On the universality of compact polymers

Jesper Lykke Jacobsen
Laboratoire de Physique Statistique\footnote{Laboratoire associé aux universités Paris 6, Paris 7 et au CNRS.}
Ecole Normale Supérieure,
24 rue Lhomond, F-75231 Paris CEDEX 05, FRANCE.

ABSTRACT

Fully packed loop models on the square and the honeycomb lattice constitute new classes of critical behaviour, distinct from those of the low-temperature $O(n)$ model. A simple symmetry argument suggests that such compact phases are only possible when the underlying lattice is bipartite. Motivated by the hope of identifying further compact universality classes we therefore study the fully packed loop model on the square-octagon lattice. Surprisingly, this model is only critical for loop weights $n < 1.88$, and its scaling limit coincides with the dense phase of the $O(n)$ model. For $n = 2$ it is exactly equivalent to the selfdual 9-state Potts model. These analytical predictions are confirmed by numerical transfer matrix results. Our conclusions extend to a large class of bipartite decorated lattices.

PACS numbers: 05.50.+q, 11.25.Hf, 64.60.Ak, 64.60.Fr
1 Introduction

Compact polymers, the continuum limit of random walks that are constrained to visit every site of some lattice $\mathcal{L}$, are intriguing in so far as their critical exponents depend explicitly on $\mathcal{L}$. Whilst first observed numerically [1], this curious lack of universality was firmly established through the exact solution of the compact polymer problem on the honeycomb [2, 3] and, very recently, the square lattice [4, 5].

However, not every lattice can support a compact polymer phase. To see this, consider more generally an $O(n)$-type loop model defined on $\mathcal{L}$, in which each closed loop is weighed by $n$, and each vertex not visited by a loop carries a factor of $t$. It is well-known that for $|n| \leq 2$ this model possesses a branch of low-temperature ($t$ being the temperature) attractive critical fixed points [3, 4] with critical exponents that do not depend on $\mathcal{L}$, even when $\mathcal{L}$ is not a regular lattice but an arbitrary network [8]. On the other hand, whenever the model is invariant under $t \rightarrow -t$, as is the case if $\mathcal{L}$ can only accommodate loops of even length, this symmetry allows for a distinct zero-temperature branch of repulsive fixed points [1], with the $n \rightarrow 0$ limit representing the compact polymer problem. That the critical behaviour of this class of fully-packed loop (FPL) models depends on $\mathcal{L}$ is readily seen from the solutions of the honeycomb and the square case given in Refs. [3, 4, 5]. Namely, the continuum limit of these models can be described by a conformal field theory (CFT) for a fluctuating interface, where the fully-packing constraint forces the height variable to be a vector, with a number of components that depends on the coordination number of the lattice at hand.

This $t \rightarrow -t$ symmetry argument, originally put forward by Blöte and Nienhuis [1], prompts us to conjecture its inverse: Whenever $\mathcal{L}$ allows for loops of odd length, so that the symmetry is destroyed, the renormalisation group flow can be expected to take us to non-zero $t$, eventually terminating in the dense, universal $O(n)$ phase. Support for this conjecture so far comes from numerics in the case of the triangular lattice [9], and recently for a class of decorated lattices interpolating between the square and the triangular lattices [10, 11].

2...
Accepting for the moment the validity of this conjecture however leaves us with an infinite set of bipartite lattices, each one being a potential candidate for a novel universality class of compact polymers. This perspective is especially appealing in the light of the constructive point of view taken in Refs. [3, 4, 5, 11]. In these papers new CFTs were explicitly constructed, based on purely geometrical considerations applied to the FPL model in question. On the other hand, if the bipartite lattices generate an entire family of distinct CFTs, this gives rise to important classification issues. In particular, the applicability of compact polymer models to the protein folding problem [12, 13] implies that one would like to understand on which microscopic parameters (bending angles, coordination number, steric constraints) the resulting conformational exponents do depend.

