

## FROM SELF-AVOIDING RANDOM LOOPS TO ISING SYSTEMS AN INTERPOLATING SPIN MODEL AND ITS MONTE CARLO STUDY<sup>☆</sup>

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We develop a new lattice model involving Ising spins on *links* with next-neighbor couplings which contains a parameter  $\xi$  that interpolates between the standard Ising model ( $\xi = 1$ ) and an ensemble of self-avoiding random loops ( $\xi = 0$ ). This model is studied by Monte Carlo techniques. We calculate the average length and its variance as a function of temperature. The reliability of our results is checked at several steps by comparison with the exactly known Ising case on finite lattices.

Until recently, Monte Carlo investigations of self-avoiding random loop or surface ensembles were plagued by two types of problems: First, in trying to simulate random geometries directly, one could not use the same techniques, by which spin and gauge models had previously been studied successfully, but had to find new procedures whose quality was unknown<sup>#1</sup>. Second, when imposing the constraint of self-avoidance, the efficiency of the simulations was strongly reduced, due to the small acceptance rate of the randomly generated configurations [1]. This problem became particularly severe near the phase transition at which the geometric objects proliferate, thereby locking up most of the available space.

Motivated by these problems we were led to develop a method by which random ensembles of loops [2] and surfaces [3] can be studied via simple models which involve spin-like variables with next-neighbor couplings. The new models had two merits: First, they opened up the difficult hot phase to simple analytic techniques, such as mean field approximations plus loop corrections. In combination with the known strong-coupling series it is now, in principle, possible to obtain good approximations to the thermodynamic properties of the ensemble. Second, the models permit-

ted the derivation of a simple local field theory which, in the critical regime, displayed clearly the universality class of the transition, showing for instance that self-avoiding loops proliferate with Ising indices, and that self-avoiding surfaces with more than one color in three dimensions do not proliferate at all.

In spite of these merits, the models are unsatisfactory in that they are not accessible to Monte Carlo studies due to their non-Boltzmann form of the partition function.

For loops, this obstacle was removed recently [4] by Hofssäss and Kleinert (HK) who were able to reexpress these models in terms of Ising spin variables.

The purpose of this note is twofold: First, we want to extend the HK spin model by a new term with a parameter  $\xi$  in such a way that the extended model interpolates between the self-avoiding random loops ( $\xi = 0$ ) and the proper Ising model ( $\xi = 1$ ). Second, we want to simulate this model in two dimensions on the computer. The new model has the advantage that we can convince ourselves of the reliability of our results, at each step, by taking the case  $\xi = 1$  and cross-checking it with the known exact finite lattice results of the Ising model [5].

Let us first recall the result of ref. [2] according to which the partition function of self-avoiding random loops is given by

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<sup>#1</sup> For simulations of certain kinds of loops and surfaces see ref. [1].

$$Z_{s.a.} = \prod_{\mathbf{x}} \left( \int_{-\pi}^{\pi} \frac{d\theta(\mathbf{x})}{2\pi} \{1 + [U^*(\mathbf{x})]^2\} \right) \times \prod_{\mathbf{x}, i} [1 + vU(\mathbf{x})U(\mathbf{x} + i)] , \quad (1)$$

where  $\mathbf{x}$  runs through all sites of a simple cubic lattice,  $i$  denotes the oriented links,  $U(\mathbf{x})$  are pure phase variables  $\exp[i\theta(\mathbf{x})]$ , and  $v \equiv \exp(-\epsilon/T)$  is the Boltzmann factor, by which each loop element of energy  $\epsilon$  is suppressed. It is easy to see that the product on the right-hand side places chain elements randomly upon all links, whose ends are then connected by the integrations

$$\int_{-\pi}^{\pi} \frac{d\theta}{2\pi} [1 + (U^*)^2] .$$

Each site can harbor at most two elements. Thus  $Z_{s.a.}$  has the low-temperature expansion

$$Z_{s.a.} = \sum_{s.a.} v^L = \sum_{s.a.} \exp[-(\epsilon/T)L] , \quad (2)$$

where the sum covers precisely all self-avoiding random loop configurations.

