Ordering Field, Order Parameter, and Self-Avoiding Walks

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(Received 13 August 1984)

We consider a grand canonical ensemble of self-avoiding walks and study its properties on a Bethe lattice of coordination number $q=3$ and in one dimension, without using the $n\to 0$ trick. The study enables us to identify the ordering field as the activity for the walk ends. We also identify the order parameter of the problem for the first time: The order parameter *is* the probability of obtaining an infinite self-avoiding walk (reaching the "boundary"), having started at the origin in some direction.

PACS numbers: 02.50.+s, 05.50.+q

Our understanding of polymers has greatly advanced over the past ten years or so, mainly because of a remarkable observation by de Gennes,[1] who argued that polymers can be described very simply by a formal $n\to 0$ limit of an n-component field theory. The analogy was further extended by des Cloizeaux[2] to describe polymers in a solution. This analogy is found to be much more transparent if we restrict ourselves to a lattice and consider a self-avoiding walk (SAW) as an idealized representation of a polymer chain. It is found[3,4] that the activity κ for a bond and the activity η for an end point of a SAW are related to the ferromagnetic coupling K and the magnetic field H of an n-vector model as $n\to 0$. However, the analogy is not complete for the following two very important reasons: (i) The physical significance of the spontaneous magnetization m is completely lost when $n\to 0$.[4] Even the nature of the ordered state is not very clear in this limit. However, since the corresponding polymer problem is a physical one, we must be able to describe the "ordered" state by a suitable and physically significant "order" parameter. (ii) The proof of the correspondence between polymers and the $n\to 0$ limit of the magnetic system[5] assumes explicitly the full $O(n)$ symmetry. Therefore, the correspondence works only at high temperatures, i.e., above and, at most, up to the critical temperature T_c. There is no reason to believe that the analogy also works below T_c where the symmetry of the theory is explicitly broken, as has been recently argued.[5]

Because of the above two gaps in our understanding, it is imperative that we study the polymer, i.e., the SAW problem directly, without ever invoking the formal $n\to 0$ limit. In the present work, we make such an attempt and study the SAW problem on a Bethe lattice of coordination number $q=3$ and in one dimension, and successfully bridge the first gap mentioned above. The "ordering" field is identified as η. The critical behavior, which occurs at $\kappa=\kappa_c$ when $\eta=0$, is completely destroyed as soon as $\eta\neq 0$, a result we would have certainly expected from the analogy with the n-vector model when $n\to 0$. The four new and important results reported in this Letter are the following: (a) We identify the "order" parameter $P(\kappa)$ for the first time: $P(\kappa)$ is the probability that a SAW originating at the origin extends to the "boundary" of the lattice in some direction. (b) The bond density ϕ_l is zero below and nonzero above κ_c. (c) The polymer density ϕ_p is zero everywhere. (d) The ground state is basically a SAW on the lattice, which below κ_c never feels the presence of the boundary, but above κ_c, covers a *finite* fraction of the lattice sites, and describes the physics of the ordered state. All these results are valid only when $\eta=0$.

The natural object to study is the following grand canonical ensemble[6]:

$$\hat{Z}=\sum_{p\geq 0}\sum_{l\geq p}\eta^{2p}\kappa^{l}U_{p,l}, \tag{1}$$

where $U_{p,l}$ is the number of ways of putting p different SAW's of total length l on the lattice. For the sake of clarity, we only consider Bethe lattices of coordination number $q=2$ (one dimension) and $q=3$, although the method is easily generalizable to any other q. Because of the peculiar topology of the Bethe lattice ($q\geq 3$), the behavior in the "interior" of the lattice is very different from that of the whole lattice.[7-10] Hence, in order to ignore the effects of this peculiar topology (in which a finite fraction of sites belongs to the surface in the thermodynamic limit), attention is focused on the interior of the lattice. This will be achieved by the demand that all (interior) sites be equivalent [see comments following Eq. (4) below]. Thus, we expect the results to closely reflect the physics of the polymer problem on regular lattices. The correctness of the approach is then confirmed by a study of the one-dimensional case, where the physics of the problem is basically trivial.