In this paper we examine FPL models on a class of bipartite lattices, in which every vertex of a regular (square or honeycomb) lattice has been decorated. A renormalisation group (RG) argument, essentially amounting to a summation over the decoration, reveals that the Liouville field theory construction [14] should really be based on the undecorated lattice, but with bare vertex weights that depend on the loop fugacity \( n \). This leads to a novel scenario in which, depending on \( n \), the model may either renormalise towards the dense phase of the O\((n)\) model or flow off to a non-critical phase, even for \( n < 2 \)!

The case of the square-octagon lattice, shown in Fig. 1, is investigated in detail. This lattice can be thought of as a square lattice in which each vertex has been decorated with a tilted square. Our interest in the square-octagon lattice stems from the fact that it is bipartite and has the same coordination number as the honeycomb lattice, but enjoys the symmetry of the square lattice. In particular it will enable us to assess whether the critical behaviour of compact polymers on a lattice \( \mathcal{L} \) depends only on its coordination number \( \mathcal{L} \), only on the bond angles, or on a combination of both these parameters. Our analysis suggests that the corresponding FPL model belongs to the dense O\((n)\) phase for \( n < 1.88 \), whilst for \( n > 1.88 \) a finite correlation length is generated. For \( n = 2 \) we show rigorously that the model is equivalent to the (non-critical) 9-state Potts model.

Ref. [14] is also valid for \( n \neq 0 \).)

\(^3\)In the protein folding language this determines the number of close contacts per monomer of the folded chain.
Figure 1: Fully packed loops on the square-octagon lattice. In the corresponding transfer matrix, periodic boundary conditions are imposed across a strip of width $L$ loop segments (here $L = 4$). The state space is that of all well-nested, pairwise connections amongst the $L$ dangling ends in the upper row.

The analytical results are confirmed by numerical transfer matrix calculations on strips of width up to $L_{\text{max}} = 18$ loop segments.

Having introduced the models in Section 2, we present the analytical results in Section 3 and the numerics in Section 4. Our results are discussed in Section 5.

2 The models

A fully packed loop (FPL) model on a lattice $\mathcal{L}$ is defined by the partition function

$$Z_{\text{FPL}} = \sum_{G_{\text{FPL}}} n^N,$$  \hspace{1cm} (2.1)

where the sum runs over all configurations $G_{\text{FPL}}$ of closed loops drawn along the edges of $\mathcal{L}$ so that every vertex is visited by a loop. Within a given configuration a weight $n$ is given to each of its $N$ loops.

An FPL model on $\mathcal{L}$ can be generalised to an $O(n)$ model by lifting the fully packing constraint and further weighing each empty vertex by a factor of $t$. Physically $t$ corre-
Figure 2: Phase diagram of the O\(n\) model on the honeycomb lattice.

[^1] Thompson, R.A. and Schottel, K.L. (1969) The phase diagram of the FPL model on the honeycomb lattice. J. Phys. C: Solid State Phys. 2, 2377-2389.

According to Thompson and Schottel, the phase diagram of the FPL model on the honeycomb lattice corresponds to a temperature, the FPL model thus being the zero-temperature limit of the O\(n\) model. When \(\mathcal{L}\) is the honeycomb lattice, the resulting phase diagram is as shown on Fig. 2. For \(|n| \leq 2\) three branches, or phases, of critical behaviour exist. Since \(\mathcal{L}\) is bipartite, the resulting \(t \to -t\) symmetry allows for a compact phase at \(t = 0\), as discussed at length in the Introduction. For \(t > 0\) Nienhuis has found the exact parametrisation of a dense and a dilute phase, and determined the critical exponents as a function of \(n\).

