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An explicit formula for the interface tension of the 2D Potts model

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Abstract. — We consider the exact correlation length calculations for the two-dimensional Potts model at the transition point β_t by Klümper, Schadschneider and Zittartz, and by Buffenoir and Wallon. We argue that the correlation length calculated by the latter authors is the correlation length in the disordered phase and then combine their result with duality and the assumption of complete wetting to give an explicit formula for the order-disorder interface tension σ_{od} of this model. The result is used to clarify a controversy stemming from different numerical simulations of σ_{od}.

1. Introduction.

First-order phase transitions play a major role in many physical systems [1, 2]. A quantity of central importance for the kinetics of first-order phase transitions is the interface free energy between coexisting phases [1, 2]. In most applications exact results are not available and one has to rely on numerical computations [3-7]. One exception is the two-dimensional Ising model where an analytic expression for the interface free energy between the two ordered phases at low temperatures has been known for a long time [8]. But already for the temperature driven first-order phase transition in the two-dimensional q-state Potts model [9], where many exact results are available [10], the interface free energy has so far eluded any analytical treatment. In this situation, the discrepancy between different numerical estimates of the order-disorder interface free energy σ_{od} is particularly challenging: for $q = 7$, the predictions of references [3, 4] and reference [5] differ by a factor of eight, see table I. Recent exact results for the correlation length of the two-dimensional q-state Potts model now give the rare opportunity to test Monte Carlo predictions which were made without prior knowledge of the result. In fact, we consider both the result of Klümper, Schadschneider and Zittartz (KSZ) [11] and of Buffenoir and Wallon (BW) [12] for the correlation length ξ at the transition point β_t. Observing that these results

Table I.— *Numerical results for the interfacial free energy of the order-disorder interface of the two-dimensional q-state Potts model as obtained from Monte Carlo simulations.*

q	$2\sigma_{\mathrm{od}}$	authors
7	0.1886(12)	Potvin and Rebbi (Ref. [3])
7	≈ 0.20	Kajantie *et al.* (Ref. [4])
7	0.0241(10)	Janke *et al.* (Ref. [5])
8	≈ 0.045	Janke (Ref. [7])
10	0.09781(75)	Berg and Neuhaus (Ref. [6])
10	≈ 0.10	Janke (Ref. [7])

do not agree, we use the large q expansion to argue that the correlation length calculated by BW is actually the correlation length ξ_{d} of the disordered phase. Combined with duality and the assumption of complete wetting we then obtain an explicit formula for the order-disorder interface tension σ_{od}.

2. Theory.

We study the two-dimensional q-state Potts model defined by the energy

$$E = -\sum_{<xy>} \delta(s_x, s_y), \tag{1}$$

where the sum goes over the nearest neighbor pairs of a simple square lattice, $\delta(\cdot,)$ denotes the Kronecker symbol and $s_x \in \mathbf{Z}_q = \{1, \mathrm{e}^{2\pi i/q}, \cdot \quad, \mathrm{e}^{2\pi(q-1)i/q}\}$. For $q > q_{\mathrm{c}} = 4$, this model is known [10] to exhibit a first-order phase transition at the inverse temperature $\beta_{\mathrm{t}} = \log(1+\sqrt{q})$. We use the symbols σ_{oo} and σ_{od} to denote the reduced interfacial free energies per unit length of the order-order and the order-disorder interface. As usual we define the inverse correlation length (also called mass gap) $1/\xi_{\mathrm{d}} = m_{\mathrm{d}}$ in the disordered phase as

$$m_{\mathrm{d}}(\beta) = -\lim_{|x-y|\to\infty} \frac{1}{|x-y|} \log \left\langle \delta(s_x, s_y) - q^{-1} \right\rangle_{\mathrm{f}}, \tag{2}$$

where $\langle\cdot\rangle_{\mathrm{f}}$ denotes the infinite volume limit of expectation values with free boundary conditions, $|x-y|$ is sent to infinity in such a way that $x-y$ is parallel to one of the coordinate directions and $\beta = 1/k_{\mathrm{B}}T$ is supposed to be smaller or equal β_{t}.

