ON THE PHASE DIAGRAM OF THE $q \to 1$ EXTENDED POTTS MODEL AND LATTICE ANIMAL COLLAPSE

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The phase diagram of the two-dimensional extended $q$-states Potts model is investigated in the $q \to 1$ limit. This is equivalent to studying the phase diagram of a two-dimensional infinite interacting lattice animal. An exact solution on the Bethe lattice and a Migdal-Kadanoff renormalization group calculation predict a line of $\theta$ transitions from an extended to a compact phase in the lattice animal. We compare this with the phase diagram predicted from previous numerical studies.

The collapse transition of polymers in dilute solution has been a subject of much current attention. Here, we are interested in the collapse of interacting, two-dimensional branched polymers, as modelled by lattice animals. A lattice animal is a connected graph of occupied sites. Some examples are shown in Fig. 1. Two neighboring occupied sites may or may not be immediately connected. If they are, we say there is a bond between them. If they are not, we say there is a contact between them. The statistical mechanics is

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{lattice_animals.png}
\caption{Some examples of lattice animals.}
\end{figure}

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conveniently described in terms of a generating function

\[ Z = \sum_{n} x^n Z_n(y, \tau) = \sum_{n, b, k} a_{n, b, k} x^n y^b \tau^k \]

where \( a_{n, b, k} \) is the number of animals with \( n \) sites, \( b \) bonds and \( k \) contacts and \( x, y, \tau \) are fugacities. The infinite lattice animal can be described either by taking \( n \to \infty \) or by fixing one of the fugacities in terms of the other two, say \( x \equiv x_c(y, \tau) \).

This system has been extensively studied numerically, using Monte Carlo simulations, exact graph enumerations and transfer matrix methods. The results for the phase diagram, shown in Fig. 2, are however controversial.

![Phase diagram of the infinite lattice animal.](image)

Figure 2: Phase diagram of the infinite lattice animal. The dark squares mark the exactly known percolation critical point and the strong embedding transition. Open squares denote the results from transfer matrix calculation and open and closed circles are the results from graph enumeration. C labels the compact and E the extended phase.

It is generally agreed upon that, as \( y \) or \( \tau \) is increased, the animal undergoes a \( \theta \)-transition from an extended to a compact phase. The point in question is the possible existence of a phase transition between two distinct compact phases.

Physically, compact and extended phases can be distinguished from the scaling behaviour of the mean radius of gyration, \( \langle R \rangle \), with the number of
monomers $N$, $\langle R \rangle \sim N^\nu$. In the compact phase, $\nu = 1/d$ and in the extended phase, $\nu = 0.6408(3)$ in two dimensions. Existing numerical results agree well with each other on the location and the nature of the extended–compact transition, see Fig. 2. At $y = \tau = 2$, the $\theta$ point coincides with the critical point of percolation. In the $y \to 0$ limit, the strong embedding case is recovered. This fixed point is unusual for a two-dimensional system as it is not conformally invariant. For $0 \leq \tau < 2$, the $\theta$ line should be controlled by the strong embedding fixed point, which leads to $\nu = \frac{1}{2}$ and $\phi = \frac{2}{3}$, respectively, where $\phi$ is the cross-over exponent. On the other hand, the $\theta$ line for $\tau > 2$ should be in a different universality class and it was conjectured that $\nu = \phi = \frac{8}{15}$.

On the other hand, graph enumeration studies suggest the existence of a further transition between two distinct compact phases, a cycle-rich branched polymer for large $y$ and a contact-rich state for large $\tau$. No sign of this transition was found using a transfer matrix approach. This discrepancy led to the investigations whose results will be reviewed here.

We shall approach the problem by using the known exact mapping between the lattice animal and the extended $q$–state Potts model described by the classical Hamiltonian

$$
\mathcal{H} = -J \sum_{(i,j)} \delta_{\sigma_i,\sigma_j} - L \sum_{(i,j)} \delta_{\sigma_i,1} \delta_{\sigma_j,1} - H \sum_i \delta_{\sigma_i,1}
$$

where $\sigma_i = 1, 2, \ldots, q$ and the fugacities are expressed in terms of $J, L, H$ as

$$
x = \exp[-H - \gamma(J + L)], \quad y = (e^J - 1) e^{J+L}, \quad \tau = e^{J+L}
$$

where $\gamma$ is the coordination number. The relation of the extended Potts model to the lattice animal problem

$$
\mathcal{Z} = \lim_{q \to 1} \frac{\partial}{\partial q} \ln \tilde{Z}, \quad \tilde{Z} = \sum_{\{\sigma\}} e^{-\mathcal{H}}.
$$

Thus by calculating the phase diagram of the extended Potts model information about the phases of the animal problem is obtained. The limit $n \to \infty$ corresponds to finding critical points of the Hamiltonian. Transitions between different states of the infinite lattice animal correspond to multicritical points within the critical manifold of the extended Potts model.

