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LETTER TO THE EDITOR

Pseudo-critical behaviour of smoothness of self-avoiding loops

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Abstract. It is shown that the critical point and the logarithmic singularity of the specific heat for the self-avoiding loop model on the square lattice can be found by introducing an exactly solvable auxiliary model. Evaluations of correlation functions of the latter model show the psuedo-critical behaviour of the density of rectilinear polymer segments.

In a recent paper (Karowski *et al* 1983) the statistical behaviour of self-avoiding loops on d-dimensional hypercubic lattices has been studied numerically. The partition function of the investigated model is defined by (Rys and Helfrich 1982)

$$Z(t) = \sum_{n,s} g(n; s) m^s t^n, \tag{1}$$

where t is the monomer fugacity and $g(n; s)$ denotes the number of configurations of self-avoiding loops with total length n in units of the lattice spacing, containing s non-intersecting contours with multiplicity m. Different values of m describe different physical systems. So, the limit $m \to 0$ corresponds to the single polymer ring without self-intersection.

The aim of the present letter is to consider the case $m = 1$ and to discuss an exactly solved model related to the self-avoiding ring polymers model on the simple square lattice. In this case we can rewrite the partition function (1) in the form

$$Z(t) = \sum_{n} G(n) t^n, \tag{2}$$

where $G(n)$ is the number of all configurations of self-avoiding loops with total length n.

Consider a square $M \times N$ lattice with periodic boundary conditions. The problem of calculating the partition function (2) is equivalent to solving the eight-vertex model with the following parameters,

$$w_1 = 0, \qquad w_2 = 1, \qquad w_i = t, \qquad i = 3, \ldots, 8, \tag{3}$$

where all types of configurations labelled by the index i are shown in figure 1. Unfortunately, the set of parameters (3) belongs neither to the Baxter condition (Baxter 1972)

$$w_1 = w_2, \qquad w_3 = w_4, \qquad w_5 = w_6, \qquad w_7 = w_8, \tag{4}$$

nor to the free-fermion condition (Fan and Wu 1970)

$$w_1 w_2 + w_3 w_4 = w_5 w_6 + w_7 w_8 \tag{5}$$

under which the eight-vertex model has an exact solution.

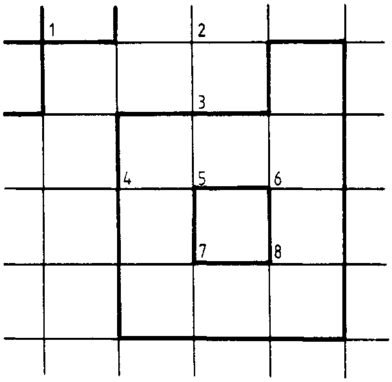

Figure 1. Typical loop configuration. The site of type 1 is forbidden.

Several years ago an auxiliary model was proposed (Priezzhev 1978) which is closely related to the self-avoiding loops problem. The idea is to put $w_3 = w_4 = \sqrt{2}\, t$ in (3) and to consider the sites of types 3 and 4 as defects on a polymer chain. Every two defects double the number of loops configurations, so the partition function of the auxiliary model can be represented in the form

$$Z^*(t) = \sum_n G^*(n) t^n. \qquad (6)$$

Here $G^*(n)$ is the number of arrangements of a set of closed chains with total length n in which the above property of defects is fulfilled. The partition function (6) can be easily calculated by the method of Pfaffians. In the large N and M limit the result is (Priezzhev 1978)

$$Z^*(t) = \exp\left(\frac{MN}{8\pi^2} \int\int_0^{2\pi} d\alpha\, d\beta\, \ln[1 + 4t^2 + 2\sqrt{2}\, t \cos\alpha + 2\sqrt{2}\, t(1 + \sqrt{2}\cos\alpha)\cos\beta]\right). \qquad (7)$$

The model has an Ising-like singularity at $t_c = \sqrt{2}/4$, e.g. the specific heat tends to infinity by the law $C \sim \ln|t - t_c|$.

In this letter we shall use the properties of correlation functions of the auxiliary model to relate the partition functions (2) and (6) and to derive the critical behaviour of the original model.

Consider the correlation function corresponding to the defect density $\eta_D(t)$ defined as the probability of a site configuration weighted by w_3 or w_4. By the standard procedure described by Montroll (1964) the correlation function function is given by

$$n_D = 2|X + Q|^{1/2}, \qquad (8)$$

where X is the 4×4 matrix

$$X = \begin{bmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \qquad (9)$$

and the components of the 4×4 matrix Q are

$$Q_{ii}=0, \qquad i=1,2,3,4,$$

$$Q_{12}=Q_{34}=\frac{1}{(2\pi)^2}\int\int^{2\pi} d\alpha\, d\beta\,[1+2t^2+2\sqrt{2}\,t\cos\alpha + \sqrt{2}\,t(1+\sqrt{2}\,t\cos\alpha)\cos\beta]/\mathscr{D}(t),$$

