FIRST-ORDER PHASE TRANSITIONS IN POTTS AND ISING SYSTEMS

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We use an equivalence between the q-state Potts model on a d-dimensional lattice for $q = 2^n$, n = 1, 2, ... and a spin 1/2 Ising model on n copies of the lattice with $2n$-spin ferromagnetic interactions to obtain some exact new results for both systems. In particular we prove the existence of first-order phase transitions for a class of ferromagnetic Ising systems obtained as perturbations of the large q Potts–Ising system and the non-vanishing of the surface tension for the Potts model (with $q = 2^n$) at all temperatures below their transition temperature.

1. Introduction. The q-state Potts model is defined as follows: at each site $i \in Z^d$ there is a variable $s_i = 0, 1, 2, ..., q-1$, the hamiltonian in a finite box $\Lambda \subset Z^d$ is

$$H_{\Lambda,\mathrm{bc}} = J \sum_{\langle ij\rangle \subset \Lambda} \delta_{s_i s_j} + J \sum_{\langle ij\rangle} \delta_{s_i \tilde{s}_j} . \qquad (1)$$

The two sums are over nearest-neighbour pairs, $\delta_{ss'}$ is the Kronecker delta, and J is the coupling constant. In the second sum, $\tilde{s}_j$ is fixed outside Λ, and represents boundary conditions (bc). We shall consider the q pure bc (l) obtained by fixing $\tilde{s}_j = l$ outside Λ, $l \in \{0, ..., q-1\}$, the free bc (f) where the second sum in (1) is omitted, and the mixed (l, l') bc defined, for a rectangular Λ, by fixing $\tilde{s}_j = l$ for the top half of the box and $s_j = l'$ for the bottom half. The Gibbs measures in Λ are:

$$\mathrm{d}\mu_{\Lambda,\mathrm{bc}} = Z^{-1}_{\Lambda,\mathrm{bc}} \exp(-\beta H_{\Lambda,\mathrm{bc}}) , \quad \beta = 1/kT .$$

We let $\langle\ \rangle_{\mathrm{bc}}$ denote the expectation with respect to the thermodynamic limit, $\Lambda \uparrow Z^d$, of the Gibbs measure with a particular bc.

What makes the Potts model (1) interesting is that its simple structure permits a rather precise analysis of its phase diagram. Thus, for certain lattices in two dimensions, Baxter [1] found the exact transition temperature and, for $q > 4$, also the jump discontinuity in the energy. For $q \leqslant 4$ he found the transition to be second order. In three dimensions it is expected [2] that the transition will be first order even for $q = 4$. What can be proven rigorously is that [3] for sufficiently large q the transition is first order in *all* dimensions $d \geqslant 2$.

For $q = 2$ the Potts model is identical to a ferromagnetic Ising model. Ferromagnetic Ising systems have been studied very extensively and there are a lot of exact results available from various inequalities. E.g. the surface tension τ is known to be zero for $T > T_c$ [4] and non-zero for $T < T_c$ [5]. A relationship between the ferromagnetic Ising model and the Potts model for $q > 2$ could therefore be useful for our understanding of both. Such a relation is in fact used

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for $q = 4$ ($d = 2$) where Potts ↔ Ashkin–Teller [6]. In this note we generalize this relation to all $q = 2^n$, $n = 1, 2, \ldots$ Potts models and derive additional results about the existence of first order transitions in modified Potts models and their Ising analogs.

2. Potts ↔ Ising isomorphism. Consider a $q = 2^n$ state Potts model on a lattice $\mathcal{L}$. The states s_i can then be put in one-to-one correspondence with a configuration of n spins $\sigma_i^\alpha = \pm 1$, $\alpha = 1 \ldots n$, which may be thought of as all being on the same site i, or as living on n copies of $\mathcal{L}$, e.g. in $d = 2$ we imagine n layers of $\mathcal{L}$. We have that

$$\delta_{s_i, s_j} = \prod_{\alpha=1}^{n} \tfrac{1}{2}(1 + \sigma_i^\alpha \sigma_j^\alpha) = 2^{-n} \sum_E \prod_{\alpha \in E} \sigma_i^\alpha \sigma_j^\alpha + 2^{-n} , \tag{2}$$

where the sum runs over all non-empty subsets of $\{1, \ldots, n\}$. Identifying the configuration $\sigma_i^\alpha = 1$ (-1) for all α with $s_i = q - 1$ (0), the bc $s_j = q - 1$ (0) become the + (−) bc in the Ising model.

We remark that the main point of this representation (when $q = 2^n$) is that it is ferromagnetic. Indeed for all q we can use a variety of spin $\frac{1}{2}$ representations, (e.g. Griffiths' method [7]) but these are in general not ferromagnetic.