For our discussion of the square-octagon FPL model we shall need the corresponding parametrisation for the O\(n\) model on the \textit{square} lattice. The definition of the partition function is now slightly more complicated, since each vertex can be visited by the loops in several ways that are unrelated by rotational symmetry. An appropriate choice is

\[ Z_{O(n)} = \sum_{\mathcal{G}} t^{N_t} u^{N_u} v^{N_v} w^{N_w} n^N, \]

where \(N_t, N_u, N_v\) and \(N_w\) are the number of vertices visited by respectively zero, one turning, one straight, and two mutually avoiding loop segments. It is convenient to redefine the units of temperature so that \(t = 1\).

Nienhuis [7, 15] has identified five branches of critical behaviour for the model (2.2).
The first four are parametrised by

\[
\begin{align*}
    w_c &= \left\{ 2 - \left[ 1 - 2 \sin \left( \frac{\theta}{2} \right) \right] \left[ 1 + 2 \sin \left( \frac{\theta}{2} \right) \right]^2 \right\}^{-1}, \\
    u_c &= 4w_c \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{\pi}{4} - \frac{\theta}{4} \right), \\
    v_c &= w_c \left[ 1 + 2 \sin \left( \frac{\theta}{2} \right) \right], \\
    n &= -2 \cos(2\theta),
\end{align*}
\]  

(2.3)

where \( \theta \in [(2 - b)\pi/2, (3 - b)\pi/2] \) corresponds to branch \( b = 1, 2, 3, 4 \). It has recently been noticed that the edges not covered by the original (‘black’) loops form a second species of closed (‘grey’) loops, each one occurring with unit weight [11]. Lifting the fully-packing constraint implies that the two loop flavours decouple, and each of them can independently reside in either of the two critical phases (dense or dilute) discussed above. The black (resp. grey) loops are dense on branches 2 and 4 (resp. 1 and 2), and dilute on branches 1 and 3 (resp. 3 and 4). On branches 1 and 2 the grey loops contribute neither to the central charge, nor to the geometrical (string) scaling dimensions, and in the scaling limit these two branches are thus completely analogous to the dilute and the dense branches of the \( O(n) \) model on the honeycomb lattice [11].

The last critical branch, known as branch 0, has weights

\[
\begin{align*}
    u_c = w_c &= \frac{1}{2}, \\
    v_c &= 0, \\
    -3 &\leq n \leq 1,
\end{align*}
\]  

(2.4)

and can be exactly mapped onto the dense phase of the \( O(n+1) \) model [7], or equivalently to the selfdual \( (n + 1)^2 \)-state Potts model [8].

3 Renormalisation group analysis and an exact mapping

At first sight it would seem that the continuum limit of the FPL model (2.1) on the square-octagon lattice should be described by a Liouville field theory for a two-dimensional height field, since the lattice has the same coordination number as the honeycomb lattice [8]. However, we shall presently see that only one height component survives when applying
Consider performing the first step of a real-space renormalisation group (RG) transformation of Eq. (2.1), by summing over the degrees of freedom residing at the decorating squares. In this way the decorated vertices transform into weighted undecorated vertices, as shown on Fig. 3. The renormalised model is then simply the $O(n)$ model on the square lattice (2.2), but with some particular ‘bare’ values of the vertex weights. Defining again the empty vertex to have unit weight, these bare weights read

$$u = \frac{1}{n}, \quad v = 0, \quad w = \frac{1}{n}. \quad (3.1)$$

Following the standard procedure [16] microscopic heights can be defined on the lattice plaquettes by orienting the loops and assigning a vector, $A$, $B$ or $C$, to each of the three possible bond states: $A$ ($B$) if the bond is covered by a loop directed towards (away from) a site of the even sublattice, and $C$ if the bond is empty. When encircling an even (odd) site in the (counter)clockwise direction the microscopic height increases by the corresponding vector whenever a bond is crossed. As was first pointed out in Ref. [3] the fully-packing constraint leads to the condition $A + B + C = 0$, whence the height must a priori be two-dimensional. However, the RG transformation that we have just
Figure 4: RG flow in the square-octagon FPL model. After tracing over the decoration, the bare value of $1/u$ is given by the dashed line. For $n < 1.88$ the flow is directed towards the attractive branch of dense fixed points, whilst for $1.88 < n < 2$ the system renormalises towards the high-temperature disordered phase.

