SELF-AVOIDING RANDOM LOOPS VERSUS ISING MODEL IN THREE DIMENSIONS ☆

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Received 5 February 1988; accepted for publication 25 February 1988
Communicated by A.A. Maradudin

On the basis of a recently developed lattice model for ensembles of random loops which contains a parameter interpolating between self-avoiding and Ising-like loops, we calculate the average length and the length fluctuations of self-avoiding loops in three dimensions, using analytic as well as Monte Carlo methods, and compare the results with the Ising case. Applying finite-size scaling techniques, we show that the critical behavior of self-avoiding random loops is consistent with universality predictions based on the Ising model.

1. Introduction

The statistical mechanics of line-like geometrical objects appears to be a useful tool in many different fields of physics (for a general overview and many references see ref. [1]). Its applications range from quite abstract investigations of polymer-representations of quantum field theory to more practical topics such as phase-transitions in condensed matter. In many cases these transitions can be explained by a proliferation of line-like excitatons. Well-known examples are the λ-transition in liquid helium which is caused by the proliferation of vortex-lines, and ordinary crystal melting where the growth of defect lines causes the breakdown of crystalline order. In this note, we want to focus on a third type of application where line-like objects have a direct physical meaning, namely polymerization processes [2]. A standard example is the polymerization of liquid sulphur (for a review of the properties of liquid sulphur see ref. [3]) which, around 115°C, consists mainly of S_8 rings. With increasing temperature the system can lower its free energy by opening up the S_8 rings, joining the ends, and forming long loops and chains. Each opened S_8 ring will be considered as one polymer element (=monomer).

☆ Supported in part by Deutsche Forschungsgemeinschaft under grant no. Kl.256.

Open chains are suppressed by the high energy of their end points. In the limit of infinite end point energy, there will be only loops. Then, as the temperature approaches the critical point at $T_c \approx 160°C$, the configurational entropy dominates and creates a condensate of infinitely long loops. Since infinitely long loops have infinitely many possibilities of breaking into pieces, also the breaking entropy becomes very large. In an actual polymer system, the end point energy is large but finite, and hence it can be compensated by the large breaking entropy. This is why a real polymer system contains always a sizable fraction of open chains above T_c [2,4]. Also, even at very large but finite end point energy, none of the polymers can become any more infinitely long so that the system does no longer have a phase transition in the strict sense. Still, the experimental transition is signaled by a sharp peak in the specific heat [5], just as in a second order phase transition, indicating the largeness of the end point energy.

Since we want to study the truly critical transition, we shall confine ourselves to an ensemble of pure loop-like polymers which, for simplicity, are assumed to lie on the links of a simple hypercubic lattice. Furthermore, we require that each link can be occupied at most by one monomer, so that backtracking loops cannot appear. If loops are allowed to touch each other at their corners then, by a duality transformation, this ensemble is seen to be equiva-

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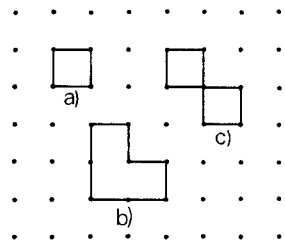

Fig. 1. A typical configuration of *Ising* loops. In the *self-avoiding* loop gas, loops which touch each other at their corners like in graph (c) are not allowed.

lent to the Ising model, and we shall call it an Ising loop gas. When excluded volume effects are taken into account and such crossing-points are forbidden, we get an ensemble of self-avoiding random loops (for examples, see fig. 1). Recalling the duality with the Ising model, it can be shown that open chains act like an external magnetic field. This analogy provides just another way to see that open chains destroy a well-defined phase transition [#1].

The purpose of this note is to study the quantitative differences between ensembles of self-avoiding and Ising loops, and to compare their critical behavior near the phase transition. We perform Monte Carlo simulations in the recently developed spin representation of loop gas models [6,7] and analyze the data for self-avoiding loops using finite-size scaling techniques.

The present note is an extension of an earlier (and much simpler) study of the two-dimensional case [8].

