The Statistics of Self-Avoiding Walks on a Disordered Lattice

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The relevance of lattice disorder on the "critical behaviour" of self-avoiding walks is discussed. A crossover from nonclassical to classical behaviour seems to take place.

The self-avoiding walk (SAW) picture has been fruitfully utilized to describe the excluded volume effect in linear polymers [1]. The mean square average of the end-to-end distance for SAWs has the following form [1]:

\[ R^2 \sim N^{2v} \]  

(1)

where \( N \) is the number of steps in the SAW and \( v \) is a universal exponent depending only on the lattice dimensionality \( d \). The exponent \( v \) for homogeneous lattices in different dimensions has been calculated in several ways: using Monte Carlo simulations [2], series expansions [2], direct renormalization of SAWs [3] and field theoretic renormalization group methods [4]. The field theoretic method, based on the connection established by de Gennes [4] between SAW statistics and the \( n \)-vector model in the \( n \rightarrow 0 \) limit, has lead to considerable understanding about the universal properties of the SAWs. In this formalism the length of a chain \( (N) \) is conjugate to \( \Delta T \), the critical temperature interval of the magnetic system, and the exponent of the correlation length is then identified with the exponent \( v \) in (1). Using the field theoretical results one estimates [5]:

\[ v = 0.588 \]  

(2)

for SAWs in three dimensions, in excellent agreement with numerous experiments [1, 2].

In a magnetic system the presence of impurities can have nontrivial effect on the critical behaviour if the specific heat exponent \( \alpha \) is positive [6, 7]. Using the scaling relation [1]:

\[ dv = 2 - \alpha \]  

(3)

with (2) one gets \( \alpha = 0.236 \) for the \( n \)-vector model in the \( n \rightarrow 0 \) limit in \( d = 3 \). The positivity of \( \alpha \) and its unusually large value therefore indicates, that in this limit the \( n \)-vector model is sensitive and infact the pure-system fixed point is unstable with respect to quenched [6] or annealed [7] impurities. In such cases the system should show the random \( n \rightarrow 0 \) critical behaviour [8] or the Fisher-renormalized critical behaviour [7], respectively. In the presence of both quenched and annealed disorder the fixed point corresponding to the quenched disorder seems to govern the ultimate critical behaviour [9]. We are thus interested in the quenched disordered \( n \)-vector model in the \( n \rightarrow 0 \) limit.

Let us consider the \( n \)-vector model (with zero external magnetic field) on a randomly diluted lattice, represented by the Hamiltonian:

\[ H = \sum_{\langle i,j \rangle} K_{ij} \xi_{ij} \mathbf{s}_i \cdot \mathbf{s}_j \]  

(4)

where the exchange constant \( K_{ij} \) depends only on the interlattice separation between sites \( i \) and \( j \), the summation runs over nearest neighbours and \( \xi_{ij} = 1 \) if the bond is active between the sites \( i \) and \( j \) and 0 otherwise (\( \xi_{ij} = \xi_i \xi_j \), \( \xi_i = 1 \) or 0 corresponds to site disorder). The length of each spin is normalized to \( \sqrt{n} \):

\[ s_i^2 = \sum_{a=1}^{n} s_i^a s_i^a = n. \]  

(5)

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In the limit \( n \to 0 \) the partition function \( Z \) for the model in a particular distribution of dilution can be expressed as [4]:

\[
Z = \prod_{i<j} \left( 1 + \xi_{ij}(K_{ij}/T) s_i s_j + (1/2) \xi_{ij}^2(K_{ij}/T)^2 (s_i s_j)^2 \right)
\]

(6)

where \( T \) denotes the temperature and \( \langle \rangle \) means the angular averaging satisfying (5). The successive terms of \( Z \) may again be represented by graphs on the lattice, where to each nearest neighbour link \( K_{ij} \) a continuous line can be associated if the bond is active \((\xi_{ij}=1)\). In the \( n \to 0 \) limit the average spin-spin correlation function can be written as

\[
\langle s_i^z s_j^z \rangle = \sum_N (K/T)^N G(N, R_{12})
\]

