

SIMPLE LATTICE MODEL FOR SELF-AVOIDING RANDOM LOOPS[☆]

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Received 24 April 1984

We show that the partition function of an ensemble of self-avoiding random loops $Z = \sum_{\text{loops}} \beta^{\text{length}}$ can be reexpressed as a local lattice model involving Ising spins. We present an approximation evaluation for $D = 2$ and large β where the loops are prolific, and compare the results with Monte Carlo data obtained from a direct summation of random loops.

In two recent notes we have developed a technique by which the partition function of ensembles of self-avoiding random loops [1] or surfaces [2], of m colors, can be transformed into a variety of local lattice models involving only next-neighbor interactions. These models can be converted into simple field theories which have led to an understanding of the universality class of the corresponding second-order phase transitions. In contrast to earlier lattice models, which involved n -component spins with $n \rightarrow 0$ [3,4] our models do not contain any forbidden line elements (such as "loops", involving a single link, or "single site walks" [4], which were hoped not to modify the universality class). Apart from this, they have the decisive advantage that they allow for an approximate evaluation of the partition function via the usual methods (strong coupling expansion for small β , mean field plus loop corrections for large β).

Our models do, however, have an unesthetic feature. It consists in the fact that the integrand in the partition function is not real. This is an obstacle to a direct Monte Carlo study of the models. It is the purpose of this note to present and analyze a better representation in terms of simple Ising spins, in which the integrand is real and positive for a range of β which starts with zero and reaches beyond the phase transition, such that the transition region becomes accessible to simulations.

Starting point is the partition function of self-avoiding random loops on a simple cubic lattice as developed in ref. [1]^{†1},

$$Z = \prod_{\mathbf{x}} \int dU(\mathbf{x}) [1 + U^{*2}(\mathbf{x})] \prod_{\mathbf{x}, i} [1 + \beta U(\mathbf{x})U(\mathbf{x} + i)], \quad (1)$$

where $U(\mathbf{x}) = e^{i\gamma(\mathbf{x})}$ are pure phases and $\int dU(\mathbf{x}) \equiv \int_{-\pi}^{\pi} d\gamma(\mathbf{x})/2\pi$. It is easy to see [1] that expanding Z in a power series in β gives the correct loop sum with a Boltzmann factor $\beta^L = e^{-\epsilon L/T}$, where ϵ is the activation energy per link and L the total number of links in the loop ensemble. Let us factorize the second product as follows:

[☆] Work supported in part by Deutsche Forschungsgemeinschaft under Grant No. KI 156/10-1.

^{†1} All our considerations are valid on any lattice in which case i runs through q neighbors where q is the coordination number.

$$\prod_{\mathbf{x}, i} [1 + \beta U(\mathbf{x})U(\mathbf{x} + i)] = \prod_{\mathbf{x}, i} \frac{1}{2} \sum_{s_i(\mathbf{x})=\pm 1} [1 + \sqrt{\beta} s_i(\mathbf{x})U(\mathbf{x})][1 + \sqrt{\beta} s_i(\mathbf{x})U(\mathbf{x} + i)]$$

$$= \frac{1}{2^{DN}} \prod_{\mathbf{x}, i} \sum_{s_i(\mathbf{x})=\pm 1} [1 + \sqrt{\beta} s_i(\mathbf{x})U(\mathbf{x})][1 + \sqrt{\beta} s_i(\mathbf{x} - i)U(\mathbf{x})]. \tag{2}$$

The Ising spin variables $s_i(\mathbf{x})$ are associated with the oriented links i emerging from the sites \mathbf{x} , the variables $s_i(\mathbf{x} - i)$ with those pointing towards \mathbf{x} . It will be useful to redefine them as $s_{-i}(\mathbf{x})$. Performing the product over \mathbf{x}, i we may keep only terms $U^n(\mathbf{x})$ with $n = 0, 2$ since higher powers of $U(\mathbf{x})$ (as well as all odd ones) do not survive the integrations in (1). Hence, under the integrand, the product (2) can be replaced by