2. The model

If ϵ is the energy per monomer, T the temperature, and $v \equiv \exp(-\epsilon/T)$ the corresponding fugacity, we want to sum the partiton function

$$Z = \sum_{\text{loop conf.}} \mathrm{e}^{-L\epsilon/T}, \tag{1}$$

where L is the number of monomers (or the total length of all polymers) in a loop-configuration which can be chosen to contain self-avoiding or Ising loops, respectively (see fig. 1). For simplicity, we shall assume these to lie on the links of a simple hypercubic lattice.

For self-avoiding loop configurations, it was pointed out by Hofsäss and Kleinert [6] that the partition function (1) can be rewritten as an infinite product of integrals over pure phase variables $U(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}\Theta(\boldsymbol{x})}$ (HK partition function):

$$Z = \prod_{\boldsymbol{x}} \left(\int_{-\pi}^{\pi} \frac{\mathrm{d}\Theta(\boldsymbol{x})}{2\pi} \left[1 + U^{*2}(\boldsymbol{x})\right] \right) \times \prod_{\boldsymbol{x},\boldsymbol{i}} \left[1 + vU(\boldsymbol{x})U(\boldsymbol{x}+\boldsymbol{i})\right] . \tag{2}$$

That this is true can easily be verified a posteriori by noticing that the second product distributes randomly, with a statistical weight v, pairs of phase variables $U(\boldsymbol{x})U(\boldsymbol{x}+\boldsymbol{i})$ over all oriented links $\boldsymbol{i}$ whose end points are knitted together by the integrals over $U^{*2}(\boldsymbol{x})$. The fact that the measure of integration contains only U^{*2} ensures that each lattice site can accommodate at most two end points. This is what distinguishes the HK partition function of self-avoiding loops from that of the Ising model, which can also be written as an integral of the form (2) but with an infinite sum of powers of U^{*2} in the integrand [#2]

$$Z = \prod_{\boldsymbol{x}} \left(\int_{-\pi}^{\pi} \frac{\mathrm{d}\Theta(\boldsymbol{x})}{2\pi} \left[1 + U^{*2}(\boldsymbol{x}) + U^{*4}(\boldsymbol{x}) + \ldots\right] \right) \times \prod_{\boldsymbol{x},\boldsymbol{i}} \left[1 + vU(\boldsymbol{x})U(\boldsymbol{x}+\boldsymbol{i})\right] . \tag{3}$$

The HK partition function is not yet very useful for Monte Carlo simulations. A better version was found in ref. [7]. It is based on introducing an auxiliary sum over Ising variables $s_i(\boldsymbol{x})$ living on links [#3] and rewriting

[#1] This is well known for Ising loops – but it is obvious that it holds also in the self-avoiding case.

[#2] We have omitted the trivial overall factor $2^N(\cosh\beta_{\mathrm{Is}})^{ND}$ (N = number of lattice sites, D = space dimension) when going from the usual Ising model partition function $Z_{\mathrm{Is}} = \prod_{\boldsymbol{x}}(\sum_{s(\boldsymbol{x})=\pm 1})\exp[\beta_{\mathrm{Is}}\sum_{\boldsymbol{x},\boldsymbol{i}} s(\boldsymbol{x})s(\boldsymbol{x}+\boldsymbol{i})]$ to the form (3). For Ising loops, the fugacity is $v \equiv \tanh\beta_{\mathrm{Is}}$.

[#3] This must not be confused with the usual Ising variables $s(\boldsymbol{x})$ which live on *sites*.

$$\prod_{x,i}[1+vU(x)U(x+i)]$$
$$=\prod_{x,i}\tfrac{1}{2}\sum_{s_i(x)=\pm 1}[1+\sqrt{v}\,U(x)s_i(x)]$$
$$\times[1+\sqrt{v}\,U(x+i)s_i(x)]$$
$$=2^{-ND}\prod_{x,i}\sum_{s_i(x)=\pm 1}[1+\sqrt{v}\,U(x)s_i(x)]$$
$$\times[1+\sqrt{v}\,U(x)s_i(x-i)]\,, \qquad (4)$$

where D is the space dimension and N is the total number of lattice sites. The product over i can be carried out most easily by introducing the notation $s_{-i}(x)\equiv s_i(x-i)$ and numbering the 2D Ising variables around each site by $s_a(x)=s_{-D}(x)$, ..., $s_D(x)$. If $s(x)\equiv\sum_{a=-D}^{D}s_a(x)$ denotes the sum over these then