The recent Ising spin HK model was obtained by taking the "square root" of the factors  $\prod_{\mathbf{x}, i} [1 + vU(\mathbf{x})U(\mathbf{x} + i)]$  via an auxiliary sum over Ising variables  $s_i(\mathbf{x})$  living on links

$$\prod_{\mathbf{x}, i} \left( \frac{1}{2} \sum_{s_i(\mathbf{x})=\pm 1} \right) [1 + \sqrt{v}U(\mathbf{x})s_i(\mathbf{x})] \times [1 + \sqrt{v}U(\mathbf{x})s_i(\mathbf{x} - i)] , \quad (3)$$

and observing that under the integral measure (3) only powers  $U^p$  with  $p=0$  and  $p=2$  can survive. Hence the product can be replaced by

$$2^{-ND} \prod_{\mathbf{x}, i} \left( \sum_{s_i(\mathbf{x})=\pm 1} \right) \times \prod_{\mathbf{x}} \left( 1 + vU^2(\mathbf{x}) \sum_{\substack{\pm i, \pm j \\ i \neq j}} s_i(\mathbf{x})s_j(\mathbf{x}) \right) ,$$

where  $s_{-i}(\mathbf{x}) \equiv s_i(\mathbf{x} - i)^{\#2}$ . Now, the  $U$  integration

<sup>#2</sup> In our notation,  $i$  covers only the oriented links emerging from a site  $\mathbf{x}$ ,  $\pm i$  runs through *all* links.

gives [4]

$$Z = 2^{-ND} \sum_{\{s_i(\mathbf{x})=\pm 1\}} \prod_{\mathbf{x}} \left[ 1 + \frac{1}{2}v \left( \sum_{\pm i=1}^D s_i(\mathbf{x}) \right)^2 - vD \right] = 2^{-ND} \sum_{\{s_i(\mathbf{x})=\pm 1\}} \prod_{\mathbf{x}} z(\mathbf{x}) ,$$

where the factors  $z(\mathbf{x})$  are *local* quantities involving only next-neighbor Ising spin on *links*.

After this reminder, let us now come to our first goal, namely that of bringing the Ising model to a related form. For this we rewrite  $Z_{\text{Ising}}$  as

$$Z_{\text{Ising}} \equiv \prod_{\mathbf{x}} \left( \frac{1}{2} \sum_{s(\mathbf{x})=\pm 1} \right) \exp \left( \beta \sum_{\mathbf{x}, i} s(\mathbf{x})s(\mathbf{x} + i) \right) = (\text{ch } \beta)^{ND} \prod_{\mathbf{x}} \left( \frac{1}{2} \sum_{s(\mathbf{x})=\pm 1} \right) \prod_{\mathbf{x}, i} [1 + vs(\mathbf{x})s(\mathbf{x} + i)] , \quad (4)$$

where  $s(\mathbf{x})$  are Ising variables on *sites* and  $v \equiv \text{th } \beta$ . Then we take again the square root of the right-hand product, using new Ising variables on *links*,

$$\prod_{\mathbf{x}, i} [1 + vs(\mathbf{x})s(\mathbf{x} + i)] = \prod_{\mathbf{x}, i} \left( \frac{1}{2} \sum_{s_i(\mathbf{x})=\pm 1} \right) \prod_{\mathbf{x}, i} [1 + \sqrt{v}s(\mathbf{x})s_i(\mathbf{x})] \times [1 + \sqrt{v}s(\mathbf{x})s_i(\mathbf{x} - i)] .$$

When working out the product, and inserting it into the sum over  $s(\mathbf{x}) = \pm 1$ , it cannot be truncated as in the previous case, where only two terms contributed. The maximal number of  $s(\mathbf{x})$  variables at each site is, however, limited by the dimensionality of the lattice. In two dimensions, at most four  $s(\mathbf{x})$  can fall onto one site such that  $Z_{\text{Ising}}$  becomes

$$Z_{\text{Ising}} = (\text{ch } \beta)^{2N} \prod_{\mathbf{x}, i} \left( \frac{1}{2} \sum_{s_i(\mathbf{x})=\pm 1} \right) \prod_{\mathbf{x}} z_{\text{Ising}}(\mathbf{x}) , z_{\text{Ising}}(\mathbf{x}) \equiv 1 + \frac{1}{2}v \left( \sum_{\pm i=1}^D s_i(\mathbf{x}) \right)^2 - 2v + v^2 \prod_i s_i(\mathbf{x})s_{-i}(\mathbf{x}) . \quad (5)$$

It is easy to work out the next terms for  $D = 3, 4, \dots$  dimensions.