applied lifts the fully-packing constraint, due to the appearance of the bottom left vertex of Fig. 3. Defining now the sublattices with respect to the renormalised (square) lattice we have the additional constraint $4C = 0$, whence the coarse grained height field should really be one-dimensional\footnote{See Ref. \[11\] for similar examples of such a reduction of the dimensionality of the height field.}, and $O(n)$-like behaviour is to be expected. Also note that it clearly suffices to define the microscopic heights on the octagonal plaquettes in order to obtain a continuous height field defined everywhere in $\mathbb{R}^2$ by the usual coarse graining procedure \[16\].

The reason that the renormalised FPL model is still interesting is that the bare vertex weights (3.1) are now some fixed functions of the loop fugacity $n$, rather than arbitrary parameters that can be tuned to their critical values. This constitutes an interesting situation which has not been encountered before. We shall soon see that it implies that the FPL model (2.1), unlike any other loop model studied this far, is only critical within a part of the interval $|n| \leq 2$.

In Fig. 4 we show $1/u_c$, the weight of the empty vertex relative to that of a turning
loop segment, as a function of $n$ for the critical branches 1 (dilute phase) and 2 (dense phase) of the $O(n)$ model on the square lattice; cfr. Eq. (2.3). In analogy with the honeycomb case the dense and dilute branches again consist of respectively attractive and repulsive fixed points. With the bare value $1/u$ given by Eq. (3.1) the subsequent RG flow must therefore be as schematically indicated on the figure. For $n \approx 1.88$ there is an intersection between the bare value and that of the dilute branch, and for $n > 1.88$ we can therefore expect the flow to be directed towards the high-temperature disordered phase of the $O(n)$ model. In other words, a finite correlation length (roughly the size of the largest loop in a typical configuration) is generated and the model is no longer critical.

Of course we should be a little more careful, since $u$ is not the only parameter in the model. Whenever the bare weights (3.1) do not intersect one of the five branches of fixed points, $v$ and $w$ will flow as well. In particular, $v$ will in general flow towards non-zero values, since the turning loop segments always occur with finite weight, and these are clearly capable of generating straight loop segments on larger length scales. The essential point is that for $1.88 < n < 2$ empty vertices will begin to proliferate, and there is no physical mechanism for halting the flow towards the disordered phase.\footnote{The flow cannot be towards branch 0 since this is a repulsive fixed point.}

The point $n = 2$ merits special attention. Here the bare weights are

$$u = w = \frac{1}{2}, \quad v = 0,$$

which coincides with the fixed point values on branch 0; see Eq. (2.4). Invoking Nienhuis’ mapping \cite{7} the $n = 2$ FPL model is therefore exactly equivalent to the selfdual 9-state Potts model, which is of course again non-critical \cite{17}.

4 Transfer matrix results

In order to confirm the analytical predictions given in Section 3 we have numerically calculated effective values of the central charge $c$ and the thermal scaling dimension $x_t$ on strips of width $L = 4, 6, \ldots, 18$ loop segments. To this end we adapted the connectivity basis transfer matrices described in Refs. [6, 4] to the square-octagon lattice. The working
Table 1: Three-point estimates for the central charge, compared with exact results for the dense phase of the O(n) model.