In order to derive a formula for the interface free energy σ_{od} we need three ingredients from the literature. First, we use the fact that

$$2\sigma_{\mathrm{od}}(\beta) \leq \sigma_{\mathrm{oo}}(\beta) \qquad \forall \beta \geq \beta_{\mathrm{t}} \ \forall q > 4, \tag{3}$$

by the correlation inequalities of reference [13], while

$$2\sigma_{\mathrm{od}}(\beta_{\mathrm{t}}) \geq \sigma_{\mathrm{oo}}(\beta_{\mathrm{t}}) \qquad \forall q \geq q_0, \tag{4}$$

by the large q results of reference [14]. In equation (4), q_0 is a sufficiently large constant $4 < q_0 < \infty$. While (3) is a special property of the Potts model, (4) should be valid in a much more general setting since it just expresses the thermodynamic stability of the order-order

interface (this was already observed by Gibbs, see Ref. [13] for a discussion). It therefore seems natural to assume that (4) stays valid for all q for which the transition is of first order, which, together with (3) implies complete wetting, $2\sigma_{od} = \sigma_{oo}$. In fact, all experience with Monte Carlo simulations of two-dimensional Potts models suggests that rigorous large q results hold down to all values $q > 4$. We therefore adapt the common assumption (see e.g. Ref. [13] and references therein) that actually complete wetting,

$$2\sigma_{od}(\beta_t) = \sigma_{oo}(\beta_t), \tag{5}$$

occurs for all $q > 4$.

Our second ingredient is the equality

$$\sigma_{oo}(\beta) = m_d(\beta^*) \qquad \forall \beta \geq \beta_t \ \ \forall q \geq 2, \tag{6}$$

which was proven in reference [15]. Here $m_d = 1/\xi_d$ is the inverse correlation length of the disordered phase defined in (2) while β^* is the inverse dual temperature defined by $(e^{\beta} - 1)(e^{\beta^*} - 1) = q$ (we recall that $\beta = \beta^*$ at the transition point β_t). Under the assumption of complete wetting, one therefore obtains

$$2\sigma_{od}(\beta_t) = \sigma_{oo}(\beta_t) = m_d(\beta_t) \tag{7}$$

for all $q > 4$. We remark that (7) becomes rigorous if the first equality is replaced by the inequality (3). As it stands, it is rigorous if q is large enough.

As a final ingredient, we need an expression for the correlation length $\xi_d = 1/m_d$ in the disordered phase for $\beta = \beta_t$. Starting from the representation of the Potts model as an "interaction-round-face" model [16], KSZ [11] have derived so-called inversion relations for the transfer matrix of the Potts model. They then use these relations and certain analyticity assumptions [17] to calculate the spectrum of the transfer matrix at the transition point β_t. For the infinite volume correlation length ξ their result is

$$1/\xi = -\log(4\sqrt{p}) - 4\sum_{m=1}^{\infty}(-1)^m \log(1 + p^m), \tag{8}$$

with

$$p = \left(\frac{q-2}{2} + \frac{1}{2}\sqrt{q(q-4)}\right)^{-1} \tag{9}$$

For $q \searrow 4$, ξ diverges as [11]

$$\xi \approx \frac{1}{8}\exp\left(\frac{\pi^2}{\sqrt{q-4}}\right), \tag{10}$$

in accordance with the result obtained by renormalization group techniques [18].

In a recent preprint [12], BW have derived a different formula for the correlation length ξ at β_t. Starting from the six vertex model representation of the Potts model with free boundary conditions, they first show that the spectra for the corresponding transfer matrices at the transition point β_t are identical. Then, using a Bethe ansatz, they obtain for the infinite volume correlation length ξ at β_t

$$\begin{aligned} 1/\xi &= 4\sum_{m=1}^{\infty}\frac{(-e^{-2v})^m}{m}\sinh(mv)\tanh(2mv) + 2\log\left[\frac{\cosh(3v/2)}{\cosh(v/2)}\right] \\ &= \frac{1}{4}\sum_{n=0}^{\infty}\log\left[\frac{1+w_n}{1-w_n}\right], \end{aligned} \tag{11}$$

where v is the solution of $2\cosh v = (2+\sqrt{q})^{1/2}$, i.e.

$$v = \log\left(\frac{1}{2}\left[\sqrt{\sqrt{q}+2}+\sqrt{\sqrt{q}-2}\right]\right), \tag{12}$$

and

$$w_n = \left[\sqrt{2}\cosh\left((n+\frac{1}{2})\pi^2/2v\right)\right]^{-1} \tag{13}$$

Note that the formula (11) is implicitly already contained in reference [19].