$$\prod_{a=-D}^{D}[1+\sqrt{v}\,U(x)s_a(x)]$$
$$=1+\sum_{n=1}^{2D}(\sqrt{u})^n U^n(x)c_n(s(x))\,, \qquad (5)$$

where

$$c_2(s)=\sum_{a>b}s_a s_b=\tfrac{1}{2}(s^2-2D)\,,$$
$$c_4(s)=\sum_{a>b>c>d}s_a s_b s_c s_d$$
$$=\frac{1}{4!}[s^4-(12D-8)s^2+6D(2D-2)]\,,$$
$$c_6(s)=\sum_{a>b>\ldots>f}s_a\ldots s_f$$
$$=\frac{1}{6!}[s^6-(30D-40)s^4+(180D^2-420D$$
$$+184)s^2-30D(2D-2)(2D-4)]\,,$$
$$\ldots \qquad (6)$$

Performing now the integrals over $\Theta(x)$ in eq. (2), we see that for self-avoiding loops only $c_2(s)$ contributes and we are left with the simple expression

$$Z=2^{-ND}\prod_{x,i}\Big(\sum_{s_i(x)=\pm 1}\Big)\prod_x z(x)\,, \qquad (7)$$

where

$$z(x)=1+vc_2(s)=1-vD+\tfrac{1}{2}vs^2(x)\,. \qquad (8)$$

For the Ising model, the "local partition functions" in (7) become

$$z(x)=1+vc_2(s)+v^2c_4(s)+v^3c_6(s)+\ldots+v^Dc_{2D}(s)\,. \qquad (9)$$

Hence, a simple interpolating model can be obtained by multiplying the last $D-1$ terms by a parameter ξ ($=0$ self-avoiding, $=1$ Ising) [8].

3. The Monte Carlo simulation

We have simulated the interpolating spin-model (7)–(9) for both $\xi=0$ and $\xi=1$ via standard Monte Carlo methods (heat-bath algorithm) [9] on three-dimensional simple cubic lattices with periodic boundary conditions. In this note we report on measurements of the total length of all loops and its fluctuations. The total length is found from

$$\langle L\rangle=v\partial_v\log Z=\sum_x\left\langle\frac{\dot{z}(x)}{z(x)}\right\rangle, \qquad (10)$$

where $z(x)$ is given in (8) and (9), respectively, $\dot{z}\equiv v\partial_v z$, and the average $\langle\ \rangle$ on the r.h.s. has to be taken with respect to the partition function (7). The length fluctuations are

$$\langle L^2\rangle_c\equiv\langle L^2\rangle-\langle L\rangle^2=v\partial_v\langle L\rangle=(v\partial_v)^2\log Z$$
$$=\left\langle\left(\sum_x\frac{\dot{z}}{z}\right)^2\right\rangle-\left\langle\sum_x\frac{\dot{z}}{z}\right\rangle^2+\sum_x\left\langle\frac{\ddot{z}}{z}-\left(\frac{\dot{z}}{z}\right)^2\right\rangle. \qquad (11)$$

Notice that these geometrical quantities are related to the internal energy and specific heat of the loop gas (1) by

$$U=-\partial_\beta\log Z=\epsilon v\partial_v\log Z=\epsilon\langle L\rangle \qquad (12)$$

and

$$C=-\beta^2\partial_\beta U=\epsilon^2\beta^2(v\partial_v)^2\log Z=\epsilon^2\beta^2\langle L^2\rangle_c\,, \qquad (13)$$

where $\beta\equiv 1/T$.

For low temperature we can check our simulations against the low-fugacity ($v\to 0$) series for $\langle L\rangle$ and $\langle L^2\rangle_c$, which can easily be derived from the expansion (for details of graph counting see ref. [10])

$$\frac{1}{N}\log Z=\binom{D}{2}v^4+\left[2\binom{D}{2}+16\binom{D}{3}\right]v^6$$
$$+\left[(\tfrac{5}{2}+2\xi)\binom{D}{2}+(150+24\xi)\binom{D}{3}\right.$$
$$\left.+(600+48\xi)\binom{D}{4}\right]v^8+\left[(4+8\xi)\binom{D}{2}\right.$$
$$\left.+(1380+552\xi+12\xi^2)\binom{D}{3}+\ldots\right]v^{10}$$
$$+O(v^{12})\,. \qquad (14)$$

For $\xi=1$ this expansion agrees with the well-known *high*-(Ising)-temperature series of the Ising model [11] (where +... in the last bracket means +22304 $\times\binom{D}{4}$+ 47616$\binom{D}{5}$).

