Ground state entropy and the **q** = 3 Potts antiferromagnet on the honeycomb lattice

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Abstract. We study the q-state Potts antiferromagnet with $q = 3$ on the honeycomb lattice. Using an analytic argument together with a Monte Carlo simulation, we conclude that this model is disordered for all $T \geqslant 0$. We also calculate the ground state entropy to be $S_0/k_B = 0.507(10)$ and discuss this result.

The effect of ground state disorder and associated non-zero ground-state entropy S_0 has been a subject of longstanding interest. A physical example is ice, for which $S_0 = 0.82 \pm 0.05$ cal/(K-mole), i.e. $S_0/k_B = 0.41 \pm 0.03$ [1, 2]§. Among spin models, an example is the Ising antiferromagnet (AF) on the triangular lattice. In the context of this model, Wannier argued that a non-zero ground state (GS) entropy implies the absence of long-range order, namely, staggered magnetization M_{st} for $T \geqslant 0$ [3]. Another example is the Ising AF on the kagomé lattice [4, 5]. In both of these Ising models, the non-zero GS entropy has the effect of removing a phase transition at finite temperature. The Ising AF on the triangular lattice is critical at $T = 0$ [6], while on the kagomé lattice, with a larger value of S_0, it is disordered even at $T = 0$ [5]. In these two cases, the non-zero GS entropy is associated with frustration. However, there are also spin models, such as the antiferromagnetic q-state Potts model [7–9] on the square (SQ) and honeycomb (HC) lattice, which exhibit GS entropy without frustration. Because of the absence of frustration, these models constitute ideally simple cases where one can study the effects of ground state entropy on the thermodynamics of a statistical mechanical model‖ In contrast to the ferromagnetic (FM) Potts model, which has a finite-temperature phase transition for dimensionality $d > 1$, the question of whether the q-state Potts AF has a phase transition at finite (or zero) temperature is more delicate and depends on both the value of q and the type of lattice. The $q = 3$ Potts AF on the SQ lattice has been well studied; an exact result of Baxter showed that it is critical at $T = 0$ [11], in agreement with a renormalization group argument [12], and several Monte Carlo simulations have been performed on it [13, 14]. However, to our knowledge, the behaviour of the $q = 3$ Potts AF on the HC lattice has not been definitely established. We report here the results of a study of this model.

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§ Henceforth, we shall use units such that $k_B \equiv 1$.
‖ Ground state entropy without frustration can also occur in models with continuous variables and interactions [10]. A yet more complicated case is that of quenched disorder with frustration, as in spin glasses.

The (isotropic, nearest-neighbour, zero-field) q-state Potts model on a lattice Λ is defined by the partition function $Z = \sum_{\{\sigma_n\}} e^{-\beta\mathcal{H}}$ with the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle nn' \rangle} \delta_{\sigma_n \sigma_{n'}} \tag{1}$$

where $\sigma_n = 1, \ldots, q$ are Z_q-valued variables on each site $n \in \Lambda$, $\beta = T^{-1}$, and $J < 0$ for the AF case. We define $K = \beta J$, $a = e^K$, $x = (a-1)/\sqrt{q}$, and the reduced free energy (per site) $f = -\beta F = \lim_{N \to \infty} N^{-1} \ln Z$, where N denotes the number of sites in the lattice. We consider $\Lambda = hc$ here.

We first observe that for the $q = 2$ (Ising) case, the paramagnetic–ferromagnetic (PM–FM) and PM–AFM critical points are both determined by the equation [15]