We now investigate the phase diagram of the extended Potts model by (a) solving the model exactly on the Bethe lattice and (b) using the Migdal-Kadanoff renormalization group. The results are reinterpreted in terms of the lattice animal providing additional evidence that there is no compact–compact transition.
We first outline the exact solution of the $q \to 1$ limit of the extended Potts model (2) on the Bethe lattice. The following relationship greatly simplifies the calculations: We are interested in the lattice animal free energy $F = \lim_{n \to \infty} n^{-1} \ln Z_n$. On the other hand, the animal generating function $Z$ diverges at the critical point $x_c$ given by

$$F = -\ln x_c. \quad (5)$$

Thus, working in the grand canonical ensemble, it is sufficient to find $x_c$ as a function of the other fugacities $y$ and $\tau$ to obtain the canonical free energy of the infinite lattice animal.

Following Baxter, it is easy to see that on a Bethe lattice with $\gamma = 3$ nearest neighbors for each site and central spin $\sigma_0$, the extended Potts model partition function factorizes into contributions $Q_n(\sigma_0 | s^{(j)})$ from the $j^{th}$ sub-branch with spins $s^{(j)}$

$$\bar{Z} = \sum_{\sigma_0} e^{H\delta_{\sigma_0,1}} \sum_{s} \prod_{j=1}^{3} Q_n(\sigma_0 | s^{(j)}). \quad (6)$$

Now the thermodynamics is completely specified by $g_n(\sigma_0) = \sum_{s} Q_n(\sigma_0 | s)$ where $n$ refers to the number of iterations performed in the construction of the Bethe lattice. Recursion relations for the $g_n$ are

$$g_n(\sigma_0) = \sum_{s_1=1}^{q} \exp \left( J\delta_{\sigma_0,s_1} + L\delta_{\sigma_0,1} \delta_{s_1,1} + H\delta_{s_1,1} \right) \left( g_{n-1}(s_1) \right)^2. \quad (7)$$

In analogy with the mean-field treatment of the Potts model, the analysis can be simplified by introducing the variables

$$\Xi_n = \frac{g_n(\sigma_0 \neq 1, 2, 3)}{g_n(1)}, \quad \Upsilon_n = \frac{g_n(2)}{g_n(1)}, \quad \Omega_n = \frac{g_n(3)}{g_n(1)}. \quad (8)$$

Besides simplification, the introduction of these variables provides a sufficient number of order parameters to enable the model to have a phase diagram rich enough to be compared with Fig. 2. As $n \to \infty$, these variables tend to fixed point values $\Xi, \Upsilon, \Omega$, which can be determined from the recursion relations (7).

At this stage, we take the $q \to 1$ limit (see (4)) and find the self-consistency relations.
\[
\begin{align*}
\Xi &= \frac{x^{-1} \tau^{-3} + \Upsilon^2 + Z^2 + (y/\tau - 2)\Xi^2}{x^{-1} \tau^{-2} + \Upsilon^2 + Z^2 - 2\Xi^2}, \\
\Upsilon &= \frac{x^{-1} \tau^{-3} + (y/\tau + 1)\Upsilon^2 + Z^2 - 2\Xi^2}{x^{-1} \tau^{-2} + \Upsilon^2 + Z^2 - 2\Xi^2}, \\
Z &= \frac{x^{-1} \tau^{-3} + \Upsilon^2 + (y/\tau + 1)Z^2 - 2\Xi^2}{x^{-1} \tau^{-2} + \Upsilon^2 + Z^2 - 2\Xi^2}, 
\end{align*}
\] (9)

These equations can be decoupled and reduced to an equation for the fugacity \(x\) which is at most quadratic. Using eq. (5), we can then read off the free energy.

Thus we obtain \(x = x(p; y, \tau)\) as a function of \(p = (\Xi + \Upsilon)\tau\) which plays the role of an order parameter. The value of \(p\) is fixed by maximising \(x(p)\) with respect to \(p\). This gives the critical surface of the extended Potts model.

A detailed analysis of eqs. (9) shows that the equilibrium phases can be described in terms of two functions \(x = x(p; y, \tau)\). One is

\[
A(p; y, \tau) = \frac{2(p - 2)}{yp^2},
\] (10)

and corresponds to the extended phase and the other one is

\[
C^{-}(p; y, \tau) = x^{(C)}(p; y, \tau) = \frac{2(1 - \tau)p - y^2/4}{py(p^2 - 4\tau p - y^2/4)} - \frac{\sqrt{p(4\tau^2 - 8\tau + 4 + y^2/4) - y^2/4}}{\sqrt{p^2 - 4\tau p - y^2/4}y}.
\] (11)

and corresponds to the compact phase. In particular, it can be shown that if two of the variables \(\Xi, \Upsilon, Z\) are equal, all three of them have to coincide. Therefore only two distinct phases are possible for the infinite lattice animal. For case A

\[
F = -\ln x^{(A)} = -\ln \left(\frac{2(p - 2)}{p^2 y}\right), \quad \frac{\partial F}{\partial p} = \frac{p - 4}{p(p - 2)}, \quad \frac{\partial^2 F}{\partial p^2} \bigg|_{p=4} = \frac{1}{8} > 0
\] (12)

and \(F\) has a single minimum at \(p = 4\). Indeed, \(F\bigg|_{p=4} = \ln(4y)\) is concave in \(y\). The solutions \(A, C^{-}\) meet at \(p = 4\).