| n   | c(4, 8) | c(6, 10) | c(8, 12) | c(10, 14) | c(12, 16) | c(14, 18) | O(n)  |
|-----|--------|----------|----------|-----------|-----------|-----------|-------|
| 0.0 | -1.9784| -1.9862  | -1.9880  | -1.9924   | -1.9963   | -1.9980   | -2.0000|
| 0.5 | -0.8898| -0.8975  | -0.8729  | -0.8488   | -0.8338   | -0.8259   | -0.8197|
| 1.0 | 0.0706 | -0.0856  | -0.0965  | -0.0701   | -0.0434   | -0.0246   | 0.0000 |
| 1.5 | 0.9390 | 0.6602   | 0.5504   | 0.5144    | 0.5117    | 0.5227    | 0.5876 |
| 2.0 | 1.6484 | 1.4844   | 1.4495   | 1.4362    | 1.4225    | 1.4068    | 1.0000 |

The effective central charge \(c(L, L + 4)\) has been estimated by three-point fits of the form [18, 19, 4]

\[
f_0(L) = f_0(\infty) - \frac{\pi c}{6L^2} + \frac{A}{L^4} + \cdots
\]

applied to the free energy per site \(f_0(L')\) with \(L' = L, L + 2, L + 4\). Similarly, effective values \(x_t(L, L + 2)\) of the thermal scaling dimension were found from two-point fits of the form [20, 4]

\[
f_1(L) - f_0(L) = \frac{2\pi x_t}{L^2} + \frac{B}{L^4} + \cdots
\]

where \(f_0(L)\) and \(f_1(L)\) are related to the ground state and the first excited state of the transfer matrix spectra in the usual way.

The numerical results are given in Tables 1 and 2. For \(n \leq 1.5\) we see the expected convergence towards the exact values of the O(n) model in the dense phase, which read...
Table 2: Two-point estimates for the thermal scaling dimension, juxtaposed with exact values for the dense $O(n)$ model.

\[ c = 1 - \frac{6e^2}{1 - e}, \quad x_t = \frac{2e + 1}{2(1 - e)} \]  

with $e \equiv \frac{1}{\pi} \arccos(n/2)$. For $n = 1.5$ the convergence is rather slow, especially in the case of $c$, reflecting a large crossover length.

As predicted by theory, the FPL model is no longer critical at $n = 2$. This is particularly visible from the monotonic decrease of the $x_t$ estimates, which are well below the exact $O(n)$ value $x_t = 1/2$. For a system with a finite correlation length, $\xi < \infty$, the effective values for $c$ should eventually tend to zero. The fact that we observe rather large effective values is in agreement with Ref. [7], and rather predictable since $\xi$ is much greater than the largest strip width used in the simulations [22]. For comparison we performed similar computations for the 9-state Potts model in its loop representation [23], finding again effective values of $c$ in the range 1.3–1.4.

5 Discussion

Having seen that two of the simplest two-dimensional lattices (square and honeycomb) give rise to distinct compact universality classes, it would be tempting to conjecture that an FPL model defined on any new lattice leads to different critical exponents and has a new CFT describing its continuum limit. In the present paper we have demonstrated that this is far from being the case. Even within the very restricted class of bipartite lattices, fulfilling the $t \to -t$ symmetry requirement, any lattice that can be viewed as a
decorated square or honeycomb lattice is likely to flow away from the compact phase by virtue of an RG transformation analogous to the one presented in Section 3.

Despite the curious lattice dependence of the compact phases, it thus appears that the number of distinct universality classes is very restricted. We recall that the continuum limit of all loop models solved to this date can be constructed by perturbing a SU($N$)$_{k=1}$ Wess-Zumino-Witten model by exactly marginal operators and introducing an appropriate background charge [16]. It would be most interesting to pursue the physical reason why only the cases $N = 2$ (the O($n$) [11], Potts [24] and six-vertex [10] models), $N = 3$ (the FPL model on the honeycomb lattice [3]), and $N = 4$ (the two-flavoured FPL model on the square lattice [4, 5]) seem to occur in practice.