For small values of $q-4$ the parameter v in (12) has an expansion

$$v = \frac{1}{4}\sqrt{q-4}+\ldots, \tag{14}$$

and the second expression in (11) converges rapidly. In fact, keeping only the $n=0$ term in leading order, we obtain an approximation

$$\xi \approx \frac{1}{8\sqrt{2}}\exp\left(\frac{\pi^2}{4v}\right). \tag{15}$$

Inserting (14) we arrive at the formula

$$\xi \approx \frac{1}{8\sqrt{2}}\exp\left(\frac{\pi^2}{\sqrt{q-4}}\right), \tag{16}$$

which differs from (10) by a factor of $\sqrt{2}$. While equation (16) is correct in the limit $q \to 4$, already for $q=5$ it is a very bad approximation, see table II. On the contrary, equation (15) is extremely accurate up to reasonably large values of q ($=20$, say). In fact, a formula of the form (15) has already been derived in reference [18] using renormalization group arguments.

In reference [12] it was observed that the correlation length ξ according to (11) agrees with $\xi_d = 1/m_d$ in the leading order of a large q expansion. However, this also holds for the result (8) of KSZ which is *identical* to (11) in the *leading* order of the large q expansion. In order to calculate the next to leading corrections for ξ_d, we use equation (7) and the fact that, for sufficiently large q, the methods of references [14] allow us to rigorously control the interface tension σ_{od} by convergent cluster expansions. It is a straightforward exercise to extract the leading orders of the large q expansion from these cluster expansions. We obtain

$$\sigma_{od}(\beta_t) = \frac{1}{4}\log q - 2q^{-1/4} + q^{-1/2} + O(q^{-3/4}). \tag{17}$$

For sufficiently large q, equation (7) is rigorous, which proves that at β_t

$$1/\xi_d = \frac{1}{2}\log q - 4q^{-1/4} + 2q^{-1/2} + O(q^{-3/4}). \tag{18}$$

Equation (18) should be compared with the large q expansions of ξ following from equation (8),

$$1/\xi = \frac{1}{2}\log q - \log 4 + O(q^{-1}) \qquad \text{(KSZ)}, \tag{19}$$

and from equation (11),

$$1/\xi = \frac{1}{2}\log q - 4q^{-1/4} + 2q^{-1/2} + O(q^{-3/4}) \qquad \text{(BW)}. \tag{20}$$

Table II.— *Correlation length ξ at the first-order transition point of the two-dimensional q-state Potts model as calculated by KSZ (Ref. [11], see Eqs. (8) and (22), below) and BW (Ref. [12], see Eq. (11)). The last two columns are the $q \searrow 4$ approximations to ξ (BW).*

q	ξ_{diag} (KSZ)	ξ (BW)	approx. (15)	approx. (16)
5	2512.246818	2512.246820	2512.246822	1708.872831
6	158.892663	158.892696	158.892729	94.902407
7	48.095798	48.095907	48.096015	26.369384
8	23.877986	23.878204	23.878422	12.290014
9	14.900755	14.901105	14.901454	7.299502
10	10.559026	10.559519	10.560013	4.969076
11	8.097408	8.098051	8.098694	3.685273
12	6.547225	6.548020	6.548815	2.896250
13	5.495888	5.496835	5.497783	2.372284
14	4.742632	4.743729	4.744827	2.003765
15	4.179709	4.180954	4.182200	1.732876
16	3.744789	3.746178	3.747568	1.526678
17	3.399605	3.401134	3.402666	1.365227
18	3.119510	3.121176	3.122844	1.235836
19	2.887982	2.889781	2.891583	1.130100
20	2.693574	2.695502	2.697434	1.042254

The comparison with equation (18) strongly suggests that the correlation length calculated by BW is actually the correlation length ξ_{d} of the disordered phase.

In fact, the infinite volume limit of the spectrum of the transfer matrix with *free* boundary conditions at β_{t} should give the spectrum of the infinite volume transfer matrix[1] in the *disordered* phase since expectation values with free boundary conditions turn into expectation values in the disordered phase once the thermodynamic limit is performed[2]. We therefore take it for granted that the correlation length ξ calculated by BW *is* actually the pure phase correlation length $\xi_{\mathrm{d}} = 1/m_{\mathrm{d}}$ of the disordered phase at β_{t}. Adopting this assumption, we combine (7) and (11) to obtain the desired explicit formula for the interface free energies σ_{oo} and σ_{od} at β_{t},

$$\boxed{2\sigma_{\mathrm{od}} = \sigma_{\mathrm{oo}} = \frac{1}{4}\sum_{n=0}^{\infty} \log\left[\frac{1+w_n}{1-w_n}\right].} \tag{21}$$

KSZ, on the other hand, have argued that the boundary conditions used in their calculations are equivalent to periodic boundary conditions in the infinite volume limit. Since periodic boundary conditions at the transition point β_{t} correspond to a convex combination of the ordered and the disordered phase, this would lead to the interpretation of the correlation length ξ calculated by KSZ as the maximum of ξ_{d} and ξ_{o}, where ξ_{o} denotes the correlation length of the ordered phase. As pointed out to us by Klümper [21], reference [11] contains a small inconsistency. The correlation length ξ(KSZ) according to equation (8) is *not* the *vertical*

(1) As constructed, e.g., in section 2a of reference [20].

