Potts models with invisible states on general Bethe lattices

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Abstract
The number of so-called invisible states which need to be added to the q-state Potts model to transmute its phase transition from continuous to first order has attracted recent attention. In the q = 2 case, a Bragg–Williams (mean-field) approach necessitates four such invisible states while a 3-regular random graph formalism requires seventeen. In both of these cases, the changeover from second- to first-order behaviour induced by the invisible states is identified through the tricritical point of an equivalent Blume–Emery–Griffiths model. Here we investigate the generalized Potts model on a Bethe lattice with z neighbours. We show that, in the q = 2 case, \( r_c(z) = \frac{4}{\pi(\frac{z-1}{z})^2} \) invisible states are required to manifest the equivalent Blume–Emery–Griffiths tricriticality. When \( z = 3 \), the 3-regular random graph result is recovered, while \( z \to \infty \) delivers the Bragg–Williams (mean-field) result.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The ferromagnetic q-state Potts model is defined through the Hamiltonian

\[ H_q = -\sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j} , \]

with nearest-neighbour interactions between spins \( \sigma_i \), defined at the sites \( i \) of a suitable d-dimensional lattice [1]. In the standard set-up, the spins \( \sigma_i \) each take one of \( q \) possible values, sometimes referred to as ‘colours’. A phase transition is induced by breaking the underlying q-fold symmetry of the model and the nature of the transition, including its order,
is a function of \( q \). In \( d = 2 \) dimensions, the Potts model has a second-order phase transition for \( q \leq 4 \) and a first-order transition for higher \( q \)-values. For \( d \geq 3 \) dimensions, only the two-state Potts (Ising) model has a continuous transition and transitions for higher \( q \)-values are of first order.

Recent experimental studies have suggested that some models with \( q \)-fold symmetry breaking in two dimensions do not display the same transition order as the corresponding ferromagnetic \( q \)-state Potts model \([2–4]\). Motivated by such discrepancies, Tamura \textit{et al} investigated an extended Potts model with a number of ‘colourless’ or ‘invisible’ states \([5–8]\). These redundant states do not contribute to the internal energy of the system, nor do they alter its symmetry or the number of ground states available. However, they change the entropy of the model as they increase the overall number of microstates available to the system. Tamura \textit{et al} showed that such invisible states can change the order of a phase transition. Indeed, in \([9]\) the invisible state Potts model was used to successfully model the Heisenberg model on distorted triangular lattices with competing interactions where such atypical transition orders are seen.

The new Hamiltonian introduced in \([5–8]\) is

\[
\mathcal{H}_{(q,r)} = - \sum_{\langle i,j \rangle} \delta_{s_i,s_j} \sum_{a=1}^{q} \delta_{s_i,a} \delta_{s_j,a}, \quad s_i = 1, \ldots, q, \; q + 1, \ldots, q + r, \tag{2}
\]

where the second summation ensures that only the first \( q \) spins contribute to the Hamiltonian (i.e., to the energy). While the remaining \( r \) spins do not contribute to the Hamiltonian, they are traced over in the partition function and thus contribute to the entropy. The new Hamiltonian defines a \((q, r)\)-state Potts model with \( q \) visible and \( r \) invisible states.

Using numerical simulations, Tamura \textit{et al} found that the introduction of a sufficiently large number of invisible states changes the nature of the two-dimensional, \( q \leq 4 \), Potts-model phase transition from (continuous) second order to first order. The strength of these first-order transitions increases with the addition of yet more invisible states; the latent heat increases and the transition temperature decreases. On the analytic side, Tamura \textit{et al} also applied a Bragg–Williams (mean-field) approximation to the \((q, r)\)-state Potts models. For \( q = 2 \), this delivers a second-order transition for \( r = 1, 2 \) and 3 and a first-order transition for \( r \geq 4 \). If \( q \geq 3 \), mean-field theory gives a first-order transition even in the ordinary Potts model and this transition remains first order with the introduction of invisible states.