To begin with, let us consider the case $q=3$. We

denote the Bethe lattice by L_B and denote its dual (triangular cactus) by L_D. Let N be the total number of sites on L_B. The number of sites N_D on L_D is $3N/2$ ($q=3$). The number of triangular figures on L_D is, however, $N_T=N$. We now put an Ising spin S on each site of L_D. If the spin is up, denoted by 0 (down, denoted by 1), this corresponds to an occupied (unoccupied) bond on L_B. If the interaction energy is properly chosen (see below), so that *no* triangular figure has *all* three spins up, which corresponds to three bonds coming out of a site on L_B, we find that we have only SAW's on L_B. Let N_S, $N_{S_1S_2}$, and $N_{S_1S_2S_3}$ denote the number of spins in state S, the number of bonds with spins S_1 and S_2, and the number of triangles with spins S_1, S_2, and S_3, respectively; then it is easily seen that

$$N_0=l,\quad N_1=3N/2-l,\quad N_{01}=2(l+p),\quad N_{00}=l-p,\quad N_{11}=3N-3l-p,$$
$$N_{000}=0,\quad N_{001}=l-p,\quad N_{011}=2p,\quad N_{111}=N-(l+p).$$

Here p denotes the number of SAW's and l the total number of bonds in the configuration. The interaction on L_D is taken to be of the following form:

$$\mathcal{H}=\sum_{(T)}\mathcal{H}_T,\quad \mathcal{H}_T=K_0+K_2(S_1S_2+S_2S_3+S_3S_1)+K_3S_1S_2S_3+\tfrac{1}{2}H(S_1+S_2+S_3). \tag{2}$$

Here, T denotes a triangular figure on L_D and the sum is over all T.

For convenience, the parameters K_0, K_2, K_3, and H are chosen in the following manner: $K_0=k_0-1/a$, $K_2=k_2-1/a$, $K_3=k_3-1/a$, and $H=h-2/a$. With use of the values of the various N's given above, it is easily seen that

$$\mathcal{H}=N(k_0+3k_2-k_3-3h/2)+2l(h-2k_2)+4p(k_3-k_2),$$

which is independent of a. If we define $\eta^2=\exp[4(k_3-k_2)]$ and $\kappa=\exp[2(h-2k_2)]$, we find that the partition function Z corresponding to (2) is related to (1) as follows: $Z=e^{NC}\hat{Z}$, where $C=k_0+3k_2-k_3-3h/2$. The four possible states of a T are shown in Fig. 1. The corresponding weights are

$$\omega_0=D,\quad \omega_1=E(\kappa^{1/2}/\eta)^{1/2},$$
$$\omega_2=E(\eta/\kappa^{1/2})^{1/2},\quad \omega_3=\omega_1/\kappa, \tag{3}$$

where $D=\exp(8/a+k_0+3k_2+k_3+3h/2)$ and $E=\exp(k_0-k_2)$. It is evident from Fig. 1(a) that by taking $a\to 0^+$, $\omega_0\to 0$ and hence $N_{000}\to 0$. In this limit, ω_1, ω_2, and ω_3 remain unchanged, as they do not depend upon a. Thus, we can study $\hat{Z}$ by studying Z, and this requires no formal limit of the kind $n\to 0$.

The study of Z on the Bethe lattice is easily carried out in a recursive manner[7-10] by satisfaction of certain consistency conditions. Let us consider the mth level of the Bethe lattice and evaluate $Z_m(S)$, the partial partition function of a spin in state S at the mth level, obtained by summation of the effects of all the "outer" spins.[7-10] We expect that

$$Z_m(S)=A_m\exp(H_m'S). \tag{4}$$

The partition function Z is easily seen to be given by $Z=Z_0^2(0)+Z_0^2(1)$. The consistency condition for all sites to be equivalent, so that we explore only the interior of the lattice, requires that all H_m' be identical. Let H' be this value. The recursion relations between $Z_m(S)$ and $Z_{m-1}(S)$ are easily seen to be given by