(2) This statement is true as long as β is chosen in such a way that the disordered phase is stable, i.e. as long as $\beta \leq \beta_{\mathrm{t}}$.

correlation length as stated in KSZ. Instead, ξ(KSZ) is actually $\sqrt{2}$ times the correlation length ξ_{diag} along the diagonal,

$$\xi_{\text{diag}} = \frac{1}{\sqrt{2}}\,\xi(\text{KSZ}), \tag{22}$$

with ξ(KSZ) as in equation (8). Note that this gives

$$\xi_{\text{diag}} \approx \frac{1}{8\sqrt{2}} \exp\left(\frac{\pi^2}{\sqrt{q-4}}\right), \tag{23}$$

as $q \searrow 4$, in accordance with equation (16). This corresponds to the well known fact that the correlation length becomes isotropic when q approaches the critical value $q_c = 4$. On the other hand, it is not expected that ξ and ξ_{diag} are identical away from criticality. In practice, however, ξ and ξ_{diag} only differ by an amount which is numerically difficult to detect up to values of q as large as $q = 20$, see table II. The fact that $\xi/\xi_{\text{diag}} = \sqrt{2}(1 - 2\log 4/\log q + \ldots) \to \sqrt{2}$ in the limit $q \to \infty$, cf. equations (19), (20) and (22), shows that the small differences in table II are not due to numerical inaccuracies. Due to the logarithmic dependence on q, however, this limit is approached extremely slowly: $\xi/\xi_{\text{diag}} \approx 0.9\sqrt{2}$ for $q = 4^{20} \approx 10^{12}$; $\xi/\xi_{\text{diag}} \approx 0.99\sqrt{2}$ for $q = 4^{200} \approx 10^{120}$.

Numerically, the (vertical) correlation length of the 10-state Potts model has been computed by Peczak and Landau [22] and by Gupta and Irbäck [23]. The quoted results are $\xi = 5.9 \pm 0.7$ and $\xi = 5.66 \pm 0.09$, and are interpreted as the correlation length of the ordered phase [23]. For the Ising model, $2\sigma_{\text{oo}} = 1/\xi_{\text{o}}$ for all $\beta > \beta_c$. Assuming that such a relation also holds for the Potts model, a limiting argument would lead to the prediction $2\xi_{\text{o}} = \xi_{\text{d}}$ at the transition point β_t, which is consistent with the numerical data of references [22, 23].

3. Discussion.

The numerical values of $2\sigma_{\text{od}}$ according to equation (21) are given in table III. A comparison with the Monte Carlo results for $q = 7$ compiled in table I is clearly in favor of the estimate given in reference [5], which is based on a histogram method proposed a long time ago by Binder [24]. This is further supported by the good agreement with the numerical estimates for $q = 8$ and $q = 10$ derived by the same method. Even if we only use the inequality (3) instead of the complete wetting assumption (5), we obtain an *upper bound*, $2\sigma_{\text{od}} \leq 0.02079\ldots$ for $q = 7$, which is clearly violated by the estimates of references [3, 4]. Our analytical result thus supports the heuristic argument given in reference [5] that the methods of references [3, 4] overestimate the interface free energy.

The methods of references [3, 4] were subsequently applied to compute the interface free energy at the deconfining phase transition of SU(3) lattice gauge theory [25, 26], which is an important parameter for cosmological models. An exploratory analysis [5] based on the histogram method indicated again a lower value and led to the suggestion to investigate this problem once again more carefully with improved data [27]. In view of the present analytical results for the Potts model a large scale project clarifying the origin of the discrepancies between different numerical predictions for the same quantity seems to be even more urgent than before.

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Table III. — *Interface free energy at the first-order transition point of the two-dimensional q-state Potts model as calculated from our equation (21). For comparison also the Monte Carlo (MC) estimates of references [5, 6, 7] using the histogram method are given.*

q	$2\sigma_{\mathrm{od}}$	$2\sigma_{\mathrm{od}}$ (MC)	q	$2\sigma_{\mathrm{od}}$
5	0.000398		13	0.181923
6	0.006294		14	0.210805
7	0.020792	0.0241(10)	15	0.239180
8	0.041879	0.045	16	0.266939
9	0.067109		17	0.294020
10	0.094701	0.09781(75)	18	0.320392
11	0.123487		19	0.346047
12	0.152718		20	0.370988

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