The existence of a first-order transition to a low-temperature, broken-symmetry phase for the \((q, r)\)-state models has been rigorously proven using random-cluster methods in \([10]\) for \( q > 1 \) and sufficiently large \( r \). The transmutation of some second-order transitions into first-order transition by invisible states is therefore well established. In \([11]\) the case of \( q = 2 \) visible states was investigated using 3-regular random graphs as an alternative route to mean-field calculations. A curious feature was that seventeen invisible states were required to induce a first-order transition using this route, compared to that of Bragg–Williams, which required only \( r = 4 \) to effect this change.

Here we investigate the \( q = 2 \), generalized Potts model defined on the Bethe lattice with a general number of nearest neighbours \( z \). In the absence of invisible states this model exhibits a continuous phase transition. We derive a general formula for the critical number of invisible states \( r_c(z) \) above which the transition transmutes to first order. In the case of \( z = 3 \) this recovers the random graph result of \([11]\). In the \( z \to \infty \) limit, our formula recovers the Bragg–Williams (mean-field) result that \( r = 4 \) invisible states are required to render the transition first order.

Following \([5]\) it is convenient to rewrite equation (2) by introducing spins \( \sigma_i \), where \( \sigma_i = s_i \) if \( s_i = 1, \ldots, q \) and \( \sigma_i = 0 \) otherwise. This leads to an effective Hamiltonian \( \mathcal{H}'_{(q,r)} \) with \( q \)
standard spins and one additional spin which does not contribute to the nearest neighbour energy term but is coupled to a temperature dependent external field,

$$\mathcal{H}'(q,r) = - \sum_{\langle i,j \rangle} \delta_{\sigma_i,\sigma_j} + \sum_{a=1}^{q} \delta_{\sigma_i,a} \delta_{\sigma_j,a} - T \ln r \sum_{i} \delta_{\sigma_i,0}, \quad \sigma_i = 0, 1, \ldots, q. \quad (3)$$

By construction, the partition functions for $\mathcal{H}(q,r)$ and $\mathcal{H}'(q,r)$ are identical, so we may employ whichever formulation is most convenient. For the particular case where $q = 2$, direct consideration of the Boltzmann weights in the latter formulation shows equivalence to a Blume–Emery–Griffiths (BEG) Hamiltonian,

$$\mathcal{H}_{\text{BEG}} = - \frac{1}{2} \sum_{\langle i,j \rangle} t_{i,j} - \frac{1}{2} \sum_{\langle i,j \rangle} t_{i,j}^2 - \mu \sum_{i} (1 - t_{i}^2), \quad t_i = +1, 0, -1 \quad (4)$$

with a temperature-dependent, crystal-field term $\mu = T \ln r$ and equal couplings for the two nearest-neighbour interaction terms [12]. The crystal-field term may also be interpreted as the chemical potential of an annealed Potts lattice gas, which was studied in the classic paper of Berker et al [13].

The tactic is then to exploit knowledge of the phase diagram of the BEG model to investigate the effects of varying the number of invisible states $r$ in the equivalent $(2, r)$-state Potts model. Analytical calculations are possible in various circumstances. In particular, Tamura et al used a Bragg–Williams (mean-field) calculation to show that four invisible states were sufficient to transmute the $(2, r)$-state Potts-model transition into a first-order transition. In [11], on the other hand, it was found that a different mean-field calculation on 3-regular random graphs required seventeen invisible states to effect such a change. The mechanism for changing the order of the transition in both cases is identical and can be understood by examining the phase diagram of the BEG model in the $\mu, T$ plane (figure 1).

The BEG model manifests a line of phase transitions which changes from first to second order at a tricritical point. The $(2, r)$-state Potts system accesses the BEG phase transitions by following lines of increasing slope for increasing $r$ as $T$ is varied. For $r = 1$ the $(2, r)$-state

![Figure 1. A schematic drawing of an equal-coupling, mean-field, BEG-model phase diagram in the $\mu, T$ plane. The second-order transition regime is shown as a solid line and the first-order region as a dashed line. The arrowed, sloped lines marked (a) and (b) represent the trajectory of the system as $T$ is increased for different values of $r$, using $\mu = T \ln r$.](image)
Figure 2. Two shells around the central vertex (circled) of a Bethe lattice with $z = 3$ nearest neighbours. In the full lattice the branching continues ad infinitum. For the recursive calculation of the partition function the spin $t_0$ resides on the central vertex.