$$\sqrt{q} + 3x - x^3 = 0. \tag{2}$$

These are $a_c = 2 + \sqrt{3}$ (PM–FM) and $a_{c,AF} = a_c^{-1} = 2 - \sqrt{3}$ (PM–AFM). (The third root of equation (2) is a complex-temperature (CT) singular point at $a = -1 \equiv a_s$.) An equivalent representation of the partition function is $Z = \sum_{G' \subseteq G} v^{b(G')} q^{n(G')}$ [16, 17, 9], where G' denotes a subgraph of $G = \Lambda$, $v = (a - 1)$, $b(G')$ is the number of bonds and $n(G')$ the number of connected components of G'. This enables one to analytically continue the model from positive integral q to real q [17, 9]. Carrying out this analytic continuation and analysing equation (2) for the critical points, one sees that the points $a_c(q)$ and $a_{c,AF}(q)$ increase and decrease, respectively, reflecting the fact that as q increases, one must go to lower temperature to achieve FM and AFM long-range order. As q reaches the value $q_z = (3 + \sqrt{5})/2 = 2.618\ldots$, $a_{c,AF}$ decreases to 0, i.e. the AFM phase is squeezed out, and there is no longer any finite-temperature AF critical point, which now occurs only at $T = 0$. Note that $q_z = B_5 = 1 + \tau$, where $B_r = 4\cos^2(\pi/r)$ is the r'th Beraha number [18] and τ is the golden mean. When $q > q_z$, $a_{c,AF}$ is negative, i.e. an unphysical, CT singular point. It follows that for $q > q_z$ and, in particular, for $q = 3$, the HC Potts AF has no critical point or associated continuous phase transition at any $T \geqslant 0$†. As q increases from q_z to $q = 3$, the root of equation (2) which, for $q < q_z$, was the PM–AFM critical point $a_{c,AF}(q)$, moves left from the origin. Since for $q > q_z$, there is no longer any physical AFM phase, we shall denote this point as a_{c2}; it moves from $a_{c2}(q_z) = 0$ left to $a_{c2}(3) = -0.1848\ldots$. Meanwhile, as q increases from 2 to 3, (i) the PM–FM critical point $a_c(q)$ moves to the right, through $a_c(q_z) = \frac{1}{2}(3 + \sqrt{15 + 6\sqrt{5}}) = 4.1654..$ to $a_c(3) = 4.4115\ldots$, and the disordered, paramagnetic (PM) phase (and its CT generalization) expands accordingly; (ii) the root $a_s(q)$ of (2) moves left, from -1, through $a_s(q_z) = \frac{1}{2}(3 - \sqrt{15 + 6\sqrt{5}}) = -1.1654\ldots$, to $a_s(3) = -1.2267\ldots$.

In particular, this argument by analytic continuation in q excludes the possibility, for the HC lattice, of a massless low-temperature phase with algebraic asymptotic decay of correlation functions of the type discussed in [21]. However, this leaves open the possibility that the model might have a first-order transition (with finite correlation length, and hence noncritical). Indeed, this is what did happen for the $q = 3$ Potts AF on the triangular

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† From these exact results, recalling the connection $Z(q, \Lambda, K = -\infty) = P_\Lambda(q)$, where $P_G(q)$ is the chromatic polynomial for the graph G [19], we would expect that the behaviour of $P_{hc}(q)$ (where $\Lambda = hc$ denotes the thermodynamic limit of the HC lattice) would differ for $q < q_z$ and $q > q_z$, as would follow if the zeros of $P_{hc}(q)$ formed a boundary curve in the complex q plane which crossed the real axis at q_z and separated the regions which include the segments $q < q_z$ and $q > q_z$. Given the observation that the crossing point of a boundary curve increases by about $\Delta q \simeq 0.4$ from an 8×8 triangular lattice with cylindrical boundary conditions (CBCs) to the thermodynamic limit [20], our expectation is consistent with the finding [20] that there is a crossing curve on the 8×8 HC lattice with CBCs at $q \simeq 2.2$.

lattice [22, 23], although for that case, the ground state is only finitely degenerate, so that $S_0 = 0$, and M_{st} is non-zero below the transition. In contrast, given that S_0 is non-zero in the present case of the HC lattice, the Wannier argument implies that $M_{st} = 0$ for all $T \geqslant 0$, so that the discontinuity at such a hypothetical transition would have to occur in U but not in M_{st}. We consider this to render such a transition unlikely but do not know of a proof which precludes a discontinuity in short-range order (which enters into U) while long range order, M_{st}, remains zero.

An effective way to study this possibility of a phase transition is to perform Monte Carlo simulations of the model, and we have done this†. For the Monte Carlo simulation, we have used two different algorithms to update the spins: the Metropolis algorithm and the Swendsen–Wang cluster algorithm (SWCA) [24]. Since the SWCA reduces critical slowing down in simulations of models exhibiting a critical points with divergent correlation lengths, the agreement of the results obtained from these two algorithms serves as a confirmation of our conclusion from the analytic argument above that the model is not critical at $T = 0$. For Metropolis, we used lattices with periodic boundary conditions (BCs) of sizes ranging from 8×8 to 40×40. For SWCA, following [24], we used lattices with helical BCs in the horizontal direction and free BCs in the vertical direction (where the HC lattice is represented as a brick lattice with horizontal bricks) with sizes ranging from 19×19 to 39×39. Typically, we ran for several thousand sweeps through the lattice for thermalization before calculating averages. Each average was calculated from 10 000 sweeps through the lattice. The full data was obtained as a thermal loop, to test for any hysteresis associated with either critical slowing down or metastability. No such hysteresis was observed. The results obtained with these two different algorithms were in excellent agreement, differing at most by only about 1%. In figure 1 we show measurements of the internal energy per site, U, from the SWCA simulation.

