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Numerical Study of Phase Transitions in Potts Models

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Abstract

A model is defined that interpolates between integer dimension and integer q-state Potts models. Phase transitions in these models are studied, and in particular the critical value q_c where the phase transition changes from second into first order is determined for several dimensions. For (d, q_c) the values (2.0;4.05), (2.5;2.68), (3.0;2.21), (3.5;2.15) and (4.0;2.07) are obtained.

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1 Introduction

For the past few decades, Potts models have provided a continuous source of research [1, 2]. This is mainly due to the fact that these models exhibit a rich critical behaviour, although they have a simple definition. In particular it is known that in the space $\{(d, q)\}$ of d-dimensional q-state Potts models, a critical line $(d, q_c(d))$ exists, separating the models with a second order phase transition ($q \leq q_c(d)$) from those with a first order phase transition ($q > q_c(d)$). The only points that are known to be exactly on this line are $(d, q) = (2, 4)$ [3] and for $d > 4$ $(d, 2)$ [4], and there is convincing evidence that $q_c(3) < 3$ [5, 6, 7, 8, 9, 10, 11, 12]. Further progress is difficult because models with noninteger d and q are hard to treat numerically. The only results known to us for noninteger (d, q) are $(1.58; 12.6)$, $(2; 4.08)$ and $(2.32; 2.85)$, which follow from a renormalization group analysis [5]. Recently, the Ising model has been studied in noninteger dimensions [13, 14], but these calculations have not been extended beyond $q = 2$.

In this paper we will define a family of models labeled by two parameters (d^*, q^*), which we expect to be a reasonable approximation of the (d, q) Potts model, and which for integer (d^*, q^*) agrees with the (d, q) Potts model. The (d^*, q^*) is essentially an anisotropic Potts model equipped with a certain non-local cluster dynamics, analogous to the one introduced by Swendsen and Wang [15, 16]. The latter has been quite successfully applied to a number of problems (for instance to the Potts model, see e.g. [17, 18, 19], or using the related Wolff algorithm [20], see e.g. [21]). We will perform a numerical study of the (d^*, q^*) models. In particular we will determine the critical temperature and try to measure the discontinuity in the internal energy which exists in case of a first order phase transition. Our results are in reasonable good agreement with the known theoretical results. A novel feature is that a considerable part of the simulations will be done at constant internal energy rather than constant temperature. This dramatically improves the statistics in the neighbourhood of the critical point. For more information about Monte Carlo simulations see e.g. [22].

This paper is organized as follows. In section 2 we define the model and recall some exact results from $d = 2$ for later use. In section 3 we determine the critical temperature of these models using a Monte-Carlo Renormalization Group Analysis [23, 24]. This method is known to be highly insensitive to finite size effects. In two dimensions we find that the critical temperature of the $(2, q^*)$ models agrees with the theoretical value of the q^*-state Potts models at least up to 0.1%. In section 4 we describe our method to determine the discontinuity in the internal energy for first order phase transitions, and how to use this to distinguish the different types

of critical behaviour. In section 5 we present our results, which were obtained from extensive simulations of a large number of (d^*, q^*) models on a three-processor Apollo DN-10000 workstation. In particular we determine $q_c^*(d^*)$ where d^* runs from 2 to 4 with steps of 0.5. We end with some conclusions in section 6.

2 The Model

Consider the following Hamiltonian of an anisotropic Potts model in d-dimensions, $\sigma_i \in \{1, \ldots, q\}$

$$\beta H = \sum_{r=1}^{d} J_r \sum_{\langle ij \rangle_r} \left(1 - 2\delta_{\sigma_i \sigma_j}\right), \tag{1}$$

where $\langle ij \rangle_r$ means a pair of neighbouring spins in the $\vec{e_r}$-direction, and $\beta = 1/k_B T$. We assume the spins live on a d-dimensional lattice with L^d sites and periodic boundary conditions. We also define the following quantities s and s_r

$$s_r = \frac{1}{L^d} \sum_{\langle ij \rangle_r} \left(2\delta_{\sigma_i \sigma_j} - 1\right), \tag{2}$$