Thus, up to the trivial factor  $(ch\beta)^{2N}$ , the self-avoiding random loops and the Ising model in two dimensions become the two extremes of the single interpolating partition function

$$Z = \prod_{x,i} \left( \frac{1}{2} \sum_{s_i(x)=\pm 1} \right) \prod_x z(x),$$

$$z(x) \equiv 1 + \frac{1}{2}v \left( \sum_{\pm i=1}^D s_i(x) \right)^2 - 2v$$

$$+ \xi v^2 \prod_i s_i(x) s_{-i}(x), \quad (6)$$

for  $\xi = 0$  and  $\xi = 1$ , respectively. This is the desired extension of the model which not only stresses the common universality class of the two systems but specifies *quantitatively* the differences. We now turn to the second goal of simulating this model via Monte Carlo techniques. Due to limitations in space, we describe here only measurements of the mean loop length

$$\langle l \rangle \equiv N^{-1} \langle L \rangle = (NZ)^{-1} \sum_{\text{s.a.}} L \exp[-(\epsilon/T)L]$$

$$= N^{-1} v (\partial/\partial v) Z, \quad (7)$$

and its variance

$$\langle l^2 \rangle_c \equiv N^{-1} [\langle L^2 \rangle - \langle L \rangle^2]$$

$$= N^{-1} \left[ Z^{-1} \sum_{\text{s.a.}} L^2 \exp[-(\epsilon/T)L] - \left( Z^{-1} \sum_{\text{s.a.}} L \exp[-(\epsilon/T)L] \right)^2 \right]$$

$$= N^{-1} (v \partial/\partial v)^2 \log Z, \quad (8)$$

where  $N$  is the number of sites. Applying these formulas to (6) we find more explicitly

$$\langle l \rangle = N^{-1} \left\langle \sum_x \frac{\dot{z}(x)}{z(x)} \right\rangle,$$

$$\langle l^2 \rangle_c = N^{-1} \left\{ \left\langle \sum_x \left[ \frac{\ddot{z}(x)}{z(x)} - \left( \frac{\dot{z}(x)}{z(x)} \right)^2 \right] + \left( \sum_x \frac{\dot{z}(x)}{z(x)} \right)^2 \right\rangle - \left[ \left\langle \sum_x \frac{\dot{z}(x)}{z(x)} \right\rangle \right]^2 \right\}, \quad (9)$$

where the dots denote the operation  $\equiv v \partial/\partial v$ .

The expectation  $\langle (\dots) \rangle$  is defined as

$$Z^{-1} \prod_{x,i} \left( \frac{1}{2} \sum_{s_i(x)=\pm 1} \right) (\dots) \prod_x z(x).$$

The boundary conditions are chosen to be periodic.

In order to apply Monte Carlo techniques we first observe that as long as  $v < \xi^{-1}(1 - \sqrt{1 - \xi})$  (which

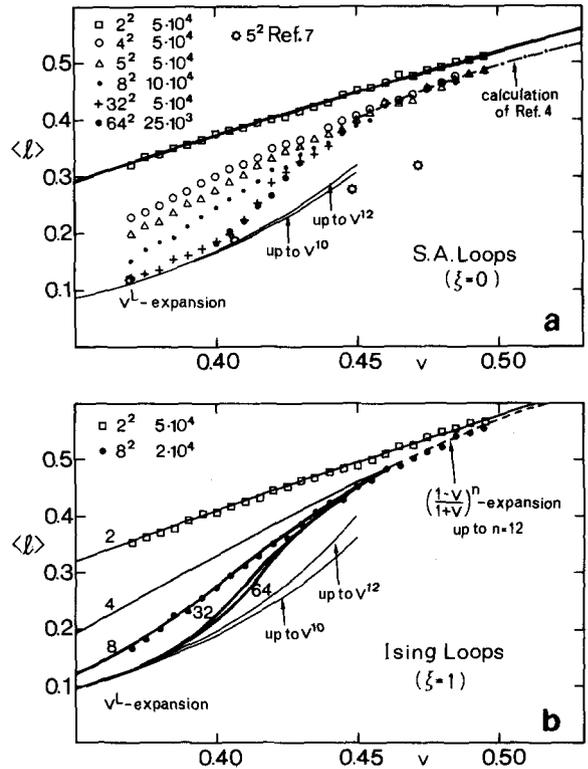


Fig. 1. (a) The mean loop length per site  $\langle l \rangle$  as a function of the fugacity  $v = \exp(-\epsilon/T)$  where  $\epsilon$  is the energy per line element. The data are for 2-dimensional s.c. lattices of sizes  $2 \times 2, 4 \times 4, 5 \times 5, 8 \times 8$ , and  $32 \times 32, 64 \times 64$ . The numbers behind the data symbols give the numbers of runs done for equilibration, the same numbers of runs were done for measurement. The curve through the  $2 \times 2$  data gives the exact solution. The thin lines come from a  $v^L$  expansion up to  $v^{10}$  and  $v^{12}$ . The dash-dotted line shows the analytic results of ref. [4]. (b) The corresponding curves for the Ising model, but in the dual loop gas interpretation. The upper five solid curves denote the exact results on finite lattices. We also have given a few data from ordinary MC runs of the Ising model, for comparison. The thin lines come again from a  $v^L$  expansion, the dashed curve from the dual  $[(1-v)/(1+v)]^L$  expansion up to the 12th power.