$$Z_{m-1}(0)=A_m^2(2\omega_1+\omega_2/x)=A_{m-1}\sqrt{x},$$
$$Z_{m-1}(1)=A_m^2(\omega_1x+2\omega_2+\omega_3/x)=A_{m-1}/\sqrt{x}, \tag{5}$$

where $x=\exp(2H')$. From (4), we find that x must satisfy

$$x=(2\omega_1x+\omega_2)/(\omega_1x^2+2\omega_2x+\omega_3). \tag{6}$$

For $\omega_2>0$, there is only *one* solution of (6). However, for $\omega_2=0$, i.e., $\eta=0$, something interesting happens. For $\omega_3>2\omega_1$, $x=0$ is the only solution. For $\omega_3<2\omega_1$, a new solution, along with $x=0$, appears, which indicates a phase transition at $\omega_3=2\omega_1$, i.e., at $\kappa=\kappa_c=\frac{1}{2}$, when the ordering field η vanishes. For $\eta=0$, the solution of (6) is given by

$$x=0\quad \text{for}\quad \kappa<\kappa_c,$$
$$x=(1/\kappa_c-1/\kappa)^{1/2}\quad \text{for}\quad \kappa>\kappa_c. \tag{7}$$

It appears from (7) that x can be taken as a suitable order parameter for our polymer problem.

It will be seen below [see (9)] that the following

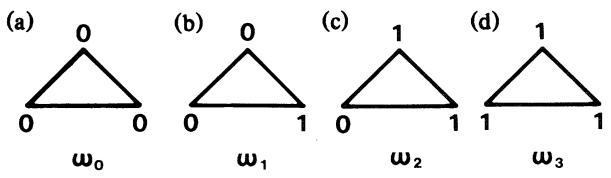

FIG. 1. Four possible states of T and their corresponding weights.

quantity

$$P(\kappa)=3x/2\kappa(x^2+1) \tag{8}$$

is a better choice for the order parameter and has strong physical appeal. From (7), we observe that $P(\kappa)$ vanishes as $\kappa\rightarrow\kappa_c^+$ according to $P(\kappa)\sim(\kappa-\kappa_c)^\beta$, $\beta=\frac{1}{2}$. To understand the physical significance of the order parameter $P(\kappa)$, let us go back to (5) and make the following observation: When $\eta=0$, i.e., when $\omega_2=0$, we find that only Fig. 1(b) contributes in the recursion relation for $Z_m(0)$. This figure continues the SAW coming in from the mth level to the $(m-1)$th level. Let us now compute the probability that this SAW terminates at the origin. For this, we need not only $Z_m(0)$, but also $\tilde{Z}_m(0)$, which has the same meaning as $Z_m(0)$ but with the condition that the SAW from the $(m+1)$th level does not continue to the mth level. Evidently, $\tilde{Z}_{m-1}(0)=\omega_2 A_m^2/x$. Thus, the required probability that there is an end point of a SAW at the origin is given by the following expression:

$$P(\kappa)=[3Z_0(0)\tilde{Z}_0(0)/\eta Z]_{\eta=0}=3x/2\kappa(x^2+1). \tag{9}$$

The factor of 3 is due to the fact that $q=3$ and there are three different directions for the SAW to come in. Also, we must divide by η, the activity for the end point to account for the fact that an end point is already present there at the origin. Thus, $P(\kappa)$ is the probability of having a SAW starting (ending) at the origin and going out to (coming in from) infinity in any one direction, and is shown in Fig. 2.

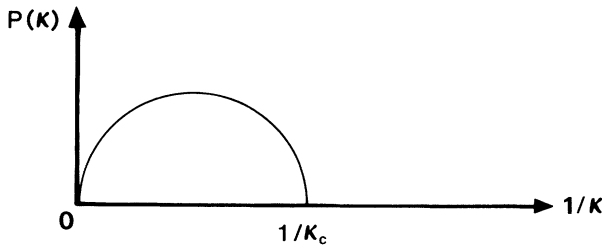

FIG. 2. The schematic form of the order parameter $P(\kappa)$ as a function of $1/\kappa$ for $q=3$.