4. Numerical results

Let us start with a *quantitative* comparison of the self-avoiding ($\xi=0$) and Ising ($\xi=1$) loop gas models. Our results on a 8^3 lattice are shown in figs. 2a, 2b where we plot the mean total loop length corresponding to the internal energy (a) and the length fluctuations corresponding to the specific heat (b) versus $v\equiv\exp(-\epsilon/T)$. As a check of the $\xi=1$ case, we have also included data from a simulation of the ordinary Ising model with spins on the sites. The agreement is excellent. Up to the transition around $v\approx 0.22$, self-avoiding and Ising loops are practically indistinguishable, in agreement with the remarks of Cordery [12]. This is also seen in the low-fugacity ($v\to 0$) expansions derived from (14) which are almost identical for $\xi=0$ and $\xi=1$. The curves labeled "LTS" are the usual low-(Ising)-temperature expansions [13] of the Ising model.

Let us now turn to the critical behavior of the self-avoiding loop gas model. To this end, we have simulated the $\xi=0$ model on lattices with linear sizes $L=6$, 8, 10, 16 and 20 and analyzed the data using finite-size scaling techniques [14,9]. Our raw data for the length fluctuations ($\triangleq$ specific heat) are displayed in fig. 3. For most of these points we have used 200000 Monte Carlo sweeps through the lattice, after discarding 50000 sweeps for thermalization. To improve the accuracy near the peaks, we have averaged two such runs with different start configurations (typically completely ordered or completely random).

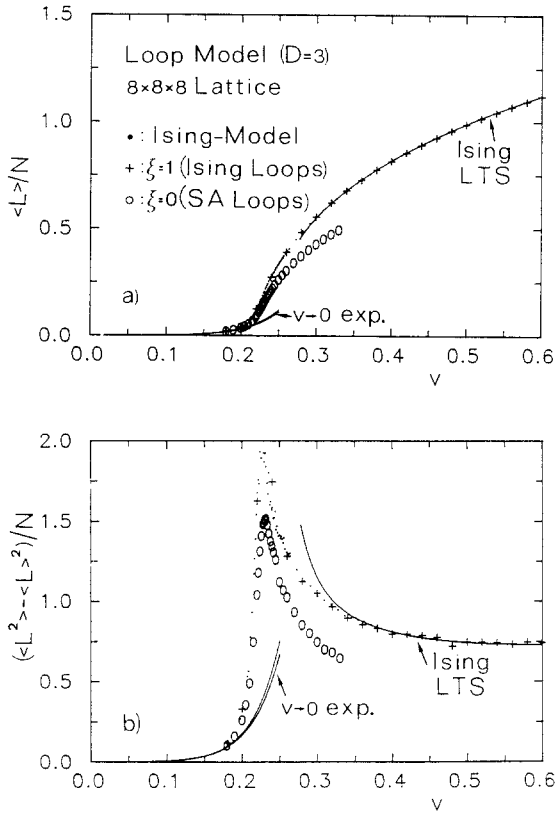

Fig. 2. The mean loop length per site (a) and the length fluctuations per site (b) of self-avoiding (○) and Ising (+) loops on a 8^3 lattice versus the fugacity $v=\exp(-\epsilon/T)$. For comparison, we also have plotted data from a Monte Carlo simulation of the ordinary Ising model (●). The $v\to 0$ curves are derived from the low-fugacity expansion (14), and the curves labeled "LTS" are the usual low-(Ising)-temperature expansions [13] of the Ising model.