The intercept and slope at $K = 0$ follow from the high-temperature expansion $-U/J = (g/2)[1/q + ((q-1)/q^2)K + O(K^2)]$, where g is the coordination number of the lattice, so $U/|J| = \frac{1}{2} + \frac{1}{3}K + O(K^2)$ for the $q = 3$ Potts AF on the HC lattice. Clearly, at $T = 0$, i.e. $K = -\infty$, the spins on each bond must be different, so $U = -(g/2)\langle \delta_{\sigma_n \sigma_{n'}} \rangle = 0$. As a check on our program, we have also simulated the $J > 0$ model and obtained excellent agreement with the PM–FM phase transition known from equation (2) to occur at $K_c = 1.484$. Evidently, the data smoothly curves down from the $K = 0$ value toward the $K = -\infty$ value as K decreases to -5; there is no indication of any phase transition, in particular, a first-order one. The absence of any critical slowing-down for large negative K is in agreement with our analytic argument from equation (2) that the model is not critical at $T = 0$. The fact that the data for the 19×19 and 39×39 lattices are very close to each other (as was also true for the intermediate sizes that we used) shows that it is not necessary to go to larger lattice sizes; the present ones are adequate for our conclusion. Indeed, this is not surprising, in view of our result that the lattice is disordered for $T \geqslant 0$ (if there had been any indication of critical behaviour as signalled, e.g. by critical slowing-down, then we would also have run simulations on larger lattices).

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† Two other methods would be (i) to analyse high-temperature series expansions (a first-order transition could manifest itself in a peculiar behaviour of exponents, as in [23]); and (ii) to calculate CT zeros of the partition function and search for a new phase boundary which crosses the positive real a axis at a point not included in the roots of (2). (This relies on the fact that in the thermodynamic limit, these zeros typically merge to form curves which separate CT generalizations of phases. If such a boundary were found, the density of zeros near the real axis would yield the critical exponent α, and $\alpha = 1$ would suggest a first-order transition.) While these methods are of interest in their own right, we were able to obtain convincing evidence for our conclusion from the Monte Carlo method alone.
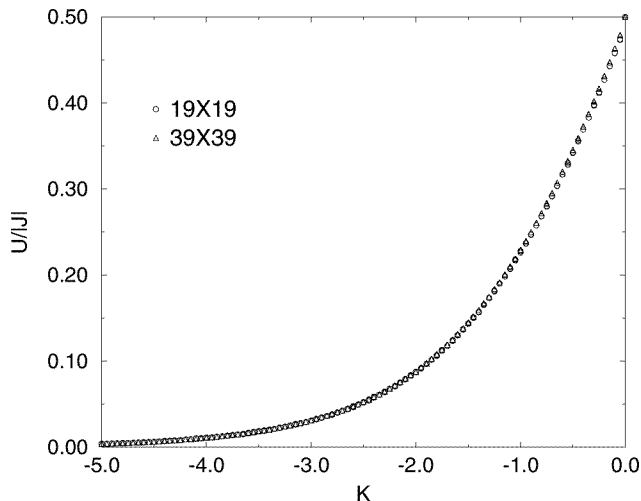
Figure 1. Measurements of internal energy U, as a function of $K = \beta J$, for the $q = 3$ Potts AF on the HC lattice. See text for details.

Our results imply that the $q = 3$ Potts AF on the HC lattice has the property that in the complex a plane, the points $a = 1$ ($K = 0$) and $a = 0$ ($K = -\infty$) are analytically connected and $a = 0$ does not lie on a CT phase boundary. We have calculated CT zeros of Z on small lattices with periodic BCs and have obtained results which are consistent with this conclusion†. We note that previous studies of the CT zeros of the square-lattice Potts model for $q = 3$ and 4 have shown that the pattern of zeros in the $\mathrm{Re}(a) < 0$ region exhibits a significant dependence on the boundary conditions [25–27].

For $q \geqslant 4$, it has been proved that the Potts AF on the HC lattice is disordered for all $T \geqslant 0$ [28]. This result is quite consistent with our finding, since increasing q increases the disorder in the model.

As part of our study, we have calculated the GS entropy $S_0(\Lambda, q) = S_0(hc, 3)$ of the model, using the relation

$$S(\beta) = S(\beta = 0) + \beta U(\beta) - \int_0^\beta U(\beta')\,\mathrm{d}\beta' \tag{3}$$