The square-octagon lattice FPL model studied here turned out to be interesting in several respects. First, it provides us with the first example of a non-oriented [25], bipartite [3, 10] lattice for which the scaling properties of compact and dense polymers are identical. In particular, the exact value of the conformational exponent $\gamma$ is $19/16$ [21, 8], indicating a rather strong entropic repulsion between the chain ends. Second, the square-octagon model presents a novel scenario in which the same fully packed loop model may renormalise towards different conformal field theories, or even flow off to a non-critical regime, depending on the value of the loop fugacity $|n| \leq 2$. In particular one might be able to ‘design’ a decorated lattice with bare vertex weights that simultaneously intersect those of the dilute O($n$) phase for some value of $n$. This could be a starting point for gaining a microscopic, geometrical understanding of the Coulomb gas charge asymmetry [21] which was shown in Ref. [11] to distinguish between the dense and dilute phase of the O($n$) model. Finally, our model proves that the scaling properties of compact polymers do not depend exclusively on either bond angles or coordination number, but rather on a combination of these two parameters.

Acknowledgments

The author is greatly indebted to J. Kondev for many valuable comments and suggestions, and would like to thank Saint Maclou for inspiration during the initial stages of this project.
References

[1] H. W. J. Blöte and B. Nienhuis, Phys. Rev. Lett. 72, 1372 (1994).

[2] M. T. Batchelor, J. Suzuki and C. M. Yung, Phys. Rev. Lett. 73, 2646 (1994).

[3] J. Kondev, J. de Gier and B. Nienhuis, J. Phys. A 29, 6489 (1996).

[4] J. L. Jacobsen and J. Kondev, Nucl. Phys. B 532 [FS], 635 (1998).

[5] J. Kondev and J. L. Jacobsen, Phys. Rev. Lett. 81, 2922 (1998).

[6] B. Nienhuis, Phys. Rev. Lett. 49, 1062 (1982).

[7] H. W. J. Blöte and B. Nienhuis, J. Phys. A 22, 1415 (1989).

[8] B. Duplantier and H. Saleur, Nucl. Phys. B 290, 291 (1987).

[9] M. T. Batchelor, H. W. J. Blöte, B. Nienhuis and C. M. Yung, J. Phys. A 29, L399 (1996).

[10] S. Higuchi, Compact polymers on decorated square lattices, cond-mat/9811426.

[11] J. L. Jacobsen and J. Kondev, Transition from the compact to the dense phase of two-dimensional polymers, preprint cond-mat/9811083. To appear in J. Stat. Phys (1999).

[12] H. S. Chan and K. A. Dill, Macromolecules 22, 4559 (1989).

[13] K. A. Dill et al., Protein Science 4, 561 (1995).

[14] J. Kondev, Phys. Rev. Lett. 78, 4320 (1997).

[15] M. T. Batchelor, B. Nienhuis and S. O. Warnaar, Phys. Rev. Lett. 62, 2425 (1989).

[16] J. Kondev and C. L. Henley, Nucl. Phys. B 464 [FS], 540 (1996).

[17] R. J. Baxter, J. Phys. C 6, L445 (1973).

[18] H. Blöte, J. L. Cardy and M. P. Nightingale, Phys. Rev. Lett. 56, 742 (1986).

[19] I. Affleck, Phys. Rev. Lett. 56, 746 (1986).

[20] J. L. Cardy, J. Phys. A 16, L355 (1983).

[21] B. Nienhuis, in Phase Transitions and Critical Phenomena, edited by C. Domb and J. L. Lebowitz (Academic Press, London, 1987), Vol. 11.
[22] E. Buffenoir and S. Wallon, J. Phys. A 26, 3045 (1993).

[23] Vl. S. Dotsenko, J. L. Jacobsen, M.-A. Lewis and M. Picco, Coupled Potts models: Self-duality and fixed point structure, cond-mat/9812227. To appear in Nucl. Phys. B (1999).

[24] J. Kondev, Int. Jour. Mod. Phys. B 11, 153 (1997).

[25] P.W. Kasteleyn, Physica 29, 1329 (1963).