The Potts model is identical to the BEG model with vanishing crystal field. For small values of $r$, the generalized Potts model remains in this universality class. However, for sufficiently large values of $r$, such a line traverses the first-order portion of the BEG phase diagram, rather than the second-order part. The number of invisible states required to transmute the phase transition from second to first order is therefore given by the position of the tricritical point on the BEG-model phase diagram.

In the next section, we follow [14, 15] and use recursion relations to derive the tricritical point of the BEG model on the Bethe lattice with equal couplings for the two nearest-neighbour interaction terms. This is compared to a saddle-point calculation on regular random graphs in section 3. Although the methods used are rather different, the solutions are identical. It proves easier to generalize the Bethe-lattice calculation to an arbitrary number of nearest neighbours, and we give the general formula for the tricritical point, and hence the critical number of invisible states, for any number $z$ of nearest neighbours on the Bethe lattice.

2. The BEG model on a Bethe lattice and its tricritical point

The Bethe lattice offers a convenient way to formulate mean-field models in statistical mechanics since the hyperbolic nature of its geometry means that it is effectively infinite-dimensional [16]. The shell-like nature of its construction also means that statistical mechanical models formulated on the Bethe lattice lend themselves to exact solutions via recursion relations. The first two generations, or shells, of a Bethe lattice with $z = 3$ neighbours are shown in figure 2. The statistical mechanical behaviour of spin models defined on the Bethe lattice is calculated ‘deep within’ the lattice, disregarding the effect of the boundary, which contains as many points as lie within the lattice itself. Regular random graphs offer an alternative way to perform what is effectively the same calculation since they appear locally identical to the Bethe lattice, but with branches that are closed off by generically large loops.

Our aim is to evaluate the partition function for the BEG model on a Bethe lattice and, in particular, to determine the tricritical point which will allow us to find the critical number
of invisible states required to effect a first-order transition. This may be done in a standard manner for the Bethe lattice by evaluating the partition function recursively, shell by shell, starting at the central vertex given by \( i = 0 \) [14, 15, 17, 18]. The partition function can be written as

\[
Z = \sum_{\{l\}} \exp \left( -\beta \mathcal{H}_{\text{BEG}} \right),
\]

or, more explicitly, as

\[
Z = \sum_{\{l\}} \exp \left( \frac{\beta}{2} \sum_{(i,j)} t_{ij} + \frac{\beta}{2} \sum_i t_i^2 - \ln r \sum_i t_i^2 \right),
\]

where we have used \( \beta \mu = \Delta = \ln r \) and ignored an inessential constant. This may be separated into the contribution of the central spin, \( t_0 \), and the \( z \) branches emerging from it

\[
Z = \sum_{t_0} r^{-t_0^2} \left[ g_l(t_0) \right]^2,
\]

where the branch partition function \( g_l(t_0) \) with \( l \) shells is given by

\[
g_l(t_0) = \sum_{x \neq t_0} \exp \left( \frac{\beta}{2} t_0 t_1 + \frac{\beta}{2} t_0^2 + \frac{\beta}{2} \sum_{i,j} t_{ij} + \frac{\beta}{2} \sum t_i^2 \right) r^{-t_0^2}.
\]

This in turn may be written recursively as

\[
g_l(t_0) = \sum_{x_l} \exp \left( \frac{\beta}{2} t_0 t_1 + \frac{\beta}{2} t_0^2 \right) r^{-t_0^2} \left[ g_{l-1}(t_1) \right]^{x_l-1}.
\]

Defining the ratios

\[
x_l = \frac{g_l(-1)}{g_l(0)} \quad \text{and} \quad y_l = \frac{g_l(+1)}{g_l(0)}
\]

allows the branch partition function recursion relations to be recast as

\[
x_l = \frac{r + x_{l-1}^{-1} e^b + y_{l-1}^{-1}}{r + x_{l-1}^{-1} + y_{l-1}^{-1}}, \quad y_l = \frac{r + x_{l-1}^{-1} + y_{l-1}^{-1} e^b}{r + x_{l-1}^{-1} + y_{l-1}^{-1}}.
\]