$$s = \frac{\sum_{r=1}^{d} J_r s_r}{\sum_{r=1}^{d} J_r}. \tag{3}$$

Clearly all s_r and hence also s are equal to 1 if all nearest neighbour spins are equal, whereas $s = -1$ if all nearest neighbour spins are different. With the partition function $Z = \sum_{\langle ij \rangle} \exp(-\beta H)$, one has

$$\langle s_r \rangle = \frac{1}{L^d} \frac{\partial}{\partial J_r} \log Z, \tag{4}$$

$$\langle s \rangle = \frac{\sum_{r=1}^{d} J_r \langle s_r \rangle}{\sum_{r=1}^{d} J_r}. \tag{5}$$

The internal energy per site is now equal to

$$\beta u = -\sum_r J_r \langle s_r \rangle = -\langle s \rangle \sum_r J_r. \tag{6}$$

In general if $J \to \infty$ $\langle s \rangle \to 1$ and if $J \to 0$ $\langle s \rangle \to -1 + \frac{2}{q}$.

In two dimensions (see e.g. [2]) phase transitions occur for pairs (J_1, J_2) satisfying

$$\left(e^{2J_1} - 1\right)\left(e^{2J_2} - 1\right) = \sqrt{q}. \tag{7}$$

If $J_1 = J_2 = J$ then at the critical coupling $J = \log(\frac{1+\sqrt{q}}{2})$ one has

$$\langle s \rangle (J_{crit}) = \frac{1}{\sqrt{q}}, \tag{8}$$

and if $q \geq 4$ the discontinuity in $\langle s \rangle$ is given by

$$\langle s \rangle (J^{\pm}_{crit}) = \frac{1}{\sqrt{q}} \pm \left(1 + \frac{1}{\sqrt{q}}\right) \tanh \frac{\Theta}{2} \prod_{n=1}^{\infty} (\tanh n\Theta)^2, \tag{9}$$

where $\cosh \Theta = \frac{1}{2}\sqrt{q}$.

The dynamics of this system that we used, resemble those proposed in [15]. Given an arbitrary spin configuration, we make clusters by creating a bond between each pair of equal nearest neighbour spins in the $\vec{e_r}$ direction, with probability $(1 - e^{-2J_r})$. Then to all sites in each cluster a new state is assigned according to the following rule: the probability that all σ's in a particular cluster obtain the value $l \in \{1, \ldots, q\}$ is p_l. Note that $\sum p_l = 1$. In the usual Swendsen-Wang algorithm $p_l = \frac{1}{q}$ for all l. We will, however, allow for the possibility that the p_l's are different. In general, the resulting system will not correspond to a Potts model. We do not know whether it is possible to write down a Hamiltonian for which these dynamics give an equilibrium distribution, but if it exists we expect that it will necessarily be non-local.

We will now try to find couplings J_r and probabilities p_l such that this system describes as closely as possible a (d^*, q^*)-Potts model with coupling J^*. To fix the p_l consider n clusters occurring in the Swendsen-Wang dynamics above. The probability that to all clusters the same spin will be assigned is equal to

$$P_n = \sum_{l=1}^{n} p_l^n. \tag{10}$$

For a q^*-state Potts model we would have $P_n = (q^*)^{1-n}$. Therefore in order to have approximately the same multi-cluster interactions as in the q^*-state Potts model we require that

$$\sum_{l=1}^{n} p_l^n = (q^*)^{1-n} \tag{11}$$

for as many values of n as possible. Alternatively, these conditions can be derived by looking at the high-temperature expansion of s. It turns out that for noninteger q^* these relations can only be realized for $n = 1, 2$ but not for $n = 1, 2, 3$ simultaneously. If we now use standard variational techniques to minimalize $(\sum p_l^3 - (q^*)^{-2})$, subject

to the conditions $\sum p_l = 1$ and $\sum p_l^2 = (q^*)^{-1}$, we find that the best choice is to take $q = [q^*] + 1$ different spin values, where $[x]$ is the Entier function, and the following values of p_l

$$p_l = \frac{1}{q}\left\{1 + \sqrt{\left(\frac{q}{q^*} - 1\right)(q-1)^{-1}}\right\} \qquad 1 \le l \le q-1, \tag{2.12a}$$

$$p_q = \frac{1}{q}\left\{1 - \sqrt{\left(\frac{q}{q^*} - 1\right)(q-1)}\right\} \qquad l = q. \tag{2.12b}$$