3. Results on the Ising model derived from the Potts model. The Potts model undergoes a first-order transition for some values of q. This was shown by Baxter for all $q > 4$ in two dimensions [1] and by Kotecky and Shlosman for q large enough in all dimensions [3]. (For $d \geqslant 3$, this presumably holds for all $q \geqslant 3$).

The phase diagram is as follows: for β large, there are q pure phases distinguished by an order parameter. (Here, and in similar statements below, we mean at least that many phases because it has not yet been shown that there are no other pure translation invariant states but their occurrence is unlikely). There is then a temperature, $\beta_q^{-1} = T_q$, where there is a transition with $q + 1$ phases: q ordered ones $\langle\ \rangle^{(l)}$ and one disordered one $\langle\ \rangle^{(\mathrm{f})}$. Above T_q, there is presumably only one state. At β_q the order parameter jumps to zero and the mean energy is also discontinuous. Using our representation for $q = 2^n$ this gives the only example known to us of a ferromagnetic spin $\frac{1}{2}$ Ising model where a first-order transition is rigorously proven.

Note that the order parameter in the phase with $l = q - 1$ bc, $\delta_{s_i, q-1} - q^{-1}$ becomes in the spin variables $\Sigma_E \Pi_{\alpha \in E} \sigma_i^\alpha$. In the other phases it is obtained by flipping an appropriate number of σ_i^α's.

The Ising model picture suggests the following question: What happens if we perturb the model by adding an external field or some other many-body interactions? The answer in the cases that we can analyse is that the low temperature phases may change but the first-order transition persists.

One type of perturbation is as follows: Consider $(n + 1)$ spins σ_i^α, define

$$\delta_\lambda(s_i, s_j) = \left(\prod_{\alpha=1}^{n} \tfrac{1}{2}(1 + \sigma_i^\alpha \sigma_j^\alpha)\right) \tfrac{1}{2}(1 + \lambda \sigma_i^{(n+1)} \sigma_j^{(n+1)}) ,$$

and insert this into the definition of the hamiltonian (1). This is a special case of the cubic model [8] and, for λ varying between 0 and 1, it interpolates between the $q = 2^n$ and $q = 2^{n+1}$ Potts models. Then one can show that for λ *or* $(1 - \lambda)$ small and n large there is a first-order transition (jump in the energy and magnetization) as β varies. More generally, consider any function $h_q(s, s')$ and such that $|h_q(s, s')| \leqslant 1$, define

$$\delta_\lambda(s, s') = \delta(s, s') + \lambda h_q(s, s') , \tag{3}$$

and insert this into (1). Of course the "universality class" of the system may change discontinuously at $\lambda = 0^+$.

These are still nearest-neighbor interactions but the perturbation is otherwise arbitrary. It may also include an external field. Then, by a modification of the proof of ref. [3], one can show:

Proposition 1. There exist q_0, λ_0 such that for each $q > q_0$ and $|\lambda| < \lambda_0$, there exist a $\beta(q, \lambda)$ where there is a first order transition in the model defined by (1) and (3). That is, the derivative of the free energy with respect to β is discontinuous at $\beta(q, \lambda)$. Moreover, at $\beta(q, \lambda)$, there exist two translation invariant equilibrium states, one with $\langle \delta_{s_i s_j} \rangle > \frac{1}{2}$ and one with $\langle \delta_{s_i s_j} \rangle < \frac{1}{2}$.

Remark: The proposition does not say that there are q states at low temperature. In fact, as the following example will show this is not in general true. Take the specific case of

$$h_q(s, s') = \tfrac{1}{2}[\delta(s, q - 1) + \delta(s', q - 1)] ,$$

i.e. an external field favoring the $q-1$ state. Then we are not restricted to small λ: for every $\lambda_0 > 0$ there exists a q_0, such that the model undergoes a first-order transition for all $q > q_0$ and all λ, $0 < \lambda < \lambda_0$. Of course, if we fix q and let λ be large, there will be no transition. Similarly, if we choose $h(q, q') = \Sigma_{\alpha,\alpha'} \sigma_i^\alpha \sigma_i^{\alpha'}$, $\alpha, \alpha' = 1, ..., n$, there will be only two ground states.

4. Results on the Potts model derived from the Ising model. The Ising representation (2) allows us to use various correlation inequalities valid for ferromagnetic spin systems. In particular one can extend results of Lebowitz and Pfister [5] on the existence of a nonzero surface tension between different phases.

We define the surface tension in the Potts model between phases l and l' by

$$-\lim_{L\to\infty} L^{-(d-1)} \lim_{M\to\infty} \log(Z_{L,M}^{l,l'}/Z_{L,M}^{l}) = \tau , \qquad (4)$$

where L, M are the dimensions of a box $\Lambda_{L,M}$ of height M and cross sectional area L^{d-1}. In $Z_{L,M}^{l,l'}$ we have mixed l, l' bc. By symmetry $Z_{L,M}^{l,l'}$ (and τ) does not depend on l, l' if $l \neq l'$. For motivation of this definition see ref. [9]. The limits in (4) are not known to exist in general, but for $q = 2^n$ one can prove that they exist, using our transformation and the results of [10]. Now we state

Proposition 2: Let $q = 2^n$.