$$\frac{1}{2^{DN}} \left(\prod_{\mathbf{x}, i} \sum_{s_i(\mathbf{x})=\pm 1} \right) \prod_{\mathbf{x}} \left(1 + \beta U(\mathbf{x})^2 \sum_{\substack{\pm i, \pm j \\ i \neq j}} s_i(\mathbf{x})s_j(\mathbf{x}) \right), \tag{3}$$

such that Z becomes

$$Z = \frac{1}{2^{DN}} \sum_{\{s_i(\mathbf{x})=\pm 1\}} \prod_{\mathbf{x}} \left(1 + \beta \sum_{\substack{\pm i, \pm j \\ i \neq j}} s_i(\mathbf{x})s_j(\mathbf{x}) \right) = \frac{1}{2^{DN}} \sum_{\{s_i(\mathbf{x})=\pm 1\}} \prod_{\mathbf{x}} \left[1 + \frac{\beta}{2} \left(\sum_{\pm i=1}^D s_i(\mathbf{x}) \right)^2 - \beta D \right]. \tag{4}$$

The mechanism, by which (4) produces the self-avoiding random loops is obvious: The products $s_i(\mathbf{x})s_j(\mathbf{x})$ attribute to each neighboring set of links, a couple of ‘‘semi-loop’’ elements, $2D(2D - 1)/2$ for each site. The sum over $s_i(\mathbf{x}) = \pm 1$ gives a contribution only if a link is empty or occupied by precisely two ‘‘semi-loop’’ elements (see fig. 1). The ‘‘semi-loop’’ character of $s_i(\mathbf{x})$ reflects the fact that the Ising spin variables have produced a kind of ‘‘square root’’ of the integrand (2). (This is similar to the way in which spin $\frac{1}{2}$ arises via Dirac’s square root of the Klein–Gordon hamiltonian.) The individual factors in Z

$$z(\mathbf{x}) = 1 + \frac{\beta}{2} \left(\sum_{\pm i=1}^D s_i(\mathbf{x}) \right)^2 - \beta D \tag{5}$$

are all real. Moreover, they are positive for

$$\beta < D^{-1}. \tag{6}$$

In ref. [1] we have listed the critical values of β in $D = 2, 3, 4, 5 \dots$ dimensions and found the values 0.414, 0.218, 0.1488, 0.1135 ($\rightarrow 1/2D$) respectively. Since $1/D$ is equal to 0.5, 0.333, 0.25, 0.2, in these cases, we expect that the new partition function

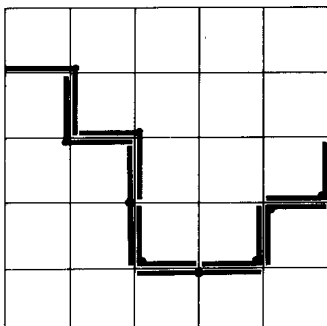


Fig. 1. Section of the way a self-avoiding loop is composed of ‘‘semi-loop’’ elements, in the partition function.

$$Z = \frac{1}{2^{DN}} \sum_{\{s_i(\mathbf{x})=\pm 1\}} \prod_{\mathbf{x}} z(\mathbf{x}) \quad (7)$$

can comfortably be interpreted in terms of probabilities, starting from low β up to a little piece above the phase transition of loop proliferation. In detail, this goes as follows: Consider the 2^{2D} spin configurations $s_{\pm i}(\mathbf{x}) = \pm 1$ associated with every site \mathbf{x} . These can be grouped into classes characterized by a common $z(\mathbf{x})$. Since $z(\mathbf{x})$ depends only on $(\sum_{\pm i=1}^D s_i(\mathbf{x}))^2/4 \equiv n^2$ we can decompose

$$z(\mathbf{x}) \equiv \sum_{n=0}^D z_n P_n(\mathbf{x}) = \sum_{n=0}^D (1 + 2\beta n^2 - \beta D) P_n(\mathbf{x}), \quad (8)$$

where

$$P_n(\mathbf{x}) = \sum_{\substack{\epsilon_i(\mathbf{x})=\pm 1 \\ (\sum_{\pm i=1}^D \epsilon_i(\mathbf{x}))^2/4=n^2}} \prod_{\substack{\pm i, \pm j \\ i \neq j}} \left(\frac{1 + \epsilon_i s_i(\mathbf{x})}{2} \right) \left(\frac{1 + \epsilon_j s_j(\mathbf{x})}{2} \right) \quad (9)$$