To fix the J_i is a much more difficult problem. The small J_i behaviour of βu can be written as an expansion in $\sum_i J_i^n$ with $n \le 1$, so it would be tempting to try to realize

$$\sum_{i=1}^{d} J_i^n = d^*(J^*)^n \tag{2.13}$$

for as many values of n as possible. However, for large J_i there is an expansion in terms of $\sum_i J_i \exp(-2nJ_i)$ and this suggests we should rather try to realize

$$\sum_{i=1}^{d} J_i e^{-2nJ_i} = d^* J^* e^{-2nJ^*}. \tag{2.14}$$

We have used a certain 'hybrid' combination of (2.13) and (2.14) which includes these equations in the appropriate limits. We try to realize

$$\sum_{i=1}^{d} \left(J_i(1-e^{-2J_i})\right)^{n/2} = d^* \left(J^*(1-e^{-2J^*})\right)^{n/2} \tag{2.15}$$

for as many values of n as possible. This has two advantages: by putting $z_i = (d^*)^{-1}\{J_i(1-e^{-2J_i})/J^*(1-e^{-2J^*})\}^{1/2}$ we see that (2.15) is equivalent to $\sum_{i=1}^{d} z_i^n = (d^*)^{1-n}$, which can be solved in the same way as the p_l were determined, and the z_i uniquely determine the J_i because $f(x) = x(1-e^{-2x})$ is an invertible function for positive x. The solution is given by ($d = [d^*] + 1$):

$$\left(J_i(1-e^{-2J_i})\right)^{1/2} = \left(J_*(1-e^{-2J_*})\right)^{1/2} \frac{1}{d}\left\{1 + \sqrt{\left(\frac{d}{d^*} - 1\right)(d-1)^{-1}}\right\} \qquad i < d,$$

$$\left(J_i(1-e^{-2J_i})\right)^{1/2} = \left(J_*(1-e^{-2J_*})\right)^{1/2} \frac{1}{d}\left\{1 - \sqrt{\left(\frac{d}{d^*} - 1\right)(d-1)}\right\} \qquad i = d,$$

in which $d = [d^*] + 1$. Note that $J_d \downarrow 0$ as $d^* \downarrow d - 1$, so that one dimension effectively decouples from the theory as expected if we reduce the dimension by one. As a further consistency check observe that all $J_i \to 0$ if $J^* \to 0$ and that all $J_i \to \infty$ if $J^* \to \infty$. This completes the description of the model.

3 Location of the Critical Point

In order to determine the critical point we use the Monte Carlo Renormalization Group Method, for details see [23, 24]. We start with a small lattice S with $L = 2^{a-b}$ and a large lattice L with $L = 2^a$. Given a configuration of spins on a lattice with $L = 2^a$ we define a renormalized configuration on a lattice with $L = 2^{a-1}$, by replacing blocks of 2^d spins with one spin that is determined by the majority rule: Let $r_1, \cdots, r_h$ be the spins that occur most often in a block of 2^d spins, then the resulting spin is picked from $r_1, \cdots, r_h$, each with probability $1/h$. Let $\langle s^{(l)} \rangle$ denote the average of s for an $l-$times renormalized lattice, then the critical point is the point where $\langle s^{(l)} \rangle_S - \langle s^{(l+b)} \rangle_L$ changes sign. The advantage of this method is that it reduces finite-size effects very efficiently. The result can be further improved by increasing a or increasing l. We used $b = 1$ and $a = 4$, and determined J_{crit} by finding the zero of a least-square fitted straight line through a set of points $(J, \langle s^{(l)} \rangle_S - \langle s^{(l+b)} \rangle_L)$ in the direct vicinity of the phase transition. The statistical error was also obtained from these fits. After this, we took the average of the values for J_{crit} obtained for $l = 1$ and $l = 2$. Comparing the results for different values of a showed that the statistical error is indeed larger than the finite-size error. The results for certain values of q^* in $d = 2$ are depicted in table 1. We took $d = 2$, because in this case we know the theoretical value of J_{crit} (2.7), so that $d = 2$ can serve as a testing ground to see how good the fractional q^* model really is. As can be seen from table 1, the agreement is better than the statistical error and no systematic errors are visible at this level of accuracy. This shows that the fractional q^* model is indeed a very reasonable approximation of the $q-$state Potts model.