Finite-size scaling theory predicts that the locations of the peaks, $v_c(L)$, scale on finite lattices of linear size L as

$$v_c(L)=v_c(\infty)+aL^{-1/\nu}\,, \qquad (15)$$

where ν is the universal critical exponent of the correlation length ($\xi\propto|1-v/v_c|^{-\nu}$), and a is a non-universal constant. The extrapolation to $v_c(\infty)$ is not very sensitive to the precise value of ν (in a reasonable range, say $\nu=0.58$, ..., 0.64), and we find the

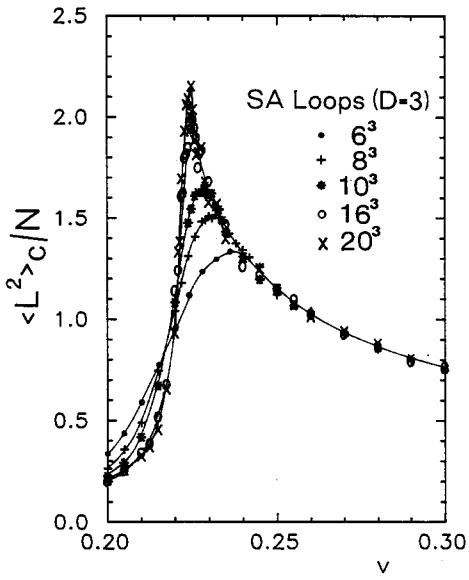

Fig. 3. Length fluctuations (≙specific heat) per site $\langle L^2\rangle_c/N=(\langle L^2\rangle-\langle L\rangle^2)/N$ of self-avoiding loops in three dimensions near the phase transition point for various lattice sizes. The curves are only to guide the eye.

almost unbiased estimate [#4]

$$v_c\equiv v_c(\infty)=0.222\pm0.001\,. \qquad (16)$$

Note that this critical value is only 1.8% larger than the corresponding one of the Ising model, $v_c^{Is}=0.218090(5)$ [16]. (The number in parentheses is the error in the last digit. See also ref. [24].)

Another important prediction of finite-size scaling theory is the scaling relation for the length fluctuations (≙specific heat) in the vicinity of v_c

$$L^{-\alpha/\nu}[\langle L^2\rangle_c(t,L)/N-b_0^{\pm}]=f_c(x)\,, \qquad (17)$$

where $t\equiv|1-v/v_c|$ and $x\equiv tL^{1/\nu}$. The critical exponent α $(=2-D\nu)$ controls the singularity of the specific heat in the infinite system ($\langle L^2\rangle_c/N\propto C/N=(A^{\pm}/\alpha)t^{-\alpha}$), and $b_0^{\pm}$ account for regular background terms above (+) and below (−) v_c. Consistency requires that for large x (in the sense $t\ll1$ fixed, $L\to\infty$)

$$f_c(x)\xrightarrow{x\to\infty}(A^{\pm}/\alpha)x^{-\alpha}\,. \qquad (18)$$

Thus if one expects, on theoretical grounds, certain values of the critical exponents ν and α, then plotting the l.h.s. of (17) versus x, the data of lattices with different sizes should fall onto a single curve. Here we perform this analysis, expecting that the self-avoiding loop gas should fall into the same universality class as the Ising model, having the exponents (the number for ν is the average of field-theory estimates using resummed g- and ϵ-expansions, reported in ref. [17])

