Finite-size scaling for branched polymers on a Bethe lattice: an analytical result

1986 J. Phys. A: Math. Gen. 19 L433

(http://iopscience.iop.org/0305-4470/19/8/005)

J. Phys. A: Math. Gen. 19 (1986) L433-L439. Printed in Great Britain

LETTER TO THE EDITOR

Finite-size scaling for branched polymers on a Bethe lattice: an analytical result†‡

S L A de Queiroz

Departamento de Física, PUC, 22452 Rio de Janeiro, Brazil

Received 28 February 1986

Abstract. The application of finite-size scaling arguments to problems defined on a Bethe lattice is discussed for the case of isolated branched polymers. Fugacities p, Λ and h are assigned respectively to monomers, branching points and end points. For coordination numbers $\sigma+1=3$ and 4, analytical expressions are found for the pseudo-critical monomer fugacity on a finite, N-generation tree which satisfy $p_c(N)-p_c\sim N^{-2}$, thus constituting an analytical verification of finite-size scaling predictions, and implying that the correlation-length exponent $\nu=\frac{1}{2}$. The relationship between 'chemical' and 'Euclidean' distance is invoked in order to show that the mean-field value of $\frac{1}{4}$ can be obtained through an appropriate exponent renormalisation. For fixed h, the crossover variable z is $N\Lambda^{1/2}$ for $\sigma=2$ and $N\Lambda^{1/3}$ for $\sigma=3$, such that the N^{-2} behaviour of $p_c(N)-p_c$ sets in for $z\gg 1$. At $\Lambda=0$ there is no pseudo-critical behaviour.

In the theoretical study of phase transitions and critical phenomena the use of approximation schemes is the rule, given the general impossibility of exactly calculating the properties of even the simplest model system in the thermodynamic limit on a realistic (two- or three-dimensional) lattice; Onsager's solution of the two-dimensional Ising model in zero external field (Onsager 1944) stood as the lone exception for a long time, and has recently been joined by a few other special cases (see the book by Baxter (1982)).

In the earlier approximate solutions one would, generally speaking, preserve the notion of an infinite translationally invariant array of sites while introducing some simplifying artificial feature either on the interactions (e.g. substituting an effective field for two-body forces, as in the standard mean-field approach to ferromagnetism) or in the underlying topological structure (e.g. substituting a Bethe lattice, which has no rings of bonds, for an actual two- or three-dimensional lattice). The equations of state thus obtained are usually amenable to analytical solutions, and the information extracted from these is more often than not qualitatively correct. On the other hand, the idea of deriving information about infinite systems from a study of their finite counterparts has proven extremely fruitful, especially after a theory (that of finite-size scaling) has been established which enables one to know precisely how to perform *extrapolations* from finite-size data to infer the behaviour of truly infinite systems (see Fisher 1971, Barber 1983). This is done, e.g., in the analysis of Monte Carlo data (Binder 1979); further, a calculational method has been developed (the phenomenological renormalisation group) whose foundations rely heavily on finite-size scaling theory

† Work supported by Brazilian agencies FINEP, CNPq and CAPES.

‡ A preliminary account of this work was presented at STATPHYS 15, Edinburgh, UK, in July 1983.

and which gives very accurate results (see e.g. Nightingale 1982). Finite-size scaling theory has been applied mainly to the analysis of numerical data; one remarkable exception arises in the discussion on the relation between finite-size correlation-length amplitudes and critical exponents (see e.g. Derrida and De Seze 1982, Privman and Fisher 1984), where long known analytical results for the Ising model (see Domb (1960) for early references) are shown to be consistent with a universality conjecture recently put forward.

In this letter we discuss the extension of finite-size scaling concepts to the problem of branched polymers on a Bethe lattice. Owing to the tree-like structure of the Bethe lattice it is possible to extract analytical data which confirm earlier numerical data (de Queiroz 1981) where applicable. This enables us to understand in full detail the roles played by the different parameters involved, as regards critical (or pseudo-critical) behaviour; also, the relationship between topological (or 'chemical') distance and Euclidean length is explored, and its implications in a finite-size scaling context are shown.