The data were obtained from a Monte Carlo simulation as described previously. For every value of q^*, the final spin configuration obtained from the Monte Carlo simulation of the previous value of q^*, was used as initial configuration, upon which 5000 thermalization steps were performed. Every new data point was obtained from another 5000 Monte Carlo steps, of which the first 2000 were used for thermalization.

4 Nature of the Phase Transition

In general it is very difficult to determine numerically the order of a phase transition, see e.g. [5, 6, 7, 8, 9, 10, 11, 12]. The method we used essentially amounts to measuring the presence of a latent heat, which is only present for a first order phase transition. Strictly speaking, the finite size effect spoils the presence of a true latent heat, but one can nevertheless try to measure the corresponding gap in the (J, s) curve, using the procedure below.

We performed simulations of Potts models for various values of (d^*, q^*), and for each we determined numerically J as a function of s. This has the advantage that much more data are obtained that are in the direct vicinity of the critical point, as opposed to measuring s as a function of J. Because s is not a parameter of the model, we used a method that is well know in e.g. constant pressure simulations in molecular dynamics, namely we build a 'thermostat' into the simulation. More precisely, after every Monte Carlo sweep we determine $s\{\sigma_r\}$, and then adjust J according to the rule $J' = J - \mu(s\{\sigma_r\} - s)$, where μ is a small multiplier. We used $\mu = 0.01$ during the 500 thermalization sweeps and $\mu = 0.002$ for the 1500 measurement sweeps performed for every point (s, J). For every value of (d^*, q^*), we obtained points (s, J) with s ranging from $-1 + \frac{q^*}{2}$ to 0.9 with steps of 0.02. As $s = -1 + \frac{q^*}{2}$ corresponds to an infinite temperature configuration, we could take a purely random initial configuration and no initial thermalization is needed. We also performed a run with s running in the opposite direction to check for the presence of hysteresis. We could not detect any, indicating that the correlation time is sufficiently eliminated by the thermalization steps. Altogether it took about 100,000 sweeps to determine one curve (s, J), each sweep taking about one second on our workstation.

From the values (s, J) thus obtained, we determined the point of minimal dJ/ds, and took 12 points at both sides of this point. In case there was a large gap visible, a few extra points were added, in case s was close to unity, one or two points were skipped at both sides. This set of points was used to perform a least square fit of a certain function $J(s)$. The function we have taken consists of two power-like branches, $J = c_l - a_l(x_l - s)^{e_l}$ for $s < \min(x_l, \frac{x_l+x_r}{2})$ and $J = c_r + a_r(s - x_r)^{e_r}$ for $s > \max(x_r, \frac{x_l+x_r}{2})$. c_l and c_r are chosen in such a way that both branches are glued together continuously. In case $x_r > x_l$, J is given by $J(s) = c_l = c_r$ for $x_l < s < x_r$. Clearly, this corresponds to the behaviour of J in the scaling region of an ideal first order phase transition. The latent heat we extract is $x_r - x_l$, and is negative if $x_r < x_l$. One might argue that due to the finite size effects, the function above is not a good description of the (s, J) curve for a finite lattice. However, we expect that the latent heat obtained from this fit will still be a reasonable approximation of the infinite lattice latent heat.

At this stage we have obtained the latent heat as function of q^*, which is negative in some cases. These negative values do not have any physical meaning, they are purely numerical artifacts. Finally, we have determined the value for q_c by defining it as the point where the latent heat changes sign. To find this point, we matched the latent heat with a function of q^* which is $-a_l(q_c - q^*)^2$ for $q^* < q_c$, and which is $a_r(q^* - q_c)^2$ for $q^* > q_c$, and optimalized a_l, a_r and q_c. This is our final result for q_c.