(a) If $\beta > \beta_q$, then $\tau \neq 0$. Moreover, $d\tau/d\beta$ (which exists at least a.e.) satisfies:

$$\frac{d\tau}{d\beta} \geqslant 2J \sum_E \left(\left\langle \prod_{\alpha\in E} \sigma \right\rangle^+\right)^2 \Big/ 2^n$$

$$\geqslant 2J\,[\langle(\delta_{s_i,q-1} - q^{-1})\rangle]^2 .$$

(b) If $\beta < \beta_c$ for the spin $\frac{1}{2}$ Ising model with nn interactions and coupling constant $J/2$, then $\tau = 0$.

Proof: (a) The proof is essentially as in ref. [5]. If we take $l = q-1$ and $l' = 0$ in (4) then we have + and − bc in the corresponding Ising model. We write

$$\frac{-d}{d\beta} \log(Z_{L,M}^{+-}/Z_{L,M}^{+}) = 2^{-n}J \times \sum_{\langle i,j\rangle} \sum_E \left(\left\langle \prod_{\alpha\in E} \sigma_i^\alpha \prod_{\alpha\in E} \sigma_j^\alpha \right\rangle^+ - \left\langle \prod_{\alpha\in E} \sigma_i^\alpha \prod_{\alpha\in E} \sigma_j^\alpha \right\rangle^{\pm} \right).$$

Using the inequalities of [5] and following the argument of [5] we end up with the first inequality. The second is just the Schwartz inequality since

$$\delta_{s_i,q-1} = \prod_{\alpha=1}^{n} \tfrac{1}{2}(1 + \sigma_i^\alpha) = q^{-1} + q^{-1} \sum_E \prod_{\alpha\in E} \sigma_i^\alpha .$$

(b) If we add to the hamiltonian (1), expressed in terms of the σ_i^α variables a term

$$\lambda \sum_{i\in\Lambda} \sum_{\alpha=2}^{n} \sigma_i^1 \sigma_i^\alpha ,$$

then, by Griffiths' inequalities τ is increasing in λ. When $\lambda \to \infty$, the σ_i^α are either all +1 or all −1. Therefore, we get a two-state Ising model where the energy difference between parallel and antiparallel spins equals $J/2$ [i.e. the same as with coupling $(J/2)\sigma_i\sigma_j$].

Remarks:

(i) We expect that, if one defines a different surface tension $\tilde{\tau}$,

$$\tilde{\tau} = -\lim_{L\to\infty} L^{-(d-1)} \lim_{M\to\infty} \log[Z_{L,M}^{l,\mathrm{f}}/(Z_{L,M}^{l} Z_{L,M}^{\mathrm{f}})^{1/2}],$$

where in $Z_{L,M}^{l,\mathrm{f}}$ we put $\tilde{s}_j = l$ on the top half of the box and free bc on the bottom half, then $\tilde{\tau}$ will be zero everywhere except at β_q where it will be strictly positive; this expectation is based on the fact that at β_q we have

$$\langle \delta_{s_i,s_j} \rangle^{\mathrm{f}} \neq \langle \delta_{s_i s_j} \rangle^{l} ,$$

and only there.

(ii) We note that, for nn Ising models, refs. [4,5] imply that the physical surface tension $K^{-1}\tau(K)$, $K = \beta J$ is monotone increasing in K: by [5] $d\tau/dK \geqslant 2(m^*)^2$ and by [4], $\tau(K) \leqslant 2(m^*)^2 K$ where m^* = spontaneous magnetization; therefore

$$\frac{d}{dK}[\tau(K)/K] = K^{-1}\, d\tau/dK - K^{-2}\tau \geqslant 0 .$$

(iii) It follows from [11] and our spin $\frac{1}{2}$ representation (2) that for $q = 2^n$ there are at most q translation invariant equilibrium states except possibly for a countable set of values of β. An argument due to Pfister actually shows that it is true for all q.

(iv) For mean field, renormalization group and computer investigations of Ising spins with two- and four-body ferromagnetic interactions showing first-order transitions we refer the reader to recent works by Mauritsen et al. [12] and references contained therein. For relevance to alloys see Connolly and Williams [13]. An interesting point there is that a first-order transition can occur even when the system has only two ground states, $\sigma_i = +1$ or -1, all i. As already noted this can also be proven rigorously for our models by choosing h appropriately in (3) and taking q large enough. In fact this includes cases when there is only one ground state.

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