It will be shown below that if $\hat{f}$ is the free energy per site in the thermodynamic limit, then $P(\kappa)=\partial\hat{f}/\partial\eta$ at $\eta=0$. Thus, the order parameter we have introduced has a very strong physical meaning.[11] It should be remarked at this point that $\beta=\frac{1}{2}$ also for the magnetic system when $n=0$.[12] Since near κ_c, $P(\kappa)$ behaves basically as x, one may just evaluate $\partial x/\partial\eta$ at $\eta=0$ to determine the exponent γ. It is found that $\gamma=1$. At κ_c, one observes that $x\sim\eta^{1/3}$, giving $\delta=3$. It is evident that all of these exponents have their classical values as expected.

Let us now calculate the density ϕ_p of SAW's and the density ϕ_l of SAW bonds.[13] To determine ϕ_p, we observe that $\phi_p=\phi_e/2$, where ϕ_e is the density of end points of SAW's. It is evident that only Fig. 1(c) gives rise to an end point. Therefore, it is not hard to see that

$$\phi_e=2\phi_p=[Z_0(0)Z_1^2(1)\omega_2+2Z_0(1)Z_1^2(0)\omega_2]/Z=3\omega_2x^2/(x^2+1)(2\omega_1x+\omega_2). \tag{10}$$

As $\eta\rightarrow 0$, $\phi_p\rightarrow 0$. However, when $\eta\rightarrow\infty$, we expect the lattice to be covered by dimers. This is certainly the case here: From (6), we find that $x=\frac{1}{2}$ in this limit, and therefore $\phi_p=\frac{1}{2}$, regardless of the value of κ. The whole lattice is covered by dimers. Moreover, comparing (9) and (10), we also observe that $P(\kappa)=\partial\hat{f}/\partial\eta$, $\eta=0$, as was claimed above.

The calculation of ϕ_l is also not very difficult. We merely observe that Fig. 1(b) yields two bonds while Fig. 1(c), which yields an end point, contributes only one bond. It is not hard to see that

$$\phi_l=(2Z)^{-1}\{2\omega_1[2Z_0(0)Z_1(0)Z_1(1)+Z_0(1)Z_1^2(0)]+\omega_2[2Z_0(1)Z_1(0)Z_1(1)+Z_0(0)Z_1^2(1)]\}.$$

The extra factor of $\frac{1}{2}$ in the front is to account for double counting of bonds. We finally find that $\phi_l=3x^2/2(x^2+1)$, and does not explicitly depend upon η.

For $\eta\rightarrow 0$ and $\kappa\rightarrow\infty$, we find that $\phi_l=1$: *All* sites of the lattice are covered. As a matter of fact, for all $\kappa>\kappa_c$, $\phi_l>0$, which implies that a finite fraction of the lattice sites are covered. As claimed at the beginning, we expect the above result also to be valid for regular lattices. Thus, we expect $\phi_l\neq 0$ above some $\kappa=\kappa_c$ for regular lattices, for example, a square lattice. (Obviously, we do not expect the exponents to be the same.) Since $\eta=0$, we expect basically a single SAW to cover a finite fraction of the lattice. (In order to understand the physics, we must first consider a finite lattice, and then consider the thermodynamic limit.) Therefore, the SAW must feel the presence of the "boundary" of the lattice. Below κ_c, $\phi_l=0$ and, therefore, there is no reason for the SAW to even know the presence of the boundary of the lattice.

Now, we are in a better position to fully appreciate the physical significance of $P(\kappa)$. As is evident

from Fig. 2, $P(\kappa) \to 0$ as $\kappa \to \infty$. This is not hard to understand. For simplicity, let us assume that we have reflecting boundary conditions. As κ starts to increase above κ_c, the probability that the other end of the SAW originating at the origin is infinitely far away from the origin (i.e., near the boundary) increases for a while, but eventually decreases when the other end is reflected back into the interior so that it finds itself close to the origin.