The different phases of the BEG model appear as different fixed points of these recursion relations as the parameters \( r \) and \( \beta \) are varied (\( x_l = x_{l-1} \equiv x \) and \( y_l = y_{l-1} \equiv y \)). Following [14, 15] we define

\[
\begin{align*}
 u &= \frac{1}{2} (x + y - 2), & v &= \frac{1}{2} (x - y), & b &= \frac{e^b - 1}{2},
\end{align*}
\]

and rewrite the fixed point equations as

\[
\begin{align*}
 r^2 &= \frac{4(b - u)^2}{u^2 - v^2} \left[(u + 1)^2 - v^2\right]^{-1}, \\
 1 &= \frac{u - v}{u + v} \left(\frac{u + v + 1}{u - v + 1}\right)^{z_l-1}.
\end{align*}
\]

As discussed in [14] there are two families of solutions to the recursion relations. The first is given by

\[
 v = 0, \quad r = \frac{2(b - u)(u + 1)^{z_l-1}}{u}.
\]
The second solution has
\[ r^2 = \frac{4(b-u)^2}{u^2 - v^2} [u + 1)^2 - v^2]^{z-1} \]  
(15)
with
\[ 1 - \frac{(z-1)u}{u+1} + \left( \frac{v}{u+1} \right)^2 \mathcal{F}(u, v) = 0, \]
(16)
where, for odd \( z \)
\[ \mathcal{F}(u, v) = \left( C^{z-1}_2 - C^{z-1}_3 \frac{u}{u+1} \right) + \cdots + \left( \frac{v}{u+1} \right)^{z-3}, \]
(17)
and for even \( z \)
\[ \mathcal{F}(u, v) = \left( C^{z-1}_2 - C^{z-1}_3 \frac{u}{u+1} \right) + \cdots + \left( z - 1 - \frac{u}{u+1} \right) \left( \frac{v}{u+1} \right)^{z-4} \]
(18)
where the \( C^{z-1}_n \) are binomial coefficients of an expansion in \( v/(u+1) \).

The \( \lambda \)-line of critical points in the BEG model is determined by the equality of the two solution sets which occurs when
\[ r = \frac{2(b-u)}{u} (u+1)^{z-1}, \quad u = \frac{1}{z-2}. \]
(19)
The \( \lambda \)-line of critical points in the BEG model is cut by the first-order transition of the quadrupolar moment at the tricritical point, which separates the second-order transition region from the first-order region. The tricritical point is defined by the condition that two different solutions of the second family of solutions of the equation of state coincide at the \( \lambda \)-line. Thus, the tricritical point is given by the solution of
\[ \frac{\delta r^2}{\delta u} = \frac{\partial r^2}{\partial u} + \frac{\partial r^2}{\partial v^2} \frac{\partial v^2}{\partial u} = 0, \]
(20)

at the point \( v = 0 \) and \( u = 1/(q-2) \), where \( r(u, v) \) is given in equation (15). This gives
\[ \frac{u+1}{b-u} = z - 2 + \frac{z-3}{2z} \frac{1}{u} \]
(21)
where \( u = 1/(q-2) \). From equations (19) and (21), we obtain values of \( b \) and \( r \) at the tricritical point on a Bethe lattice with \( z \) neighbours as
\[ b_c(z) = \frac{5z - 6}{3(z-2)^2} \]
(22)
and
\[ r_c(z) = \frac{4z}{3(z-1)} \left( \frac{z-1}{z-2} \right)^z. \]
(23)

Referring back to the equivalence between the BEG model and the \((2, r)\)-state Potts model we see that the Potts model displays a first-order transition for \( r > r_c \) invisible states.

Since the result applies for general \( z \) we have, for instance,
\[ z = 3, \quad r_c(3) = 16, \]
\[ z = 4, \quad r_c(4) = 9 \]
(24)
and we can also take the \( z \to \infty \) limit to find \( r_c(\infty) = 4e/3 \simeq 3.624 \). The monotonicity of \( r_c(z) \) as a function of \( z \) is shown in figure 3.
3. Comparison with the BEG model on random graphs

Another approach to mean-field theory in statistical mechanics is to consider the models on regular random graphs. As we have noted, they are clearly related to the same models on the Bethe lattice since the local environment for the spins is identical. The (generically) large loops which close the branches of the Bethe lattice to give the corresponding regular random graph turn out not to affect the critical behaviour, at least for the ferromagnetic transitions considered here [19, 20].