tends to 1/2 for  $\xi \rightarrow 0$ ) the factors  $z(\mathbf{x})$  are positive and the partition function has a conventional probabilistic interpretation. Guided by the experience with the Ising model, we used the heat bath updating procedure. Most data points were taken three times, first during a thermal cycle and then, independently by single measurements starting with completely random or ordered configurations. Typically, we established equilibrium by going through 50 000 Monte Carlo sweeps after which we measured  $\langle l \rangle$  and  $\langle l^2 \rangle_c$  by averaging over further 50 000 iterations. The resulting mean loop length for  $\xi = 0$  (s.a. loops) as functions of  $v$  for various lattice sizes is displayed in fig. 1a.

In order to have a check of the finite size scaling behavior, we have calculated the exact partition function on a  $2 \times 2$  lattice by direct counting of loops. With our periodic boundary conditions, the general result for all  $\xi$  is <sup>†3</sup>

$$Z^{2 \times 2 \text{ latt}} = 1 + 4v^2 + (18 + 4\xi)v^4 + 4\xi^2 v^6 + \xi^4 v^8. \quad (10)$$

This exact result produces the continuous line in fig. 1a in excellent agreement with our data.

In the infinite volume limit, another useful check is provided by an expansion of the partition function in powers of  $v$ ,  $Z = \sum_L g_L v^L$ , where  $g_L$  counts the number of loop configurations with total length  $L$ . Taking the logarithm, we find up to  $L = 12$

$$N^{-1} \log Z = v^4 + 2v^6 + \left(\frac{5}{2} + 2\xi\right)v^8 + (4 + 8\xi)v^{10} + \left(\frac{58}{3} + 12\xi + 6\xi^2\right)v^{12}, \quad (11)$$

which for  $\xi = 1$ , coincides with the well-known high temperature expansion of the Ising model (apart from a trivial term  $2 \log \text{ch } \beta$ ) [6]. Note that for  $v \lesssim 0.4$ , the 12th order contribution is so small that it cannot be seen on the scale of fig. 1a.

The opposite regime  $v \gtrsim 0.45$  of our data is in excellent agreement with another analytic calculation given in ref. [4]. For comparison, we show in fig. 1b the corresponding data for  $\xi = 1$  i.e. for the loop gas of the Ising model. In order to test the accuracy of our simulation techniques we have evaluated the corresponding curves from the finite size exact result for the Ising partition function [5]. Using the relation  $v$

$\equiv \text{th } \beta_{\text{Ising}}$  we find for the Ising loops

$$\begin{aligned} \langle l \rangle &= -[v/(1 - v^2)](u_{\text{Ising}} + Dv), \\ \langle l^2 \rangle_c &= [v^2/(1 - v^2)^2] \\ &\times [(\beta_{\text{Ising}})^{-1} C_V^{\text{Ising}} - 2D - v^{-1}(1 + v^2)u_{\text{Ising}}], \end{aligned} \quad (12)$$

where

$$\begin{aligned} u_{\text{Ising}} &\equiv -N^{-1}(\partial/\partial\beta) \log Z_{\text{Ising}}, \\ C_V^{\text{Ising}} &\equiv N^{-1}\beta^2(\partial^2/\partial\beta^2) \log Z_{\text{Ising}} \\ &= -\beta^2(\partial/\partial\beta)u_{\text{Ising}}. \end{aligned}$$