The analogy of the asymptotic conformational properties of a polymer in the limit of large number (N_M) of monomer units to the behaviour of a magnet close to its critical temperature is by now well understood (see de Gennes 1979 and references therein). For the moment, it is enough to recall that, for a single polymer in a good solvent (where the only physical constraint is that of excluded volume, that is, two monomers cannot touch each other) one has for the average mean-square radius of gyration

$$\langle R_G^2 \rangle^{1/2} \sim N_M^{\nu} \qquad N_M \to \infty \tag{1}$$

where the exponent ν (which has this name because it is the correlation-length index of the corresponding magnet) depends only on space dimensionality and on whether the polymer is linear or has a finite percentage of branching units (note that if the *number* of branching units is held constant as the number of monomers increases, the exponent in (1) is the same as if there were no branching points at all, although the amplitudes are different in either case (Redner 1979)). Above the upper critical dimensionality d_c, which is respectively 4 and 8 for linear and branched polymers, the exponent ν sticks to its mean-field (or random-walk) value: $\nu_{MF} = \frac{1}{2}$ in the former case and $\frac{1}{4}$ in the latter (de Gennes 1979, Redner 1979, Lubensky and Isaacson 1979; see also Dobson and Gordon 1964). Below d_c, where the excluded volume effect (not taken into account in mean field) is relevant, one consequently has $\nu > \nu_{MF}$. Since the Bethe lattice is usually regarded as being of infinite dimensionality (standard arguments are recalled in Baxter (1982)), one could think that mean-field results apply in this case. While this is true for 'bulk' exponents (thus e.g. $\beta = \gamma = 1$ for the Ising model on a Bethe lattice (Baxter 1982)), the situation has to be analysed more carefully when an exponent related to the divergence of a length (such as ν) is considered, as we shall see below.

As is usual in geometric problems, we begin by considering the grand partition, or generating, function for an isolated branched polymer on a lattice (McKenzie 1976, de Gennes 1979, Lubensky and Isaacson 1979):

$$\Gamma(p, \Lambda, h) = \sum_{N_M N_b N_v} A(N_M N_b N_v) p^{N_M} \Lambda^{N_b} h^{N_v} \tag{2}$$

where $A(N_M N_b N_v)$ is the number of configurations of a single polymer (allowed by the excluded volume constraint) with N_M monomers, N_b branching points and N_v

end points; p, Λ and h are the respective fugacities per monomer, branching point and end point. For simplicity, only one type of branching unit is considered. The possibility of loop formation is excluded (this does not matter as regards universality classes; see, e.g., Lubensky and Isaacson (1979) and Family (1980)).

Criticality is identified with a singularity of the generating function; although in p-Λ-h space there is a critical surface where Γ is singular, the fundamental (temperature-like) parameter is taken to be the monomer fugacity p. This can be understood from the underlying field theory where, ψ being the field density, the quantity $p-p_c$ (p_c = critical monomer fugacity) arises naturally as the coefficient of the two-spin term ψ^2 while Λ and h are respectively related to ψ^f (f = branching degree $\geqslant 3$) and ψ_1 (field component along the external magnetic field) (Lubensky and Issacson 1979). Λ and h are then irrelevant in the renormalisation group sense (as long as they are non-zero; we comment on this point below) and can be regarded as fixed parameters, for each value of which there is a critical $p_c \equiv p_c(\Lambda, h)$. Recall that $p \to p_c$ corresponds to the asymptotic behaviour $N_M \to \infty$ through the identification $N_M^{-1} \sim (p-p_c)$ (de Gennes 1979).