It is possible to enumerate undecorated 3-regular random graphs by considering them to be generated by the ‘Feynman diagram’ expansion of a scalar integral, rather than a path integral as in a quantum field theory or an integral over matrices as in a matrix model [21, 22]. The number of 3-regular random graphs with \( n \) vertices is given by evaluating the integral

\[
N_n = \frac{1}{2\pi i} \oint \frac{d\lambda}{\lambda^{2n+1}} \int_{-\infty}^{\infty} d\phi \ exp \left( -\frac{1}{2} \phi^2 + \frac{\lambda}{3} \phi^3 \right) \tag{25}
\]

using a perturbative expansion of the \( \phi^3 \)-term to the required order. Other families of random graphs can be enumerated in a similar fashion by simply replacing the potential, for instance by using a \( \phi^r \) term for \( r \)-regular random graphs. The graphs may be decorated with the appropriate weights, both edge and vertex, for the statistical mechanical model under consideration by evaluating a similar integral for an ‘action’ which generates the correct weights when expanded perturbatively. In the case of the BEG model on 3-regular random graphs such an integral is given by

\[
Z_n(\beta) \times N_n = \frac{1}{2\pi i} \oint \frac{d\lambda}{\lambda^{2n+1}} \int \frac{d\phi_1 d\phi_2 d\phi_3}{2\pi \sqrt{\det K}} \ exp(-S_{\text{BEG}}), \tag{26}
\]
where the BEG action is
\[ S_{\text{BEG}} = \frac{1}{2} \left( \phi_1^2 + \phi_2^2 + \phi_3^2 \right) - a (\phi_1 \phi_3 + \phi_2 \phi_3) - \frac{\lambda}{3} \left( \phi_1^3 + \phi_2^3 + \phi_3^3 \right) \]
(27)
and \( K \) is the propagator evaluated from the inverse of the quadratic coefficients. Since the BEG model is a spin-1 model with three spin states, \( t_i = \pm 1, 0 \), three variables \( \phi_1, \phi_2, \phi_3 \) are required to generate the perturbative expansion of \( Z_n(\beta) \).

The coefficients in \( S_{\text{BEG}} \) are chosen so that inverting the quadratic terms to obtain the propagator and including the extra factor of \( \sigma \) for any \( \phi_3^3 \) vertices gives weights to the spin configurations on 3-regular random graphs which match those coming from the BEG Hamiltonian \( H_{\text{BEG}} \). It is also possible to scale \( \phi_3 \) to remove the \( \sigma \) from the cubic coupling, but this then gives a non-canonical coefficient for the \( \phi_3 \) propagator. The coefficients in \( S_{\text{BEG}} \) required to match the Hamiltonian couplings are given by
\[ e^{-\beta} = \frac{a^2}{1 - a^2}, \]
\[ \sigma = a^3 e^{\beta \mu} = a^3 r, \]
(28)
so the physical range of the coefficient
\[ a = \sqrt{\frac{1}{e^\beta + 1}} \]
(29)
in \( S_{\text{BEG}} \) is \( 0 < a < 1/\sqrt{2} \).

The vertex coupling \( \lambda \) may be scaled out of \( S_{\text{BEG}} \) and the leading contribution in the thermodynamic limit \( n \to \infty \) evaluated using the saddle-point equations
\[ \frac{\partial S_{\text{BEG}}}{\partial \phi_1} = \phi_1 - a \phi_3 - \phi_2 = 0, \]
\[ \frac{\partial S_{\text{BEG}}}{\partial \phi_2} = \phi_2 - a \phi_3 - \phi_2 = 0, \]
\[ \frac{\partial S_{\text{BEG}}}{\partial \phi_3} = \phi_3 - a (\phi_1 + \phi_2) - a^3 r \phi_3^2 = 0 \]
(30)
whose various solutions then delineate the phase diagram.

