LETTER TO THE EDITOR

Absorption of a self-avoiding random walker by a random trap distribution

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Abstract. A particle performing a self-avoiding random walk is considered on a lattice in any number of dimensions d, which contains a fraction q of randomly distributed impurity sites. An impurity is assumed to trap the walker when stepped on. We find the average time to trapping to be $\gamma(1-q)/[q-(1-K_c)]$, where K_c and γ are the inverse critical temperature and the critical index of the susceptibility for the classical Heisenberg model of magnetism with vanishing $(n \to 0)$ internal degrees of freedom.

The average trapping time and probability distribution of trapping time have been studied by Hemenger *et al* (1972), Rosenstock (1980) and Rosenstock and Straley (1981) for a random walk on a d-dimensional lattice containing a random distribution of traps. A random walker was assumed to step on one of the nearest neighbours with equal probability after a specified time interval. Though the problem originated in the mathematical theory of probability, such as the classical gambler's ruin problem (Feller 1957), it is expected to have applications to many physical systems. A particularly important one is an organic crystal in which the quenching of migratory excited states of molecular aggregates takes place (Rosenstock 1969, Birks 1970, Hemenger *et al* 1972).

We study in this paper the case where a particle performs a random walk of the same kind as mentioned above but with an additional constraint that it can never visit the lattice sites which have already been stepped on. The walk is called a self-avoiding random walk (SAW). According to a general formula found by Rosenstock (1980), the average time to trapping is given by $1/q$ where q is the fraction of randomly distributed trapping sites, since $V(m)$, the number of distinct sites that would be visited in m steps if there were no traps, is nothing but m for such a SAW. The result is obviously erroneous since it contains no information on the type of the lattice or even the space dimensions. We derive a better estimate by applying the theorem found by de Gennes (1972) which established an isomorphic relationship between a SAW on a lattice and the spin correlation function for the ferromagnetic model with vanishing internal degrees of freedom.

Let us associate the ith lattice site with a variable ν_i which takes the value 1 if the site i is normal and 0 if it is an impurity site. The number of SAW paths which start at a normal site i and are trapped by the impurity site j after exactly m steps is given by

$$Z_m(i, j; \{\nu\}) = \sum_{i_1, i_2, \ldots, i_{m-1}} \nu_i \nu_{i_1} \nu_{i_2} \ldots \nu_{i_{m-1}} (1 - \nu_j) \tag{1}$$

for a fixed impurity distribution $\{\nu\}$, where the summation is taken over all possible paths of intermediate $m - 1$ lattice sites which forms a chain of SAW. The total number of SAW paths which start at the ith site and are quenched at any one of the trapping centres after m steps is then given by

$$Q_m(i;\{\nu\}) = \sum_j Z_m(i,j;\{\nu\}). \tag{2}$$

The average trap time can be expressed as

$$\langle m \rangle = \left[\sum_m m Q_m(i;\{\nu\}) \bigg/ \sum_m Q_m(i;\{\nu\}) \right]_{\text{av}} \tag{3}$$

where $[\ldots]_{\text{av}}$ denotes the average over possible distribution of impurities. The result is independent of the starting site i.

Our analysis will be based on the following fundamental theorem on the generating function of Z_m;

$$\sum_m K^m Z_m(i,j;\{\nu\}) = \nu_i(1-\nu_j)G(i,j;\{\nu\}). \tag{4}$$

In this theorem $G(i,j;\{\nu\})$ is a spin correlation function

$$G(i,j;\{\nu\}) \equiv \lim_{n \to 0} n^{-1}\langle S_i \cdot S_j \rangle \tag{5}$$

for the dilute ferromagnetic Heisenberg Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \nu_i\nu_j S_i \cdot S_j \tag{6}$$

where S_i is a classical n-component spin vector with constraints $S_i^2 = n$. The parameter K is related to the exchange integral through $K = \beta J$ (β being the inverse temperature of the magnetic system). The theorem (4) can be easily derived by high-temperature series expansion in a quite similar way to the one for the pure case (de Gennes 1972, Emery 1975, Daoud *et al* 1975). The problem is therefore reduced to finding the spin correlation function (or the susceptibility) of a dilute ferromagnetism with vanishing internal degrees of freedom.