$$Q_{13}=Q_{24}=0,$$

$$Q_{14}=\frac{-1}{2\pi^2}\int\int_0^{2\pi} d\alpha\, d\beta(1+\sqrt{2}\,t\cos\alpha+\sqrt{2}\,t\cos\beta)/\mathscr{D}(t), \tag{10}$$

$$Q_{23}=\frac{-\sqrt{2}\,t}{(2\pi)^2}\int\int_0^{2\pi} d\alpha\, d\beta[(1+2t^2+2\sqrt{2}\,t\cos\alpha)\cos\beta+2\sqrt{2}\,t(1+\sqrt{2}\,t\cos\alpha)]/\mathscr{D}(t),$$

$$Q_{ij}=-Q_{ji}, \qquad i>j, \qquad i,j=1,2,3,4,$$

where

$$\mathscr{D}(t)=1+4t^2\sqrt{2}\,t\cos\alpha+2\sqrt{2}\,t(1+\sqrt{2}\,t\cos\alpha)\cos\beta.$$

The plot of the ratio of the density of defects $n_D(t)$ to the polymer density $\rho = Vt(\partial/\partial t)\ln Z^*(t)$,

$$s(t)=n_D(t)/\rho(t), \tag{11}$$

is shown in figure 2. It is natural to call the function $s(t)$ the 'smoothness' of the polymer rings since the sites weighted by w_3 and w_4 correspond to rectilinear segments of the polymer. One can see that the smoothness function behaves like an order parameter. The function $s(t)$ is almost constant above the critical point t_c and rapidly decreases below t_c. The plateau of the smoothness is not just constant, but weakly changes and reaches its limit value $s_l=\frac{1}{2}$ when $t\to\infty$.

Up to now we have been dealing with the exactly solved auxiliary model. To consider the problem of calculation of the partition function (2), we should make some model assumptions. First suppose that the smoothness behaves as a true order parameter, i.e. $s(t)$ is constant above t_c. Second, assume s_l to be the value of this constant. Then for large n we have the following equality,

$$G(n)\approx G^*(n)2^{-ns_l/2}, \tag{12}$$

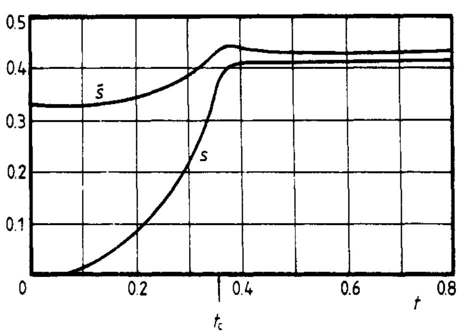

Figure 2. Smoothness s and reduced smoothness $\bar{s}$ against fugacity.

since the presence of each two defects doubles the number of possible configurations in the original problem, and the number of defects is ns_l.

From (12) a relation follows between the partition functions $Z(t)$ and $Z^*(t)$ above t_c

$$Z(t)=\sum_n G(n)t^n \approx \sum_n G^*(n)2^{-ns_l/2}t^n = \sum_n G^*(n)\tilde{t}^n = Z^*(\tilde{t}) \tag{13}$$

where the new variable $\tilde{t}$ is introduced:

$$\tilde{t}=t/2^{s_l/2}, \qquad t>t_c. \tag{14}$$

The singularity of $Z^*(t)$ is known, and therefore we can find the critical point of the model of self-avoiding loops, writing

$$t_c=\tilde{t}_c 2^{s_l/2}=2^{-5/4}=0.4204\ldots. \tag{15}$$

This result can be compared with the numerical data of Karowski *et al* (1983). These authors have observed infinite fluctuations in the system of loops at temperature $\beta_c=0.86$. Taking into account their definition $t=e^{-\beta}$, we get from (15) $\beta_c=\frac{5}{4}\ln 2=0.866\ldots$ in good agreement with numerical data. Relation (13) together with (14) means that the thermodynamic functions in the self-avoiding loops model have the same singularity as in the auxiliary model above t_c, i.e. the specific heat $C\sim\ln(t-t_c)$ which is also consistent with the results of the numerical analysis.

It should be stressed that we cannot draw any conclusions about the type of singularity below t_c since $s(t)$ is no longer constant at $t<t_c$.

To clarify the origin of the critical behaviour of the smoothness function, we have considered the contribution of the smallest loops (the elementary square in figure 1) to the value of $s(t)$. By definition the proper smoothness of such loops is zero. The density of squares ρ_{sq} can be calculated by the method of Pfaffians. The result of these calculations is presented in figure 2, where $\tilde{s}$ is given by

$$\tilde{s}=n_D/(\rho-4\rho_{sq}). \tag{16}$$

One can see that deleting the elementary squares makes the smoothness function more even. We conclude that the pseudo-critical behaviour of $s(t)$ is due to the presence of small loops and the smoothness of the long polymer chains depends weakly on the fugacity.

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