In finite-size scaling theory one usually has that, for a finite system of linear size L which displays pseudo-critical behaviour (e.g. a susceptibility maximum) at a temperature $T_c(L)$, the following proportionality holds:

$$T_c(L) - T_c \sim L^{-1/\nu} \tag{3}$$

where T_c is the critical temperature of the infinite system (Fisher 1971, Barber 1983). This is not true in some pathological cases, e.g. the spherical model (see Fisher (1971) for a thorough discussion of this point); here we shall be concerned with the applicability of (3) to branched polymers on a Bethe lattice.

On a Bethe lattice with coordination number $\sigma+1$, where the excluded volume condition is fulfilled provided 'backward' steps are not taken into account, it is easy to see that the following relation holds for the generating function Γ_{N+1} for a finite section of the lattice with $N+1$ generations:

$$\Gamma_{N+1}(p, \Lambda, h) = p(h + \Lambda p^\sigma X_N^\sigma + \sigma p X_N) \tag{4}$$

where X_N is defined by the recursion relation

$$X_N = h + \Lambda p^\sigma X_{N-1}^\sigma + \sigma p X_{N-1} \qquad X_0 = 0 \tag{5}$$

(see de Queiroz 1981). Here, $\Gamma(p, \Lambda, h) = \lim_{N\to\infty} \Gamma_N(p, \Lambda, h)$ and, for simplicity, the branching units are assumed to be of degree $\sigma+1$. Recall that, in the model, monomers are assumed to occupy bonds, whereas branching and end points are located on lattice sites.

If we assume that the equivalent of the finite linear size L in this case is the number of generations N, (3) above translates into

$$P_c(N, \Lambda, h) - P_c(\Lambda, h) \sim N^{-1/\nu} \tag{6}$$

where $P_c(N, \Lambda, h)$ ($\equiv P_c(N)$ for short) is the value of P at which $\Gamma_N(p, \Lambda, h)$ displays an incipient singularity (in numerical work, $P_c(N)$ was found by locating the point where Γ_N itself becomes greater than a given tolerance; results thus obtained were, for large $N \geqslant 100$, independent of the pre-established tolerance down to one part in 10^7, which is of course quite an indispensable feature as regards their reliability (de Queiroz 1981)). One of our goals here will be to find $P_c(N)$ analytically.

On the other hand, $P_c(\Lambda, h)$ ($\equiv P_c$ for short) can be found by imposing

$$X_{N+1}(P_c) = X_N(P_c) \equiv X^* \qquad (N \to \infty) \tag{7a}$$

and

$$(\partial/\partial X)(h + \Lambda p_c^\sigma X^\sigma + \sigma p_c X)|_{X^*} = 1 \tag{7b}$$

(de Queiroz 1981). One finds

$$(\sigma P_c)^{-1} = 1 + \left(\frac{\Lambda h^{\sigma-1}}{(\sigma-1)^{\sigma-1}}\right)^{1/\sigma}. \tag{8}$$

Note that $P_c(\Lambda = 0) = 1/\sigma$, which is the result for linear polymers (McKenzie 1976).

In order to find $P_c(N)$, we first transform recursion relation (5) into a differential equation:

$$\mathrm{d}X/\mathrm{d}N = h + \Lambda p^\sigma X^\sigma + (\sigma p - 1)X. \tag{9}$$

This is valid provided $X_{N+1} - X_N \ll 1$, that is, below (pseudo-) criticality; with the equivalence $p \equiv J/k_B T$ between monomer fugacity and bond strength in the associated zero-component ferromagnet (de Gennes 1979), $p < p_c$ corresponds to the disordered phase $T > T_c$ in a magnetic model. Equation (9) cannot be solved at once for generic σ; however, solutions for the non-trivial cases $\sigma = 2$ and $\sigma = 3$ are relatively straightforward.