(7)

where \( K=K_{ij} \), the overhead bar denotes the configurational averaging over \( \xi_{ij} \) distributions and \( G(N, R_{12}) \) is the number of configurations of SAWs with \( N \) steps and its ends fixed at sites 1 and 2 on the diluted lattice (Fig. 1). Above the percolation threshold there is an infinite cluster of occupied bonds (or sites) on which the SAWs can take place. In the large \( N \) limit the divergence of the average \( G(N, R_{12}) \) should therefore be determined by the susceptibility exponent of the diluted \( n \)-vector model in the \( n \to 0 \) limit and the exponent \( \nu \) of the correlation function of this model gives the exponent of the end-to-end distance of SAWs (1) on a diluted lattice.

For the magnetic \( n \)-vector model the effect of quenched (bond or site) impurities has been successfully investigated in the \( \varepsilon \) \((=4-d)\) expansion scheme, using the replica trick for configurational averaging [8]. The crossover exponent for the pure system fixed point is \( \alpha/\nu \) and for \( \alpha>0 \) this fixed point becomes unstable, in agreement with [6]. One finds then a stable “random” fixed point for which the exponents for general \( n \) \((\pm 1)\) are [8]:

\[
v = 1/2 + \frac{3n}{32(n-1)} \varepsilon + \frac{n(127n^2 - 572n - 32)}{4096(n-1)^2} \varepsilon^2 + \ldots \quad (8)
\]

\[
\eta = 2 - \nu/\nu = \frac{n(5n-8)}{256(n-1)^2} \varepsilon^2 + \ldots \quad (9)
\]

to \( \varepsilon^2 \) order. In the limit \( n \to 0 \) the dimensional dependence therefore vanishes and one gets the classical exponents \( v=1/2 \) and \( \eta=0 \) up to this order in \( \varepsilon \). If we suppose that the \( n \) dependence of the correction terms of the exponents is at least linear in all orders of \( \varepsilon \), as it is up to the order of \( \varepsilon^2 \) in (8) and (9), then we get for \( n \to 0 \), i.e. for the SAW statistics, a crossover from nonclassical to classical critical behaviour on diluting the lattice. Phenomenologically such a crossover is perhaps not unexpected, because the dilution itself favors selfavoidance and therefore the constraint on a walk to avoid itself becomes irrelevant. It may be noted, that a similar situation occurs also for the uniaxial ferromagnets with dipolar interaction which drives the critical behaviour of the system from the nonclassical (Ising) to the classical one (apart from logarithmic corrections in three dimensions) [10].

Equations (8) and (9) show that at least for \( d \leq 4 \) the SAW statistics on a random lattice will have a classical critical behaviour. However, using Flory’s approximate value for the exponent \( \nu \) in general dimensions [1]:

\[
v = 3/(2+d)
\]

(10)

and using the hyperscaling relation (3) one finds that the specific heat exponent for the corresponding magnetic model is always positive for \( d<4 \):

\[
\alpha = (4-d)/(2+d)
\]

(11)

and its magnitude increases rapidly for lower dimensions. The \( \varepsilon \)-expansion does not contradict this conclusion. This indicates, that the “pure” SAW critical behaviour in lower dimensional diluted lattices is even more unstable.

In the discussions above on SAWs on diluted lattices, the bond (site) occupation probability has been assumed to be far above the percolation threshold. However, just at the percolation threshold the incipient infinite cluster is the object on which the infinite SAWs can be built up. Very recently Coniglio solved the problem of thermal fluctuations on the incipient infinite cluster for both \( q \)-state Potts model and \( n \)-vector model for \( n \to 1 \) [11]. The critical behaviour we discussed above remains valid until the percolation point.