5 Results

Because the correlation time increases as the lattice size increases [25], not only will the sweeps take more time for a larger lattice, but we also need more sweeps to overcome the correlation time. This strongly limits the lattice sizes that can be used in the simulations. We used a 128×128 lattice for $d^* = 2$, a $32 \times 32 \times 32$ lattice for $d^* = 2.5, 3$ and $10 \times 10 \times 10 \times 10$ for $d^* = 3.5, 4$. The results for the latent heat and the exponents e_l and e_r have been gathered in table 2. The final results for q_c are shown in table 3, together with the typical statistical errors for the gapsizes and exponents for each dimension. Here, the values of $\triangle e+$ and $\triangle e-$ indicate the typical positive and negative deviations of the values for the exponents given in table 2. A typical plot of some (s, J)-curves is provided for $d = 2$ and $d = 3$ in figures 1 and 2. The shadowed areas indicate the fitted curve for the latent heat as a function of q^*. Finally, we have given a plot of q_c versus d^* in figure 3.

If we compare the location and the size of the measured latent heat for $d = 2$ with the theoretical values that can be computed from (2.8) and (2.9), we see that the agreement for the location is good and for the size reasonable. For $(d, q) = (3, 3)$ we can compare our result with the latent heat as obtained in [10, 11], and again the agreement is reasonable. In comparing these values with the theoretical ones, one should bear in mind that the errors as indicated in table 3 are purely statistical. We find the surprisingly good value of $q_c^* = 4.05$ for $d = 2$. The value for $d = 4$ is also in good agreement with the theoretical value $q_c = 2$. The result for $d^* = 2.5$ agrees with the results of [5] (indicated by a circle in figure 3). What is certainly clear is that the phase transition for the three-dimensional three state Potts model is of first order. On the other hand our results seem to contradict the result of [4] that $q_c(4 - \epsilon) = 2 + \epsilon + \mathcal{O}(\epsilon^2)$. The behaviour of q_c in figure 3 near the point $(4, 2)$ does not display any visible edge.

The exponents that are displayed in table 2 are for $q^* > q_c$ related to the standard exponent α via $\alpha = 1 - \frac{1}{e}$. For $q^* < q_c$ they have no direct physical meaning. Furthermore, the systematic error, due to the deviation from pure scaling in the region where we fitted $J(s)$, is quite large for the critical exponents, but small for the latent heat. Therefore, one should not have too much confidence in the values

for $q^* > q_c$ either. If one's main interest is the determination of the values of the exponents, there are better methods to obtain these. One can e.g. obtain $e_l - 1$ and $e_r - 1$ by fitting a power like curve through $(s, \frac{dJ}{ds})$, where $\frac{dJ}{ds}$ can be accurately determined as in [23]. Another method is to use the Monte Carlo Renormalization Group Method [23, 24].

A final remark concerns the systematic errors involved in this method. As the derivative dJ/ds is typically ~ 0.02 along the gaps in the (s, J) curves, we expect that the systematic errors due to the finite size effect are certainly smaller than the statistical errors. The finite size effect tends to increase the value of q_c. Comparing our value of q_c with the theoretical values for $d = 2, 4$ suggest that the systematic error is altogether not much larger than 0.05.

6 Conclusions

In summary, we have simulated a large number of Potts models and managed to confirm the suspected behaviour of q_c versus d. Of course, our model is not equivalent to a real fractional (d, q) Potts model. From the definition one sees that it does not interpolate analytically between the integer (d, q) models, but continuously. The fractional q behaviour seems to be quite unambiguously defined, in contrast to the fractional d behaviour, for which other definitions are as plausible as ours. It would be interesting to try to 'fractionalize' other systems that allow a description in terms of Swendsen-Wang dynamics.

The model can be improved in several ways. The definition of the J_i in terms of J^* can certainly be improved. One can also *define* the dimension of a Potts model by looking at the finite size scaling of the correlation length [14], or at the finite size scaling of the size of the largest cluster [18]. To determine the value of q_c one can also look at the finite size scaling of the maximum value of the specific heat, which is different for first and second order phase transitions [26, 8]. Computation speed might be improved by using the algorithm of Wolff [20], or by using other methods to obtain the (J, s) curves [27, 28]. Parallelizing or vectorizing the algorithm should also be possible. We leave these issues to future work.