are the projection operators into the spin configurations of common $(\sum_i s_i(\mathbf{x}))^2/4 = n^2$. For example, if $D = 2$, there are the following classes of spin configurations of $n = 0, 1, 2$, respectively:

$$++--, +--+ , +---, ---+, -+-+ , +-+-, \quad (9a)$$

$$+++-, ++-+ , +-++ , -+++ , +---, -+---, ---+-, ----+, \quad (9b)$$

$$++++, ----, \quad (9c)$$

with

$$P_0 = \frac{1}{16} [(1+s_1)(1+s_2)(1-s_{-1})(1-s_{-2}) + (1+s_1)(1-s_2)(1+s_{-1})(1-s_{-2}) + (1+s_1)(1-s_2)(1-s_{-1})(1+s_{-2}) \\ + (1-s_1)(1-s_2)(1+s_{-1})(1+s_{-2}) + (1-s_1)(1+s_2)(1-s_{-1})(1+s_{-2}) \\ + (1+s_1)(1-s_2)(1+s_{-1})(1-s_{-2})] = \frac{1}{16} \left(6 - 2 \sum_{\substack{\pm i, \pm j \\ i \neq j}} s_i s_j + 6s_1 s_2 s_{-1} s_{-2} \right), \quad (10a)$$

$$P_1 = \frac{1}{16} [(1+s_1)(1+s_2)(1+s_{-1})(1-s_{-2}) + (1+s_1)(1+s_2)(1-s_{-1})(1+s_{-2}) + (1+s_1)(1-s_2)(1+s_{-1})(1+s_{-2}) \\ + (1-s_1)(1+s_2)(1+s_{-1})(1+s_{-2}) + (1+s_1)(1-s_2)(1-s_{-1})(1-s_{-2}) + (1-s_1)(1+s_2)(1-s_{-1})(1-s_{-2}) \\ + (1-s_1)(1-s_2)(1+s_{-1})(1-s_{-2}) + (1-s_1)(1-s_2)(1-s_{-1})(1+s_{-2})] = \frac{1}{2} (1 - s_1 s_2 s_{-1} s_{-2}), \quad (10b)$$

$$P_2 = \frac{1}{16} [(1+s_1)(1+s_2)(1+s_{-1})(1+s_{-2}) + (1-s_1)(1-s_2)(1-s_{-1})(1-s_{-2})] \\ = \frac{1}{16} \left(2 + 2 \sum_{\substack{\pm i, \pm j \\ i \neq j}} s_i s_j + 2s_1 s_2 s_{-1} s_{-2} \right), \quad (10c)$$

having the eigenvalues 1 on their proper class and 0 on the others. Hence $\sum_{n=0}^D P_n = 1$ and

$$P_n P_m = \delta_{nm} P_m, \quad (11)$$

which shows that they are truly projection operators. We can therefore write

$$z(\mathbf{x}) = \exp \left(\sum_n \log(1 + 2\beta n^2 - \beta D + i\epsilon) P_n(\mathbf{x}) \right), \quad (12)$$

if β is such that all eigenvalues $1 + 2\beta n^2 - \beta D$ are non-zero and

$$z(\mathbf{x}) = [1 - P_m(\mathbf{x})] \exp\left(\sum_{n \neq m} \log(1 + 2\beta n^2 - \beta D + i\epsilon) P_n(\mathbf{x})\right), \quad (13)$$

if $\beta = 1/(D - 2m^2)$ for some $m = 1, \dots, D$. For $\beta < 1/D$ the representation (12) has a proper probability interpretation and can be employed for Monte Carlo simulations.