For $\sigma = 2$, (8) gives $p_c = \frac{1}{2}(1 + \sqrt{\Lambda h})$; with $\alpha \equiv (|(2p-1)^2 - 4\Lambda h p^2|)^{1/2}$, the solution of (9) is

$$X = \begin{cases} \dfrac{1-2p}{2\Lambda p^2} + \dfrac{\alpha}{2\Lambda p^2}\coth\left(\dfrac{\alpha N}{2}\right) & p < p_c \text{ or } p > \frac{1}{2}(1-\sqrt{\Lambda h}) \qquad (10a) \\ \dfrac{1-2p}{2\Lambda p^2} - \dfrac{\alpha}{2\Lambda p^2}\cot\left(\dfrac{\alpha N}{2}\right) & p_c < P < \frac{1}{2}(1-\sqrt{\Lambda h}). \qquad (10b) \end{cases}$$

Note that, for finite N, the function has no singularity at p_c; also, since we are working in the vicinity of p_c and for large N, a constant has been dropped in the integration which appears in the argument of the trigonometric (or hyperbolic) functions.

As the transformation of the recursion relation into a differential equation depends on $X_{N+1} - X_N$ being small, the above result should be valid only *below* the smallest value of p for which it diverges, for a given N. This latter value of p simulates the location of the incipient singularity of the true generating function for the finite lattice, $p_c(N)$. One then has from (10*b*) the condition

$$\tfrac{1}{2}(|(2p_c(N)-1)^2 - 4\Lambda h p_c(N)^2|)^{1/2} N = \pi \tag{11}$$

from which, assuming $1/N^2 \ll \Lambda h$ (a condition that can always be fulfilled for finite branching-point fugacity), one obtains

$$p_c(N) - p_c = \pi^2/\sqrt{\Lambda h}\, N^2. \tag{12}$$

Comparison with (6) gives $\nu = \frac{1}{2}$; we shall return to this later.

As a side remark we note that, although (10*b*) can represent the real generating function only between p_c and $p_c(N)$, above $p_c(N)$ it may be interpreted as an extension of $X_N(p)$. In this context, it is easy to show that the number of poles of (10*b*) per unit length on the p axis is linearly proportional to N, thus becoming a dense set as

$N \to \infty$. The situation bears a similarity to the problem of a randomly dilute Ising spin chain, where the zeros of the finite sub-chain partition functions, located on the complex magnetic field plane, close on the real axis as the number of spins on a sub-chain goes to infinity thus giving rise to Griffiths singularities (see e.g. Wortis 1974); it could be interesting to check whether the analogy goes any further.

Another way to obtain condition (11) which will be useful also in the case $\sigma = 3$ is by analysing the implicit expression for X_N obtained from direct integration of (9). For $\sigma = 2$, with α as defined above, one has

$$\frac{1}{i\alpha} \ln \frac{2p - 1 + 2\Lambda p^2 X - i\alpha}{2p - 1 + 2\Lambda p^2 X + i\alpha} = N \qquad p_c < p < \tfrac{1}{2}(1 - \sqrt{\Lambda h}). \tag{13}$$

When we impose the condition $X_N \to \infty$, the expression of which the logarithm is taken approaches $1 = \exp(2in\pi)$ where

$$2in\pi = i\alpha N. \tag{14}$$

For $n = 1$, result (11) above is obtained (note that for $n = 0$ one is at p_c). Higher values of n correspond to singularities of the extension of X_N above $p_c(N)$ referred to above.

For $\sigma = 3$, $p_c^{-1} = 3[1 + (\frac{1}{4}\Lambda h^2)^{1/3}]$ from (8), and (9) becomes

$$dX/dN = \Lambda p^3 (X - X_1)(X - X_2)(X - X_3) \tag{15}$$

where the X_i are the roots of

$$X^3 + \frac{3p - 1}{\Lambda p^3} X + \frac{h}{\Lambda p^3} = 0 \tag{16}$$

which, for $p_c < p < \frac{1}{3}$ (the region where $p_c(N)$ is to be found), are given by