Consideration of other spin models on such regular random graphs has shown that the content of the saddle-point equations is identical to the fixed point equations obtained when the models are formulated on the corresponding Bethe lattice with the same number of neighbours. Although it is not immediately apparent that this is also the case for the BEG recursion relations in equation (11) and the saddle-point equations in equation (30), we can show this is so by using the first two equations of (30) to write the third as
\[ \tilde{\phi}_3 = \frac{a^2}{1 - 2a^2} \left( \phi_1^2 + \phi_2^2 \right) + \frac{a^2 r}{1 - 2a^2} \tilde{\phi}_3^2, \]
(31)
where we have rescaled \( \phi_3 \to \tilde{\phi}_3/a \) for convenience. The first two equations may then be rewritten using equation (31) as
\[ \phi_1 = \tilde{\phi}_3 + \phi_1^2 = \frac{1 - a^2}{1 - 2a^2} \tilde{\phi}_3^2 + \frac{a^2}{1 - 2a^2} \phi_2^2 + \frac{a^2 r}{1 - 2a^2} \tilde{\phi}_3^2, \]
\[ \phi_2 = \tilde{\phi}_3 + \phi_2^2 = \frac{1 - a^2}{1 - 2a^2} \tilde{\phi}_3^2 + \frac{a^2}{1 - 2a^2} \phi_1^2 + \frac{a^2 r}{1 - 2a^2} \tilde{\phi}_3^2 \]
(32)
and taking the ratio of these with equation (31) recovers the fixed point equations for the recursion relations in equation (11) for \( z = 3 \) with \( x = \phi_1/\tilde{\phi}_3 \) and \( y = \phi_2/\tilde{\phi}_3 \).
Similar manipulations of the saddle-point equations may be used to demonstrate the equivalence with the Bethe lattice fixed points for general $z$, so conclusions drawn about the Bethe lattice phase diagram with $z$ neighbours may also be taken to apply to the model on $z$-regular random graphs.

4. Discussion

The number of invisible states required to obtain a first-order transition is determined by the position of the tricritical point in the BEG model, so it is a non-universal quantity. It is therefore of no surprise that it depends on the details of the lattice under consideration, such as the number of neighbours for the Bethe lattice considered here. We have seen, however, that the fixed point of Bethe lattice recursion relations and the saddle-point equations which determine the phase diagram on the regular random graphs have the same content. The tricritical point $r_c(z)$ on $z$-regular random graphs is thus determined by the same equations which give the fixed points of the recursion relations on the Bethe lattice with $z$ neighbours and the values of $r_c(z)$ are identical in these cases. The previous calculation in [11] of $r_c(3)$ for 3-regular random graphs agrees with $r_c(3) = 16$ found here for the Bethe lattice.

It is also interesting to note that the result found for the Bragg–Williams approximation, where four invisible states are sufficient to produce a first-order transition with a $(2, r)$-state Potts model, is consistent with the $z \to \infty$ value calculated here on the Bethe lattice. In this case the nearest-neighbour environment with $z \to \infty$ is closer to that in standard mean-field theory where we think of the model as living in a high dimensional space where $z$ is also large.

The fact that invisible states can produce first-order transitions on Bethe lattices is evidence for the generality of the phenomenon, while its dependence on the coordination number $z$ indicates the non-universality of the mechanism. The explicit calculations here have focussed on the $(2, r)$-state Potts model since, as we have noted, mean-field theory in all its variants gives a first-order transition for the standard $q \geq 3$-state Potts model. The happy coincidence of the correspondence with the BEG model then allows the explicit determination of $r_c(z)$. On planar random graphs continuous Potts transitions exist for $q = 2, 3, 4$ and we have already remarked in [11] that the critical number of invisible states in the $(2, r)$-state Potts model on 4-regular planar random graphs may be transcribed from the solution using matrix models [23, 24] of the BEG model on such graphs to give $r_c = 223$ states. In principle, the matrix models for the $q = 3, 4$-state Potts models with a suitable external field coupling to an invisible state in the manner of equation (3) would allow a similar determination for $q = 3, 4$ in a non-mean-field context.

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