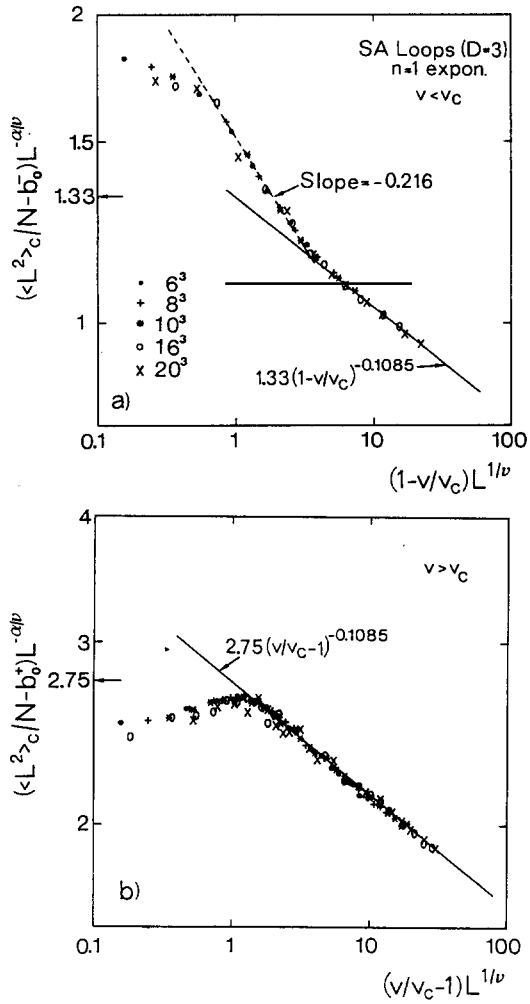

Fig. 4. Finite-size scaling plot (see eq. (17)) of the length fluctuations (≙specific heat) for $v<v_c=0.222$ (a) and $v>v_c$ (b) in log–log representation. The data are the same as those in fig. 3. For the critical exponents, we have chosen Ising values, $\nu=0.6305$, $\alpha=0.1085$, and the background parameters are $b_0^-=1.5$, $-b_0^+=-2.3$. The straight lines $\propto|1-v/v_c|^{-0.1085}$ confirm the expected $x\to\infty$ behavior (18).

[#4] We have confirmed this value by other means to be reported in a future publication [15].

$$\nu = 0.6305\,, \quad \alpha = 0.1085\,. \tag{19}$$

This is suggested by the fact that both types of loop gases follow the same field theoretic model [6], with the only difference being the numerical value of the parameter ξ. We judge the quality of the values (19) by monitoring the degree of clustering of our data. By "trial and error" we have found that with $b_0^- \approx -1.5$, $b_0^+ \approx -2.3$ the above expectations are indeed reasonably satisfied. This is demonstrated in the log–log plots in fig. 4. In this representation, the asymptotic laws (18) are given by the straight lines with slope $-\alpha$. Notice that, for $v < v_c^*$ (fig. 4a), one must be careful not to misinterpret an apparent asymptotic behavior for intermediate x, indicated by the dashed straight line with slope -0.216. As a further test of the scaling properties, from the ordinates of the asymptotic straight lines at $x = 1$, we can read off the ratio of the leading amplitudes below $(-)$ and above $(+)$ v_c

$$\frac{A^-}{A^+} \approx \frac{1.33}{2.75} = 0.48\,. \tag{20}$$

Also this ratio is consistent with estimates for the Ising universality class, which are, from series analyses, 0.51 [18] and, from ϵ-expansions, 0.54 (up to ϵ), 0.38 (up to ϵ^2), 0.44 ([1,1] Padé) [19].

5. Summary and discussion

We have rewritten the self-avoiding loop gas as a spin model with Ising variables on links and given the explicit form of the interaction in general dimensions. A parameter ξ allows interpolation to the well understood Ising loop gas. In three dimensions, Monte Carlo simulations show that below the phase transition both models are even quantitatively very similar. For self-avoiding loops, we find a critical temperature $v_c = \exp(-\epsilon/T_c) = 0.222 \pm 0.001$ which lies only 1.8% above that for Ising loops. For large volumes, these results are in agreement with a direct Monte Carlo simulation of loops [20], where the self-avoiding constraint was enforced by hand. (For finite volumes, there are differences due to boundary conditions different from our purely periodic ones.)

A finite-size scaling analysis of the length fluctuations ($\triangleq$ specifc heat) shows that the critical behavior of self-avoiding loops is *consistent* with the universality hypotheses based on Ising exponents. It must be pointed out, however, that using this technique with the presently available computer facilities and reasonable operating times, it is very hard to exclude possible other exponents of nearby universality classes such as the $n=0$ exponents ($\nu = 0.5880$, $\alpha = 0.2360$) [21] (see also ref. [17]) of a single self-avoiding loop [22]. This is not astonishing if one keeps in mind that similar finite-size scaling analyses [23] of Monte Carlo data of the Ising model, the best known model of statistical mechanics, provide at most a consistency check of critical exponents with numbers already known from large order series expansions. Only very elaborate Monte Carlo simulations on special purpose computers [16], or extremely time consuming Monte Carlo renormalization group studies [24] have provided independent results of comparable accuracy.

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