Let us make use of the new representation (4) and calculate Z for the case of $D = 2$ dimensions. For large β , the decomposition (12) suggests a simple approximation of keeping only the two $n = D$ contributions in (7) [all $s_i(\mathbf{x})$ up or down]. This gives

$$Z \sim Z_0 = (2/2^{DN})[(1 + 2\beta D^2 - \beta D)]^N. \quad (14)$$

From this we calculate the total loop length per site (=internal energy per site)

$$\langle l \rangle = \langle L \rangle / N = u = N^{-1}(\beta d/d\beta) \log Z \sim \beta D(2D - 1)/[1 + \beta D(2D - 1)], \quad (15)$$

and the variance of the length per site (=specific heat per site)

$$N^{-1}(\langle L^2 \rangle - \langle L \rangle^2) = c = N^{-1}(\beta d/d\beta)^2 \log Z \sim D(2D - 1)/[1 + \beta D(2D - 1)]^2. \quad (16)$$

In the limit of large β , $\langle l \rangle$ tends to 1, as it should do exactly, due to self-avoidance. In the polymer interpretation, however, this is an unphysical limit since the maximal value of $\beta = e^{-\epsilon/T}$ is unity. At that maximal value, our simple approximation gives $\langle l \rangle \sim 6/7 \sim 0.857$ which agrees quite well with the Monte Carlo number 0.8.

It is possible to develop a correction procedure which includes the effects of the eigenvalues z_n . Let us split $P_n(\mathbf{x})$ into new projections $P_{+n}(\mathbf{x})$ and $P_{-n}(\mathbf{x})$, which project into states with $\frac{1}{2}\sum_{\pm i} s_i(\mathbf{x}) = n > 0$ and $\frac{1}{2}\sum_{\pm i} s_i(\mathbf{x}) = -n < 0$, respectively. If r_n denotes the ratios $r_n \equiv z_n/z_D \equiv r_{-n}$, we can expand the partition function as follows:

$$\begin{aligned} Z = & \frac{1}{2^{DN}} (1 + 2\beta D^2 - \beta D)^N \left(\prod_{x,i} \sum_{s_i(\mathbf{x})=\pm 1} \right) \left(\prod_x [P_D(\mathbf{x}) + P_{-D}(\mathbf{x})] \right. \\ & + \sum_y \prod_{x \neq y} [P_D(\mathbf{x}) + P_{-D}(\mathbf{x})] \sum_{\pm n=1}^{D-1} r_n P_n(\mathbf{y}) \\ & \left. + \frac{1}{2} \sum_{y \neq z} \prod_{x \neq y, \neq z} [P_D(\mathbf{x}) + P_{-D}(\mathbf{x})] \sum_{\pm n=1}^{D-1} \sum_{\pm m=1}^{D-1} r_n r_m P_n(\mathbf{y}) P_m(\mathbf{z}) + \dots \right). \quad (17) \end{aligned}$$

For $D = 2$, the ratios r_n are displayed in table 1. We see that down to $\beta \sim \beta_c \sim 0.414$ they are sufficiently small such as to expect a reasonable convergence of the expression. Notice that even though $\langle l \rangle$ had the correct $\beta \rightarrow \infty$ limit, Z_0 itself does not since the r_n 's remain finite.

Consider now the first correction to Z_0

$$Z_1 = \frac{1}{2^{DN}} (1 + 2\beta D^2 - \beta D)^N \left(\prod_{x,i} \sum_{s_i(\mathbf{x})=\pm 1} \right) \sum_y \prod_{x \neq y} (P_D(\mathbf{x}) + P_{-D}(\mathbf{x})) \sum_{\pm n=1}^{D-1} r_n P_n(\mathbf{y}).$$

In order that the product of P_D 's be non-zero, all spins around each site, except for y , have to be 1 or -1 . But then n must also be $\pm D$ and the sum over $n = -(D - 1), \dots, (D - 1)$ gives no contribution. Hence $Z_1 = 0$.

The second correction does give a non-zero contribution. If all spins are up and one $s_i(\mathbf{x})$ is down, there is a contribution of $n = (D - 1)$ from that link and

$$Z_2 = \frac{1}{2^{DN}} (1 + 2\beta D^2 - \beta D)^N D 2N r_{D-1}^2 = Z_0 D N r_{D-1}^2. \quad (18)$$

Table 1
The coefficients of our expansion (17).