starting the integration at $\beta = 0$ with $S(\beta = 0) = \ln q$ for the q-state Potts model. We found, as in previous work [29], that this provides a very accurate method for calculating S_0. For this we used the Metropolis algorithm with periodic BCs for several lattice sizes. Since $U(K)$ rapidly approaches its asymptotic value of 0 as K decreases past about $K = -5$ (see figure 1), the RHS of (3) rapidly approaches a constant in this region, enabling one to obtain the resultant value of $S(\beta = \infty)$ for each lattice size. We then performed a fit to this data and extrapolated the result to the thermodynamic limit; the results are shown in figure 2. As a check, we also carried out the analogous calculations for the $q = 3$ Potts AF on the SQ lattice. A fit to the finite-size dependence of our sq lattice data agrees very well with the form found in [13, 30], $S_0(sq, 3) = S_0(L; sq, 3) + c_{sq,3}/L^2$ with $c_{sq,3} = 1.077$, and we get $S_0(sq, 3) = 0.4317(3)$, in excellent agreement with the exact value $S_0(sq, 3) = \frac{3}{2}\ln\frac{4}{3} = 0.4315\ldots$ [2, 8, 9]. For the HC lattice, as is evident from
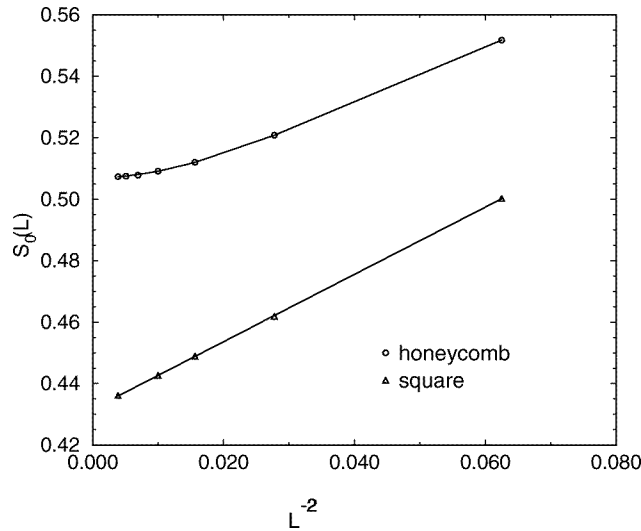
Figure 2. Measurements of GS entropy S_0, as a function of lattice size, for the $q = 3$ Potts AF on the HC and SQ lattices.

figure 2, our measurements do not exhibit the same finite-size dependence as for the sq lattice. An empirical function including terms up to L^{-6} yields a good fit to the data (see figure 2) and gives the $L = \infty$ value of the GS entropy for the $q = 3$ HC Potts AF

$$S_0(hc, 3) = 0.507 \pm 0.010 \tag{4}$$

where the error is an estimate of the uncertainty. This yields $W(hc, 3) = 1.66 \pm 0.02$, where $W(\Lambda, q) = e^{S_0(\Lambda, q)}$. We observe that our results are consistent, to within the uncertainty, with the exact expression $W(hc, 3) = \frac{5}{3}$. The ratio $R_S(\Lambda, q) = S(\Lambda, q, T = 0)/S(q, T = \infty)$ serves as a useful measure of the reduction of disorder in a given model as T decreases from ∞ to 0. Our results yield $R_S(hc, 3) = 0.4615 \pm 0.010$ for the $q = 3$ HC Potts AF, which shows that the disorder at $T = 0$ is a substantial fraction of its maximal, $T = \infty$ value.

From the basic relation $S = \beta U + f$ and the property that $\lim_{K \to -\infty} \beta U(\beta) = 0$, as is true of the q-state Potts AF models considered here, it follows that

$$S_0(\Lambda, q) = f(\Lambda, q, K = -\infty) = \lim_{N \to \infty} N^{-1} \ln(P_\Lambda(q)) \tag{5}$$

or equivalently $W(\Lambda, q) = \lim_{N \to \infty} P_\Lambda(q)^{1/N}$. That is, the GS entropy is determined by the asymptotic behaviour of the chromatic polynomial in the thermodynamic limit. Series of the form $W(\Lambda, q) = q((q - 1)/q)^{g/2} \bar{W}(\Lambda, q)$, where $\bar{W}(\Lambda, q) = 1 + \sum_{n=1}^{\infty} w_n y^n$ with $y = 1/(q - 1)$ were calculated in [31]. It is of interest to compare our result (4) with an estimate from the series for $\bar{W}(hc, 3) = 1 + y^5 + 2y^{11} + 4y^{12} + \cdots$, calculated through $O(y^{18})$ [31]. Because of the changes of sign in the HC series (the coefficients of the first five terms are positive, while those of the remaining four terms are negative), it is difficult to make a reliable extrapolation. Simply taking the sum yields $W(hc, 3) = 1.687$, which is agreeably close to our central value, 1.66.

In summary, combining analytic arguments and a Monte Carlo simulation, we have reached the conclusion that the $q = 3$ Potts AF on the HC lattice is disordered for all $T \geqslant 0$ and have calculated the GS entropy for this model.

Acknowledgment

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