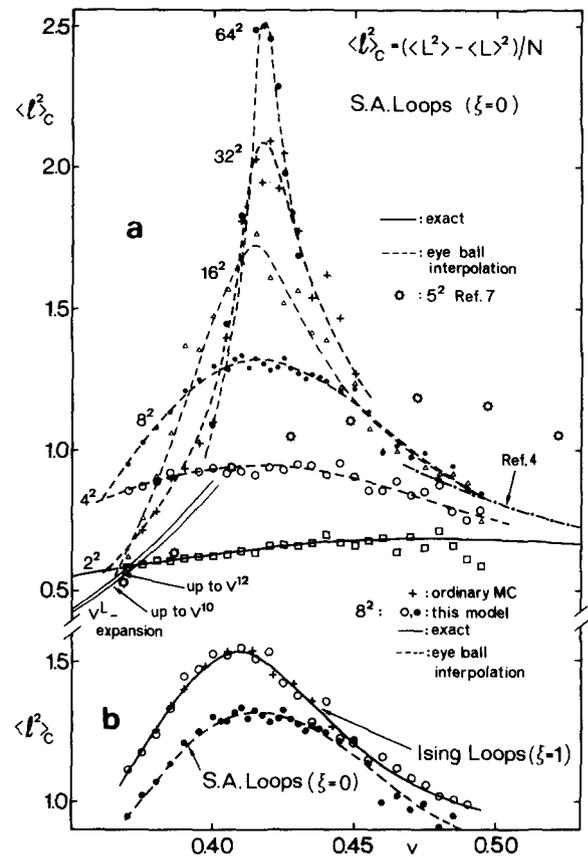


Fig. 2. (a) The variance of the loop length per site,  $\langle l^2 \rangle_c = (\langle L^2 \rangle - \langle L \rangle^2)/N$  as a function of  $v = \exp(-\epsilon/T)$ . The upper five dashed curves are to guide the eye. The data which fall completely out of our set are the  $5 \times 5$  points of ref. [7]. The other curves come from the same sources as in fig. 1a. (b) The  $8 \times 8$  curves of  $\langle l^2 \rangle_c$  in the s.a. loop gas ( $\xi = 0$ ) as compared with those of the Ising model ( $\xi = 1$ ). We also have given the exact  $8 \times 8$  curves and the data of an ordinary MC simulation of the Ising model.

<sup>†3</sup> As  $T \rightarrow \infty$ ,  $v \rightarrow 1$ , the mean length tends to  $20/23 = 0.8696$ , 1 for  $\xi = 0$  (s.a. loops),  $\xi = 1$  (Ising loops), respectively in agreement with figs. 1a, b.

We also found it useful to compare, in fig. 1b, our results for an  $8 \times 8$  lattice with a standard simulation of the Ising model using site variables  $s(\mathbf{x})$  rather than our link variables  $s_l(\mathbf{x})$ .

In fig. 2a we have displayed the variance of the length ( $\hat{=}$  specific heat) for  $\xi = 0$ . It displays a pronounced size dependence. Doubling the linear lattice size causes each time roughly the same increment of the maximum of  $\langle l^2 \rangle_c$ . This is the typical sign of logarithmic scaling  $\langle l^2 \rangle_c \approx a \log n$ . Thus, in two dimensions, the critical exponent of the s.a. loop gas is consistent with the Ising value,  $\alpha = 0$ .

Extrapolating the location of the maximum for  $n \gtrsim 8$  to infinite volume we estimate for the s.a. loop gas  $v_c \sim 0.42$ , remarkably close [2] to  $v_{c \text{ Ising}} = \sqrt{2} - 1 \approx 0.41$ . At first sight it looks unusual that the locations  $v_{\max}$  of the  $\langle l^2 \rangle_c$  are not a monotonic function of the linear lattice size  $n$ , as it is in the specific heat of the Ising model. The location moves first to the left, then, for  $n \gtrsim 8$ , to the right. The origin of this behavior lies in the fact that  $\langle l^2 \rangle_c$  is not the same as the usual specific heat [see (15)]. Indeed, when plotting  $\langle l^2 \rangle_c$  for the Ising model we find exactly the same behavior.

In fig. 2b we compare the  $\langle l^2 \rangle_c$  curves of s.a. loop gas and Ising loops ( $\xi = 1$ ) with the exact solution and with the data of an ordinary simulation.

Finally, we have tested the interpolation character of our model by running a few simulations for fixed  $v$  as a function of  $\xi$ . On the  $2 \times 2$  lattice we find com-

plete agreement with the exact curves derived from (13).

Summarizing we see that our new model permits Monte Carlo simulations of self-avoiding random loops which are just as efficient and reliable as those of the ordinary Ising model.

Let us finally mention that our results are in serious contradiction with the data of ref. [7]. Their  $5 \times 5$  values of  $\langle l \rangle$  lie practically on the strong-coupling curve for infinite volume, which they should not, due to finite size effects. The disagreement in the variance is even more dramatic, as illustrated by the  $5 \times 5$  curve in fig. 2a. The discrepancy is apparently due to the emission, in ref. [7], of closed loops which wind completely around the toroidal lattice and which are not covered naturally by their direct simulation method.

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