D	r_{D-1}, \dots, r_1	$\beta \rightarrow \infty$	$\beta = 1$	$\beta \approx \beta_c$
2	$\frac{1-2\beta}{1+6\beta}, \frac{1}{1+6\beta}$	$-\frac{1}{3}, 0$	$-\frac{1}{7}, \frac{1}{7}$	0.05, 0.29
3	$\frac{1-3\beta}{1+15\beta}, \frac{1-\beta}{1+15\beta}, \frac{1+5\beta}{1+15\beta}$	$-\frac{1}{5}, -\frac{1}{15}, \frac{1}{3}$	$-\frac{1}{8}, 0, \frac{3}{8}$	0.08, 0.18, 0.49
4	$\frac{1-4\beta}{1+28\beta}, \frac{1-2\beta}{1+28\beta}, \frac{1+4\beta}{1+28\beta}, \frac{1+14\beta}{1+28\beta}$	$-\frac{1}{7}, -\frac{1}{14}, \frac{1}{7}, \frac{1}{2}$	$-\frac{3}{29}, -\frac{1}{29}, \frac{5}{29}, \frac{15}{29}$	0.08, 0.14, 0.31, 0.6

The third correction comes from two adjacent spins being flipped with the three sites, on which they lie, having $n = D - 1$ at the ends, and $n = D - 2$ at the joint. This gives

$$Z_3 = Z_0^{\frac{1}{2}} N 2D (2D - 1) r_{D-1}^2 r_{D-2}. \quad (19)$$

The fourth correction requires a more tedious counting. One trivial contribution is the disconnected one, in which two distant links are occupied by a flipped spin. The weight is r_{D-1}^4 and the multiplicities are ND for the first link and $ND - 1 - 2(2D - 1)$ for the second, since it can lie neither on top of the first (-1) nor join with one of the end points $[-2(2D - 1)]$. With a factor $\frac{1}{2}$, to avoid double counting, this gives

$$Z_4^{(1)} = Z_0^{\frac{1}{2}} ND (ND - 4D + 1) r_{D-1}^4. \quad (20)$$

A further contribution comes from connected graphs $\#^2 \square$ which contribute $r_{D-1}^2 r_{D-2}^2$. Starting with $2ND$ links, we can attach $(2D - 1)$ links. With a factor $\frac{1}{2}$ we have

$$Z_4^{(2)} = Z_0^{\frac{1}{2}} N 2D (2D - 1)^2 r_{D-1}^2 r_{D-2}^2. \quad (21)$$

If the three links of this contribution form the boundary of open plaquette \square , it can be closed by a flipped spin to \square , to the same order giving

$$Z_4^{(3)} = Z_0^{\frac{1}{2}} ND (D - 1) T_{D-2}^4. \quad (22)$$

A fourth contribution comes from the graphs in which three links with flipped spins have one common site \diamond ,

$$Z_4^{(4)} = Z_0 N^{\frac{2}{3}} D (D - 1) (2D - 1) r_{D-1}^3 r_{D-3}. \quad (23)$$

Finally, in $D = 2$ dimensions, there is an exceptional contribution, i.e. $+$. If the background is occupied by P_D , the central site contains P_{-D} with $r_{-D} = 1$ and one has a contribution of four r_{D-1} :

$$Z_4^{(5)} = Z_0 \delta_{D,2} N r_{D-1}^4. \quad (24)$$

Collecting all these terms we arrive at

$$Z_4 = Z_0 N \left\{ \frac{1}{2} D (ND - 4D + 1) r_{D-1}^4 + D (2D - 1)^2 r_{D-1}^2 r_{D-2}^2 + \frac{2}{3} D (D - 1) (2D - 1) r_{D-1}^3 r_{D-3} + \frac{1}{2} D (D - 1) r_{D-2}^4 + \delta_{D,2} r_{D-1}^4 \right\}, \quad (25)$$

from which we obtain the free energy

$$-\beta f \equiv N^{-1} \log Z \equiv -\beta (f_0 + f_2 + f_3 + f_4 + \dots), \quad (26)$$

$\#^2$ Full lines denote links with flipped spins, dotted lines have unflipped spins.