To put things in an even better perspective, let us briefly consider the one-dimensional problem ($q=2$). The lattice is now self-dual. We follow the same procedure as for $q=3$, but with the following Hamiltonian on the dual lattice: $\mathscr{H} = K\sum_i S_i S_{i+1} + H\sum_i S_i$. It is easily found that $Z = \exp(N\{H-K\})\hat{Z}$, where $\kappa = e^{2H}$ and $\eta^2 = e^{-4K}$. Constructing the recursion relation between $Z_m(S)$ and $Z_{m-1}(S)$ and requiring that H_m' in (4) be the same for all m, we find that

$$Z_{m-1}(0) = A_m(\omega_1\sqrt{x} + \omega_2/\sqrt{x}) = A_{m-1}\sqrt{x},$$

$$Z_{m-1}(1) = A_m(\omega_2\sqrt{x} + \omega_3/\sqrt{x}) = A_{m-1}/\sqrt{x},$$

where $\omega_1 = (\kappa^2/\eta)^{1/4}$, $\omega_2 = \eta^{1/4}$, and $\omega_3 = 1/(\kappa\eta)^{1/2}$, and x is given by $x = (\omega_1 x + \omega_2)/(\omega_2 x + \omega_3)$. The solutions are

$$x = [\kappa - 1 \pm (\kappa-1)^2 + 4\kappa\eta^2]/2\eta\sqrt{\kappa}.$$

For $\eta \to 0$, i.e., $K \to \infty$, we find that $\kappa_c = 1$ and that $x = 0$ below κ_c and $x = \infty$ above κ_c. At κ_c, $x = 1$.

Following steps similar to those for $q=3$, we can evaluate the order parameter $P(\kappa)$ in one dimension. We find that $\tilde{Z}_{m-1}(0) = A_m\sqrt{\eta}$ and that

$$P(\kappa) = (2/\eta)[\tilde{Z}_0(0)Z_0(0)/Z]|_{\eta=0}$$
$$= 2x/\kappa^{1/2}(x^2+1).$$

Thus, we find that $P(\kappa) = 0$ everywhere except at $\kappa = \kappa_c = 1$, where $P(\kappa) = 1$. Moreover, for $\eta = 0$ one also finds that ϕ_l is zero below κ_c and unity above κ_c, while $\phi_p = 0$ everywhere.

It is not hard to understand the physics in one dimension. Since $\phi_l = 1$ above κ_c, the lattice is completely filled up by a SAW. [For $q=3$, this happened only in the limit $\kappa \to \infty$ ($\eta = 0$).] If we use periodic boundary conditions, we find that the two end points of the SAW are next to each other for $\kappa > \kappa_c$, which explains why $P(\kappa)$ should be zero. Since $P(\kappa)$ is κ independent, we must have $\beta = 0$. At κ_c, $P(\kappa)$ is independent of η, yielding $\delta = \infty$. Moreover, $\gamma = 1$ and $\alpha = 1$. All these exponents are consistent with the results of Balian and Toulouse[14] for $d=1$ and $n=0$.

To summarize, the SAW problem has been considered without the use of any formal $n \to 0$ limit. The problem is shown to be identical to an Ising model (with somewhat peculiar interactions or limits). This analysis has enabled us to identify the order parameter of the problem for the first time. The analysis also clarifies, for the first time, the physical nature of the ordered state: We have basically a single SAW extending in both directions to infinity, in such a way that it reaches the boundary of the lattice, since $\phi_l > 0$ in the ordered state. It should be stressed that a lattice structure is very important in our understanding of the ground state with ϕ_l bounded between zero and one. In a continuum version, ϕ_l can easily blow up, which makes it useless above κ_c unless an ultraviolet cutoff is used.[5] It appears at present that the ordered phase discussed here is identical to the new phase that appears in Ref. 5.

This research was supported by a faculty research grant at The University of Akron and by a grant from the Research Corporation.

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