Thus two distinct phases of the infinite lattice animal are described by the two solutions \(A(p; y, \tau)\) (extended) and \(C^{-}(p; y, \tau)\) (compact). To obtain the transition lines between the two phases, note that \(\partial C^{-}/\partial \tau\bigg|_{p=4} = 0\) if and only if \(\tau = 2\). Furthermore, \(C^{-}(p; y, 2)\) for \(p = 4\) has a maximum, turning point or
minimum for \( y > 8, y = 8 \) or \( y < 8 \), respectively. Thus, for \( y < 8 \), there is a first-order transition between the extended and compact phases which is given by the conditions

\[
C_-(p; y, \tau) = A(4; y, \tau) = \frac{1}{4y}, \quad \frac{\partial C_-}{\partial p}(p; y, \tau) = 0, \quad \frac{\partial^2 C_-}{\partial p^2} \leq 0. \tag{13}
\]

At this transition point, \( p \) jumps from its value \( p = 4 \) for \( \tau \) small to a new value \( p_c(y, \tau) < 4 \). On the other hand, for \( y > 8, \tau = 2 \) there is a second order transition as \( A \) and \( C_- \) merge into each other. The second order line ends at \( y = 8, \tau = 2 \) in a tricritical point.

Having found a single compact phase from the Bethe lattice calculations, we now supplement this with a Migdal-Kadanoff renormalization group study. Our eventual result that qualitatively the same phase diagram results from both schemes makes it plausible that our analytical approach is capable of capturing the relevant physics of the system.

For \( d = 1 + \epsilon \) dimensions and rescaling factor \( b = 2 \) the Migdal-Kadanoff recursion equations for the extended Potts Hamiltonian (2) are

\[
\xi' = \left( \frac{\xi(1 + \rho + (q - 2)\eta)}{1 + \xi^2 + (q - 2)\eta^2} \right)^{b^*}, \quad \eta' = \left( \frac{\xi^2 + 2\eta + (q - 3)\eta^2}{1 + \xi^2 + (q - 2)\eta^2} \right)^{b^*}, \quad \rho' = \left( \frac{\rho^2 + (q - 1)\xi^2}{1 + \xi^2 + (q - 2)\eta^2} \right)^{b^*} \tag{14}
\]

where

\[
\xi = \exp(H/2 - J), \quad \eta = \exp(-J), \quad \rho = \exp(L + H). \tag{15}
\]

Eqs. (14) were obtained by performing a one-dimensional decimation followed by bond-moving.

The fixed point structure that follows from the recursion equations (14) is complicated and \( q \)-dependent. However in the two limits of interest to us \((q \to 1 \text{ and } \epsilon \to 0)\) a clear pattern appears and 14 fixed points can be identified. They are shown in Fig. 3. They are interpreted using existing results on the \( q \)-state Potts model as a guide.

We point out that the fixed point structure changes at \( q = 1 \), as can be seen by comparison with earlier work where for \( d = b = 2 \) and \( q = 1 \) only 4 non-trivial fixed points were found. In the case of interest to us, the non-trivial fixed points are E,F,G,H and I which all have \( \rho^* \sim 1 \). (The other fixed points are trivial or merge into trivial ones for \( q \to 1 \).) Two of these (E and I) are independent of both \( q \) and \( \epsilon \) and have one relevant eigenvalue. For the fixed point E, the relevant direction is characterized by the exponent
1/\nu = d = 1 + \epsilon$, characteristic of a (single) compact phase. For the fixed point I, the single relevant eigenvalue is $1/\nu = d - 1 < d$. We thus expect the fixed point E (I) to describe the compact (extended) phase of the lattice animal. The fixed point H has three relevant eigenvalues and therefore represents the percolation fixed point (which is realized for $H = 0$ and $L = 0$ in eq. (2)). F and G are tricritical points and govern the renormalization group flow along the two critical lines leaving the percolation point H. We emphasise that the fixed point G is only found when the limit $q \to 1^+$ is carefully taken.

In summary, the collapse of an infinite branched polymer was studied using its equivalence with the extended $q$–state Potts model in the $q \to 1$ limit. The phase diagram was found from an exact solution on the Bethe lattice and using a Migdal-Kadanoff renormalization group. In both cases an extended and a single compact phase, separated by a line of \( \theta \) transitions, was found. The \( \theta \) line consists of two segments which are in different universality classes and which meet at a multicritical point which coincides with the critical point of two-dimensional percolation. This is in agreement with the available numerical results in two dimensions. Our finding of a single compact phase agrees with the transfer matrix results but is in disagreement with the expectations based on graph enumeration studies.
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