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LETTER TO THE EDITOR

Ising model on a self-avoiding walk

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Abstract. Fluctuation arguments combined with basic features of the geometry of self-avoiding walks (SAWs) are shown to lead to zero transition temperature T_c for the Ising model on a SAW. The Ising model on a non-random fractal representing the essential geometrical features of SAWs is treated exactly by a decimation method. It also leads to $T_c = 0$, and to Ising SAW critical behavior different from that on an Ising chain.

Recently the Ising model has been studied on a self-avoiding walk (SAW) in the context of the study of phase transitions on linear magnetic polymers (Chakrabarti and Bhattacharya 1983, 1985, Bhattacharya and Chakrabarti 1984a, b). In this model one considers Ising spins (with nearest-neighbour interactions) placed on a SAW embedded in a d -dimensional lattice. Unlike spins on a linear chain the spins on a SAW frequently have more than two nearest neighbours. In fact, on an infinite SAW the average number of nearest neighbours z_{eff} is given by $z_{\text{eff}} = 2 + (z - 1) - \mu$; z is the coordination number of the d -dimensional lattice and $\mu (< z - 1)$ is the connective constant for SAWs on the lattice (Bhattacharya and Chakrabarti 1984a). These extra neighbours are responsible for the system feeling the d -dimensional nature of the underlying lattice, producing a multiply connected structure with a distribution $P(L)$ for the number of loops of length L . From the mapping of the SAW onto the n -vector model as $n \rightarrow 0$ this distribution has the asymptotic form, for large L ,

$$P(L) \sim L^{-(1-\alpha)} \quad (1)$$

where α is the specific heat exponent as $n \rightarrow 0$ (de Gennes 1979).

In this letter we are principally concerned with the existence, or otherwise, of a finite-temperature phase transition. Application of various kinds of mean-field type arguments would indicate a finite transition temperature for such a system (Bhattacharya and Chakrabarti 1984a). A complementary viewpoint is that the quasi-linear nature of a finite fraction of any SAW allows fluctuations to destroy the long range order at any finite temperature. This is the position taken in this letter which will be expanded upon below.

These fluctuation arguments are difficult to formalise if exact quantitative results for the critical behaviour are required. Approximate small cell real space renormalisation group (RSRG) calculations have already been used to study the system (Chakrabarti and Bhattacharya 1985). In the last part of this letter we introduce another approach

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based on an idealised fractal system, designed to model the important features of an Ising model on a SAW, which is exactly solvable by decimation.

We now consider the stability of the ordered state of an Ising system on a SAW. The argument used is closely related to that used when discussing the Ising model on a one- or higher-dimensional lattice. However there turns out to be a crucial difference between the geometry of domain walls in an Ising system on a SAW and an Ising system on a pure Euclidean lattice in two or more dimensions, which shows that comparison of the fractal dimensionality with the usual lower critical dimensionality (of pure lattices) is not enough to determine the stability of the ordered phase in general (see also Boccara and Havlin 1984).

Let us consider two spins at sites A and B separated by a large distance. Examination of a typical randomly generated configuration indicates that the correlations between A and B are transmitted by m essentially independent paths. This independence derives from the long tail in the distribution of loop lengths given by (1). One expects m to diverge as the separation between A and B become large. One way to break the correlations between A and B is to introduce a single domain wall at an arbitrary point on each of the m independent paths between A and B. This can happen because, although the internal energy of the system will increase by mJ (J is the exchange interaction) when the domain is formed the entropy will dominate the free energy for sufficiently large separations.

Let us consider the ordered state as defining the zero of free energy for the system. Then, as stated above, to break the m bonds between A and B requires internal energy mJ . The number of ways that this break can occur can be estimated as R^m where R is the length of a typical path linking the two points. Thus an upper bound on the free energy of the system is given by

$$F = mJ - Tm \ln R. \quad (2)$$

Since R can become very large this shows that if the SAW is well described by the above picture, as we believe, then the ordered state is unstable and $T_c = 0$.

The difference between the argument given above and that for a pure lattice in more than one dimension comes in the estimate for the entropy. Since the m routes are largely independent in the SAW, the domain wall between A and B can become very rough without increasing the internal energy. Thus there are a large number of independent configurations which can destroy the order. On a pure Euclidean lattice one can ask a similar question as to the number of energetically equivalent configurations which can separate two regions of the lattice. Compared with the SAW, this number grows much less quickly with the size of the regions considered because any roughening of the domain wall involves an increase in energy. Thus long range order remains for small but finite temperatures in pure Euclidean lattices with $d > 1$. As an example consider the stability of droplets on a pure two-dimensional lattice. If the perimeter of the droplet is m then the number of distinct droplet configurations for large m , or equivalently the number of SAW loops, is of order $\mu^m m^{-(1-\alpha)}$ where μ and α are as above (de Gennes 1979). This leads to a change in free energy for formation of a droplet

$$\delta F = mJ - mT \ln \mu + O(\ln m). \quad (3)$$

This is positive for T small. Thus the ordered state is stable against droplet formation for this standard pure lattice example.