Unfortunately no exact results have been obtained for such a disordered system. We therefore introduce a simple approximation by which we take the impurity average of the numerator and the denominator separately in (3). We have

$$\langle m \rangle \approx \sum_m m [Q_m(i;\{\nu\})]_{\text{av}} \bigg/ \sum_m [Q_m(i;\{\nu\})]_{\text{av}}. \tag{7}$$

Within this approximation our result is exact. Since the impurities are assumed to be randomly and independently distributed, we find

$$[Q_m(i;\{\nu\})]_{\text{av}} = \sum_j [Z_m(i,j;\{\nu\})]_{\text{av}} = p^m q \sum_j Z_m^{(0)}(i,j)$$

$$\equiv p^m q Q_m^{(0)} \tag{8}$$

where $p \equiv 1 - q$ and $Z_m^{(0)}(i,j)$ is the number of m-step SAW paths from i to j on a *pure* lattice. The generating function for $Z_m^{(0)}$ is the spin correlation function for the pure Hamiltonian;

$$\sum_m K^m Z_m^{(0)}(i,j) = \lim_{n \to 0} n^{-1}\langle S_i \cdot S_j \rangle_0. \tag{9}$$

Hence we have

$$\sum_m K^m Q_m^{(0)} = \chi^{(0)}(K) \tag{10}$$

where $\chi^{(0)}(K)$ is the susceptibility of the 0-component pure magnetic system. Substituting (8) into (7) we find

$$\langle m \rangle \approx \sum_m mp^m Q_m^{(0)} \Big/ \sum_m p^m Q_m^{(0)} = p\left(\frac{\partial}{\partial K} \log \chi^{(0)}(K)\right)_{K=p}. \tag{11}$$

For K smaller than K_c, the inverse critical temperature of the second-order phase transition point of the $n \to 0$ Heisenberg model, it is well known that the high-temperature series expansion (10) converges to give a dominant singularity

$$\chi^{(0)}(K) = \chi_0 (K_c - K)^{-\gamma} \tag{12}$$

of the magnetic susceptibility characterised by a critical index γ, where χ_0 is a finite amplitude. This singular form leads to the final result

$$\langle m \rangle = \gamma p/(-p + K_c) = \gamma(1-q)/[q-(1-K_c)]. \tag{13}$$

For the impurity concentration q larger than the critical value q_c defined by

$$q_c \equiv 1 - K_c, \tag{14}$$

the average trapping time is finite and is given by (13). For q less than q_c, however, this time becomes infinite since the high-temperature series (10) diverges. SAW paths are infinitely extended on average for such a dilute limit of impurity concentration.

The coefficients $Q_m^{(0)}$ have been extensively enumerated for SAW's on finite lattices. They are well known to be precisely fitted by the asymptotic form

$$Q_m^{(0)} \sim K_c^{-m} m^{\gamma-1} \qquad \text{for large } m. \tag{15}$$

By expanding (12) in powers of K, one can easily be convinced that K_c and γ of this asymptotic form are identical to those parameters which appeared in (12). Watts (1975) carefully estimated them by applying the method of Padé approximants. His results are summarised in table 1. On the other hand, study of the critical phenomena of the $n \to 0$ spin model gives another estimate of them. Unfortunately the precise value of the critical temperature has not been available so far but the renormalisation group theory (Le Guillou and Zinn-Justin 1980) predicts the three-dimensional γ as

$$\gamma = 1.1615 \pm 0.0020. \tag{16}$$

γ is believed to be independent of the lattice structure.

Table 1. The critical temperature and the susceptibility index for various lattices in two and three dimensions. H (honeycomb), T (triangular), SQ (square), D (diamond), SC (simple cubic), BCC (body centred cubic), FCC (face centred cubic) and MF (molecular-field theory) (z being the number of the nearest neighbours).

Lattice	H	T	SQ	D	SC	BCC	FCC	MF
K_c	0.541	0.379	0.241	0.347	0.214	0.153	0.100	$1/z$
γ	1.342	1.335	1.330	1.157	1.162	1.165	1.166	1

Contrary to the conclusion obtained by Rosenstock (1980) for free random walks our result gives a finite critical fraction of the trapping centres at which the trapping time diverges.

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