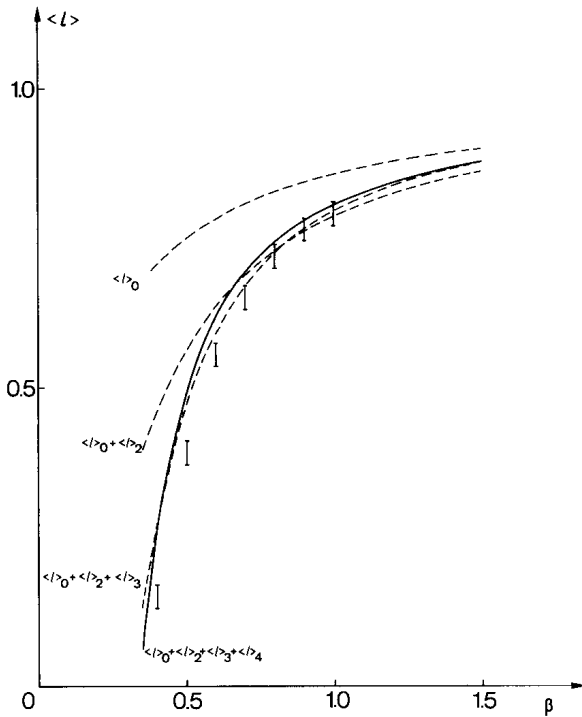


Fig. 2. The total length per site (=internal energy) as a function of $\beta = e^{-\epsilon/T}$ in comparison with the Monte Carlo data of ref. [5].

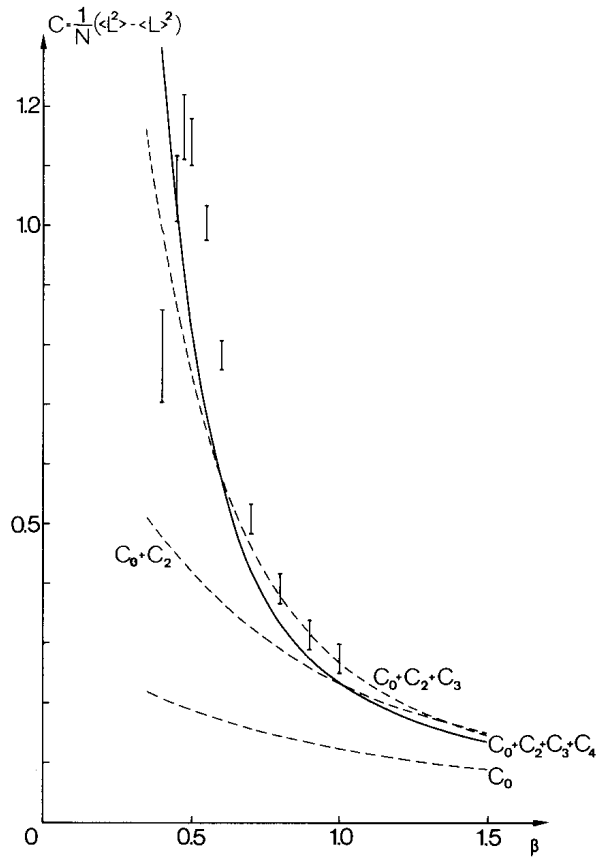


Fig. 3. The length fluctuation per site (=specific heat) as a function of $\beta = e^{-\epsilon/T}$ in comparison with the Monte Carlo data of ref. [5].

with

$$\begin{aligned}
 -\beta f_0 &= -D \log 2 + \log(1 + 2\beta D^2 - \beta D), & -\beta f_2 &= D r_{D-1}^2, & -\beta f_3 &= D(2D-1)r_{D-1}^2 r_{D-2}, \\
 -\beta f_4 &= -\frac{1}{2}D(4D-1)r_{D-1}^4 + D(2D-1)^2 r_{D-1}^2 r_{D-2}^2 + \frac{2}{3}D(D-1)(2D-1)r_{D-1}^3 r_{D-3} \\
 &+ \frac{1}{2}D(D-1)r_{D-2}^4 + \delta_{D,2} r_{D-1}^4.
 \end{aligned} \tag{27}$$

From this one can calculate $\langle l \rangle$ and $\langle (\Delta l)^2 \rangle$.

The results are displayed in figs. 2 and 3 and compared with data from Monte Carlo simulation on 5×5 lattices. We see that the agreement is quite good, if the size dependence of the simulations is extrapolated towards infinite size. For higher dimensions, the convergence of the expansion (17) slows down rapidly and other analytic methods have to be used. These will be presented elsewhere.

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