The characteristic of the SAW geometry essential for the consideration of the low temperature Ising static behaviour appears to be the existence of long chain paths folding back on themselves with a frequency related to the loop distribution (1). A non-random fractal model incorporating this feature and having a similar form for the loop length distribution is now introduced, and the Ising model critical behaviour is solved exactly for it. Again it will be found that the transition is at zero temperature.

The fractal is a limit of a hierarchy in which the n th member, shown in figure 1(b), corresponds to a single bond in the $(n + 1)$ th member (figure 1(a)).

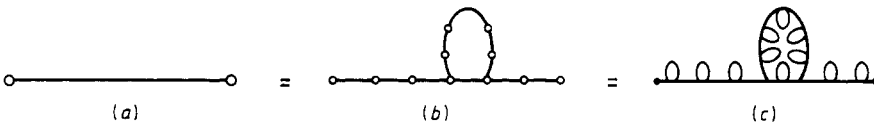


Figure 1. Successive generations in the construction of a fractal model.

To show that this construction gives rise to a loop probability distribution of type (1), consider a further member (figure 1(c)) of the hierarchy. By considering the relationship of figures 1(b) and (c) it is seen that in one step of the construction, the number of loops, and the loop length, change by $r + s$ and r respectively, where r, s are respectively the number of bonds in the chain sections and the loop in figure 1(b). A simple scaling argument then shows that the loop distribution for the fractal is (1) with

$$1 - \alpha = \ln(r + s) / \ln r. \tag{4}$$

The exact discussion of the Ising critical behaviour on the fractal uses the parameters t, t' for two successive stages in the fractal construction, where t is the usual Ising thermal variable $t \equiv \tanh K, K \equiv J/k_B T$. The relation between t and t' is found by tracing out the intermediate spins in figure 1(b). This results in

$$t' = t^r \left(\frac{t + t^s}{1 + t^{s+1}} \right) \equiv R(t). \tag{5}$$

This is the renormalisation transformation corresponding to the fractal construction, which is analogous to length scaling by a dilation factor $b = r + 1$. It can easily be shown that for $r \geq 1$ the only unstable fixed point of (5) is $t^* = 1$. Thus

$$T_c = 0. \tag{6}$$

So no fractals of this type have a finite temperature phase transition. To the extent to which these fractals have the crucial geometric characteristics of the SAW, the Ising system on the SAW would have $T_c = 0$.

$T_c = 0$ is a true critical point (the fixed point $t^* = 1$ is unstable, so the correlation length ξ diverges there, for $r \geq 1$ (see below)). Now consider whether the critical behaviour there is different from that of an Ising chain. The (thermal) eigenvalue λ of (5) at the fixed point $t^* = 1$ is $\lambda = r$, that is, the number of 'cutting bonds' in figure 1(b) (cf Stinchcombe 1983). Inserting this and the dilation factor b into the usual length scaling relationships gives the critical behaviour of the correlation length ξ as

$$\xi \propto (e^{2K})^\nu \quad \nu = \ln(r + 1) / \ln r. \tag{7}$$

(For a non-pathological result we need $r > 1$; cf Gefen *et al* (1983).) For the fractal the critical behaviour is thus in general different from the Ising chain where $\nu = 1$, and this difference must also be expected for the Ising system on the SAW, if the fractal model represents it adequately.

The Heisenberg system on the fractal representation of the SAW can be discussed in a similar manner. For the classical version of the model the low temperature thermal scaling can be found without difficulty using techniques developed elsewhere (Stinchcombe 1979), and leads, as expected, to a zero transition temperature (for $r \geq 1$). However now the low temperature critical behaviour is

$$\xi \propto T^{-\nu}, \quad \nu = \ln(r+1)/\ln(r+s/(s+1)). \quad (8)$$

In conclusion we have examined the problem of the Ising model on a SAW from a viewpoint which emphasises the importance of fluctuations occurring in the essentially linear parts of a SAW. The two calculations of this letter both indicate that fluctuations are strong enough to destroy any long range order at any finite T . Similarly the dynamics of spins on a SAW could also be studied (see e.g. Bhattacharya and Chakrabarti 1984b). Finally, we point out that in the case of Ising spins placed on the distinct sites visited by a random (non-interacting) walk one might expect a finite transition temperature on a two-dimensional lattice where the walk is sure to visit the origin many times. In high enough dimensions, where self intersections become rare, the transition would again occur at zero temperature.

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