$$X_1 = -2r \cosh(\phi/3) \tag{17a}$$

$$X_2 = r \cosh(\phi/3) + i\sqrt{3} r \sinh(\phi/3) \tag{17b}$$

$$X_3 = r \cosh(\phi/3) - i\sqrt{3} r \sinh(\phi/3) \tag{17c}$$

with $r \equiv (|3p - 1|/3\Lambda p^3)^{1/2}$, $q \equiv h/2\Lambda p^3$; $\cosh \phi = q/r^3$ (Abramowitz and Stegun 1970). The differential equation (15) is solved as

$$A \ln\left[\frac{X - X_1}{X - X_3}\right] + B \ln\left[\frac{X - X_2}{X - X_3}\right] = \Lambda p^3 N \tag{18}$$

where $A^{-1} \equiv (X_2 - X_1)(X_3 - X_1)$; $B^{-1} \equiv (X_2 - X_3)(X_2 - X_1)$. When $X \to \infty$, $(X - X_1)/(X - X_3) \to \exp(i2\pi n_1)$ and $(X - X_2)/(X - X_3) \to \exp(i2\pi n_2)$. In order to have a real solution for p, it is easy to show that one must have $2n_1 = n_2$; (18) then gives the defining equation for $p_c(N)$:

$$N\sqrt{3}\,|p_c(N) - \tfrac{1}{3}| \sinh \phi = 2\pi n_1 \cosh(\phi/3). \tag{19}$$

Along the same lines of reasoning as for $\sigma = 2$, $p_c(N)$ is given by the smallest value of p satisfying (19), and it can be shown from (19) that this value occurs for $n_1 = 1$. For $1/N^2 \ll (\Lambda h^2)^{2/3}$ we finally have

$$P_c(N) - p_c = \frac{4\pi^2}{3} \left(\frac{4}{\Lambda h^2}\right)^{1/3} \frac{1}{N^2}. \tag{20}$$

Equations (12) and (20) show that the dependence of $p_c(N)-p_c$ on N is of the form N^{-2} both for $\sigma=2$ and $\sigma=3$; on universality grounds, it is reasonable to expect that this will hold also for $\sigma>3$. The prefactors check very well with the numerical results of de Queiroz (1981). Comparing with (6), we see that (12) and (20) stand among the few analytical results available in finite-size scaling, provided that we accept $\nu=\frac{1}{2}$ for branched polymers on a Bethe lattice, which is different from the mean-field result, $\frac{1}{4}$.

As regards this point, it is important to bear in mind the distinction between 'chemical' and 'Euclidean' distance. While the former is given by the number of bonds in the shortest path between two points, the latter is, in an N-dimensional space, given as usual by

$$\left(\sum_{i=1}^{N}(X_1^i-X_2^i)^2\right)^{1/2}$$

where X_j^i is the ith cartesian coordinate of point j. No general relationship exists between these quantities, apart from the obvious one, d (Euclidean) $\leq d$ (chemical), on finite-dimensional spaces; however, if one considers a Bethe lattice as infinite dimensional in the sense that each site has only one non-zero coordinate ($=1$) along an orthogonal set of axes while every bond connects sites at Euclidean distance $=1$ (see e.g. Peruggi *et al* 1984), then one has

$$d(\text{Euclidean})=\sqrt{d}(\text{chemical}) \tag{21}$$

in the case where d(Euclidean) stands for the extension, to the Bethe lattice, of the concept of Euclidean distance.

The value $\frac{1}{2}$ for ν in (12) and (20) is then related to the 'chemical' distance (the origin of this can be traced back to our assumption of the number of generations N, which is a chemical distance, being the analogue of the finite linear size). In order to obtain an exponent related to Euclidean distance (rather, to the above-mentioned extension of this concept), (21) implies that a factor of $\frac{1}{2}$ must be present, where the mean-field result $\frac{1}{4}$ is recovered. We note in passing that the geometric origin of the present exponent 'renormalisation' is entirely distinct from the Fisher renormalisation of exponents which arises when a certain combination of fields is held constant in a field-theoretic study of branched polymers (Lubensky and Isaacson 1979).

