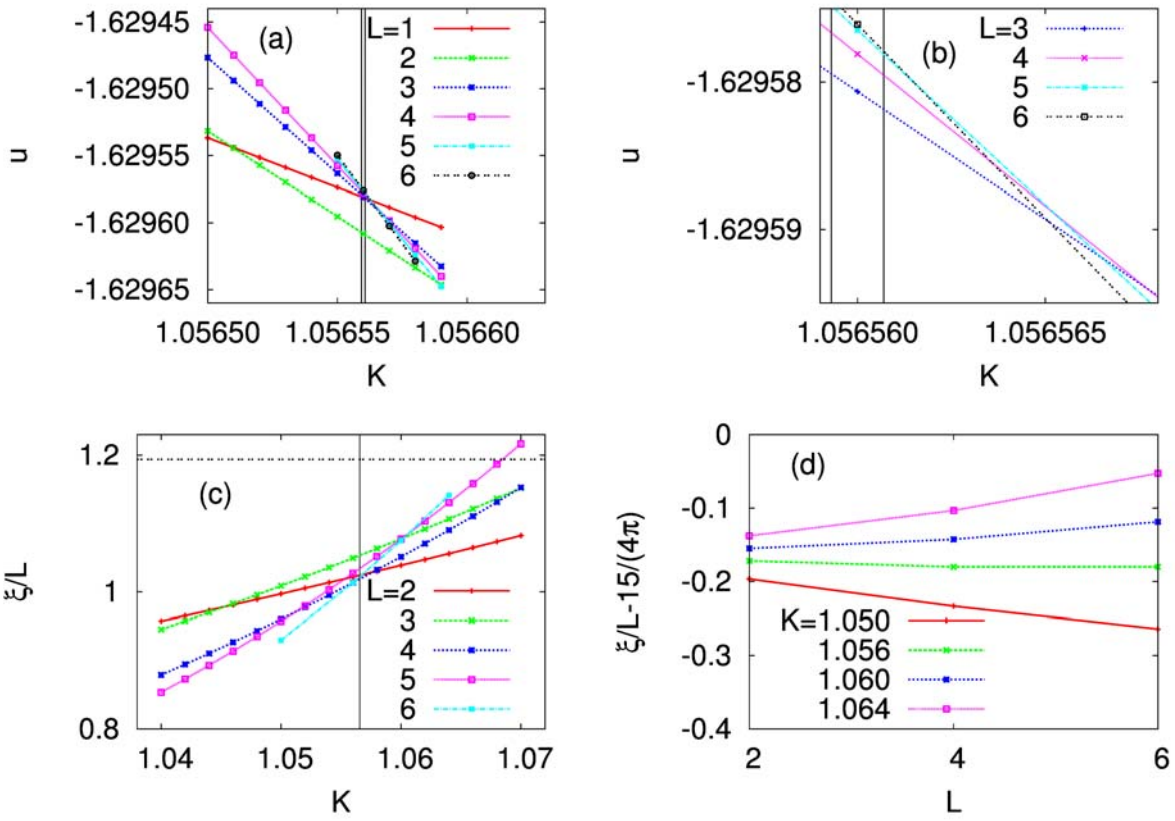

Fig. 2. (Color online) (a) Internal energy density as a function of K for each strip width L and (b) its zoomed view. (c) Correlation length ξ divided by L, where the dotted horizontal line means $1/(\pi\eta) = 15/(4\pi)$. The vertical lines in panels (a) to (c) indicate the range of K_c estimated by Jacobsen and Scullard [9]. (d) As L increases, the convergence of ξ/L to $15/(4\pi)$ is observed for $K > 1.056$.

gradually converge to K_c from above [Fig. 2(b)]. It is, therefore, plausible that K_c is located to the left of the crossing between $L = 5$ and $L = 6$ at $K \approx 1.0565615$. Although the size-dependence of u_L is known for large L at the critical point, our fitting result to estimate K_c from this critical scaling behavior is inconclusive because sub-leading corrections are not negligible for such small L's.

In order to estimate a lower bound, we use the correlation length $\xi = [\ln(\lambda_1/\lambda_2)]^{-1}$, where λ_2 is the second largest eigenvalue of T. The second largest eigenvalue can be found by applying the power iteration method to a vector orthogonal to $\mathbf{v}_R$, the eigenvector associated with λ_1. The numerical error in ξ is estimated as $O(10^{-11})$ for $L = 5$ and $O(10^{-7})$ for $L = 6$. As L increases, ξ/L is known to converge to $1/(\pi\eta) = 15/(4\pi) \approx 1.194$ at criticality, where η is the critical exponent for the two-spin correlation function [10]. Because ξ is an increasing function of K and the lines cross each other below $1/(\pi\eta)$ [see Fig. 2(c)], the crossing point will approach K_c from below if L is large enough. We thereby infer a lower bound as $K_c > 1.0560$, where the lines of $L = 4$ and $L = 6$ cross each other. The convergence of ξ/L to $15/(4\pi)$ also suggests that the borderline is around $K = 1.056$ [Fig. 2(d)]. Note that we compare results from even L's here because compared to the behavior of λ_1, that of λ_2 seems more sensitive to the boundary condition in the vertical direction.

III. SUMMARY

In summary, we have numerically calculated internal energy densities near $K = K_c^{\mathrm{conj}}$ for the three-state ($q = 3$) Potts model on kagome-type strips with various widths. The result disproves our previous conjecture that the internal energy density has no finite-size corrections at the critical point. The size dependence suggests $1.0560 < K_c < 1.0565615$, which is consistent with the recent estimate $K_c^{\mathrm{JS}} = 1.0565600(7)$ [9].

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