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q^*	J_{crit}(exp)	J_{crit}(theor)	$10^5 \triangle$J
2.0	0.44060(65)	0.44069	-09
2.2	0.45507(82)	0.45478	+29
2.4	0.46764(76)	0.46789	-25
2.6	0.47973(52)	0.48014	-42
2.8	0.49241(70)	0.49166	+75
3.0	0.50253(66)	0.50253	-00
3.2	0.51270(57)	0.51282	-12
3.4	0.52312(56)	0.52259	+53
3.6	0.53170(72)	0.53190	-21
3.8	0.54100(56)	0.54079	+21
4.0	0.54981(56)	0.54931	+50
4.2	0.55781(57)	0.55747	+34
4.4	0.56597(50)	0.56532	+65
4.6	0.57223(54)	0.57287	-64
4.8	0.58114(72)	0.58015	+99
5.0	0.58723(62)	0.58718	+05
5.2	0.59330(52)	0.59398	-67
5.4	0.60045(73)	0.60055	-11
5.6	0.60623(99)	0.60693	-70
5.8	0.61380(44)	0.61311	+69

Table 1:
Measurement of J_{crit} for various values of q^* and $d = 2$.

d^*	q^*	e_l	e_r	latent heat
2.0	5.0	1.97	2.00	0.094
	4.8	1.95	2.04	0.034
	4.6	2.14	1.92	0.005
	4.4	1.99	2.00	-0.004
	4.2	2.03	1.89	0.020
	4.0	1.97	1.97	0.019
	3.8	2.08	2.30	-0.058
	3.6	2.70	2.25	-0.172
2.5	2.9	1.73	1.82	0.076
	2.8	1.67	1.77	0.082
	2.7	1.77	1.96	0.059
	2.6	1.87	2.12	0.010
	2.5	3.29	2.00	-0.159
	2.4	3.26	2.29	-0.209
3.0	3.3	1.25	0.91	0.241
	3.1	1.15	1.55	0.233
	2.9	1.34	1.83	0.130
	2.7	1.71	1.67	0.061
	2.5	1.97	1.88	0.008
	2.3	2.01	2.11	-0.013
	2.1	1.77	2.29	0.007
	1.9	2.71	1.81	-0.111
	1.7	3.14	2.70	-0.208
3.5	2.5	1.08	1.15	0.192
	2.4	1.57	0.93	0.118
	2.3	1.37	1.17	0.097
	2.2	1.67	1.94	0.049
	2.1	1.80	2.31	-0.009
	2.0	2.04	2.15	-0.015
	1.9	3.85	2.04	-0.370
	1.8	3.27	1.88	-0.416
4.0	2.5	1.08	0.68	0.245
	2.4	1.05	0.67	0.223
	2.3	1.14	0.67	0.195
	2.2	1.14	0.91	0.180
	2.1	1.34	1.42	0.080
	2.0	1.26	1.77	0.096
	1.9	2.47	2.18	-0.083
	1.8	3.00	2.30	-0.354
	1.7	2.24	0.92	-0.428
	1.6	3.05	2.19	-0.456

Table 2:
The latent heat and exponents for
various values of d^* and q^*.
For typical statistical errors see table 3.

d^*	q_c^*	$\triangle$gap	$\triangle e+$	$\triangle e-$
2.0	4.05(16)	0.02	+40%	-15%
2.5	2.68(9)	0.05	+80%	-40%
3.0	2.21(5)	0.04	+50%	-30%
3.5	2.15(7)	0.03	+70%	-30%
4.0	2.07(9)	0.03	+80%	-25%

Table 3:
Typical statistical errors in the exponents
and latent heat as given in table 2;
q_c^* is the value of q^* where the phase
transition changes from second into first order.

Figure Captions

figure 1: The internal energy S in two dimension, as function of J, for various values of q. The shaded area represents the latent heat.

figure 2: The internal energy S in three dimension, as function of J, for various values of q. The shaded area represents the latent heat.

figure 3: Phase diagram of the (d^*, q^*) Potts model. The circle indicates a value taken from [5].