Returning to the analysis of (12) and (20) we see that, contrary to the N dependence, with dependence on Λ and h is non-universal; this is consistent with the above-mentioned idea of p as the fundamental parameter while Λ and h are secondary. On the other hand, it is easy to see that our results depend fundamentally on both Λ and h being non-zero. While the $h=0$ case brings no new insight, it is interesting to note that as Λ decreases for fixed h the regime of validity of (12) and (20) is pushed further towards larger N; one then has a crossover region (at $N^*\sim\Lambda^{-1/2}$ for $\sigma=2$, $N^*\sim\Lambda^{-1/3}$ for $\sigma=3$) above which the N^{-2} behaviour sets in, that is, branching effects are felt. On the other hand, we point out that in the extreme case $\Lambda=0$ there is no pseudo-critical behaviour at $p\neq p_c$; in this case (which is that of linear polymers) one merely has a removable singularity in the generating function at $p=p_c=1/\sigma$ for finite N. Thus, the crossover is from linear to branched polymer behaviour.

In summary, we have discussed the application of finite-size scaling arguments to the problem of branched polymers on a Bethe lattice. For coordination numbers 3 and 4, analytical expressions have been found for the pseudo-critical monomer fugacity on a finite N-generation tree which satisfy $p_c(N)-p_c\sim N^{-2}$. The implications of this

as meaning that the correlation-length exponent ν is $\frac{1}{2}$ have been examined, and the relationship between 'chemical' and 'Euclidean' distance on a Bethe lattice has been invoked in order to show that the mean-field result $\nu = \frac{1}{4}$ can be obtained through an appropriate renormalisation. The non-universality in Λ and h of the finite-size scaling expressions has been pointed out, and it has been found that (for fixed h) the crossover variable z is $N\Lambda^{1/2}$ for $\sigma = 2$ and $N\Lambda^{1/3}$ for $\sigma = 3$, such that the N^{-2} behaviour of $p_c(N) - p_c$ sets in for $z \gg 1$. Further, at $\Lambda = 0$ there is no pseudo-critical behaviour.

The author would like to thank P M Oliveira and C Tsallis for interesting suggestions and, most expecially, F Peruggi for an illuminating discussion and helpful correspondence. R R dos Santos is to be thanked for a critical reading of the manuscript and constructive remarks.

References

Abramowitz M and Stegun I 1970 *Handbook of Mathematical Functions* (New York: Dover)
Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 7, ed C Domb and J L Lebowitz (New York: Academic) p 145
Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (New York: Academic)
Binder K 1979 *Monte Carlo Methods in Statistical Physics* ed K Binder (Berlin: Springer) p 26
de Gennes P G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
de Queiroz S L A 1981 *J. Phys. A: Math. Gen.* **14** L339
Derrida B and De Seze L 1982 *J. Physique* **43** 475
Dobson G R and Gordon M 1964 *J. Chem. Phys.* **41** 2389
Domb C 1960 *Adv. Phys.* **9** 149
Family F 1980 *J. Phys. A: Math. Gen.* **13** L325
Fisher M E 1971 *Critical Phenomena: Enrico Fermi Summer School, Varenna, Italy* course 51, ed M S Green (New York: Academic) p 1
Lubensky T C and Isaacson J 1979 *Phys. Rev.* A **20** 2130
McKenzie D S 1976 *Phys. Rep.* **27C** 35
Nightingale P 1982 *J. Appl. Phys.* **53** 7927
Onsager L 1944 *Phys. Rev.* **65** 117
Peruggi F, di Liberto F and Monroy G 1984 *Physica* **123A** 175
Privman V and Fisher M E 1984 *Phys. Rev.* B **30** 322
Redner S 1979 *J. Phys. A: Math. Gen.* **12** L239
Wortis M 1974 *Phys. Rev.* B **10** 4665