

Magnetic analog of self-avoiding random walks (polymer chains) on a lattice

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It is shown that if one considers the $n \rightarrow 0$ limit of a magnetic system consisting of n -component classical spins on a lattice, one indeed obtains a correspondence with a system of self-avoiding random walks; that is, polymer chains with excluded volume in a solution, but the correspondence is not *isomorphic*. It turns out that K and H do not serve as the activities for the polymer system, which, in fact, are given by K/z and H/\sqrt{z} , where $z = 1 + H^2/2$. Moreover, the polymer free energy \hat{W} is also different from the magnetic free energy W_0 in the limit $n \rightarrow 0$. Various polymer correlation functions are calculated and are found to be different from those proposed by other authors. It is also shown that \hat{W} satisfies the proper *convexity* properties, even though W_0 does not.

I. INTRODUCTION

In order to study excluded-volume effects, which forbid the chains to overlap, one starts with a simple model of polymer chains: The chains are described by self-avoiding walks (SAW). If one is interested in long-range properties of polymers, then their chemical details are not expected to be important, and the above model seems to be quite appropriate. (The reader is referred to an excellent review article by Freed¹ for more details.) de Gennes² pointed out in 1972 an analogy between a self-avoiding random walk, i.e., a *single* polymer chain with excluded volume and $n=0$ limit of an n -component ϕ^4 field theory (described by the Landau-Ginzburg-Wilson Lagrangian) in the absence of any external field. It is possible to give a meaning to the ϕ^4 theory for nonintegral and also zero n (as a matter of fact, any n) in the usual Wick perturbation expansion in powers of the interaction: Each term in the expansion is a simple polynomial in n and can be unambiguously continued for any value of n . Later on, the above correspondence was established using other means.³⁻⁷ des Cloizeaux⁸ extended the approach of de Gennes and succeeded in providing an analogy between a system of polymer chains with excluded volume in a solution and the ϕ^4 theory in the presence of an external magnetic field as $n \rightarrow 0$.^{9,10} Moreover, he also noted that, for example, the longitudinal correlation function in the equivalent magnetic system describes the correlation between *any* two end points of polymer chains. Schäfer and Witten¹¹ provided the scheme for calculating the correlation between any two monomers of polymer chains. Recently, Moore and Wilson¹² have noted that the longitudinal susceptibility χ of the magnetic system becomes *negative* for $T < T_c$ as the magnetic field H tends towards zero, i.e., as the coexistence curve is approached in the limit $n \rightarrow 0$. They argue that a negative susceptibility

is *impossible* and provide an alternative means of computing χ which they observe to be positive. Ballian and Toulouse¹³ have shown that the magnetic system in the absence of a magnetic field has negative specific heat for $n < 1$ in zero- and one-dimensional cases.

Our aim in the present paper is to establish correctly the above correspondence between SAW's, i.e., polymers and the $n=0$ limit of the magnetic system. In order that the analysis can be carried out explicitly, we have confined ourselves to a magnetic system, and therefore a polymer system, on a *lattice*. Moreover, the length of each spin of the magnetic system is *constrained* to be \sqrt{n} : $\vec{S}^2 = n$. Our final expression differs from the one proposed by des Cloizeaux⁹ for the continuum case with unconstrained spins and this *distinction* should be emphasized: It is conceivable that the lattice version and the continuum version are distinct. It is not clear at this stage what is the connection, if any, between the constrained lattice system considered here and the continuum version considered by des Cloizeaux⁹ as $n \rightarrow 0$. We will also establish that the polymer-magnet analogy is *not* isomorphic and point out its limitations. We express various polymer correlation functions in terms of quantities describing the corresponding magnetic system. These relations among various polymer correlation functions and the magnetic correlation functions are slightly different from those proposed by other authors.^{9,11} We will also establish that the "susceptibility" $\hat{\chi}$ and the "specific heat" \hat{C} of the polymer system are always *non-negative*, even if the magnetic susceptibility χ and the magnetic specific heat C are negative. (The fact that χ and C may become negative is the subject matter of a separate paper.¹⁴) It should again be emphasized that des Cloizeaux⁹ and Schäfer and Witten¹¹ have calculated various polymer correlation functions in the continuum limit, with unconstrained spins.

The layout of the paper is as follows. We describe in Sec. II how the $n \rightarrow 0$ limit of the magnetic system on a lattice can be obtained. Section III describes the correct correspondence between the polymer system and the magnetic system. This correspondence is different from the one quoted in the literature and implies that the activities of the polymer system are given by $\kappa = K/z$ and $\eta = H/\sqrt{z}$, $z = 1 + H^2/2$. This is the first of the two major modifications required for a correct correspondence between the polymer system and the $n \rightarrow 0$ limit of the magnetic system. Section IV is the most important part of the paper and describes the correct definitions of the correlation functions for the polymer system in terms of those of the magnetic system in the $n \rightarrow 0$ limit. It is shown that the chemical potentials for the polymer system are given by $\lambda = \ln \kappa$ and $\zeta = \ln \eta$, and this observation constitutes the second major modification. It should be *emphasized* that the two modifications are independent of each other, and it is the *second* modification and not the first one that *saves* the convexity properties of the polymer system. A brief summary of these results has been reported earlier.¹⁵ The last section gives a summary of our results.

II. THE $n \rightarrow 0$ LIMIT OF THE MAGNETIC SYSTEM

Even though there are several expositions available in literature describing the analogy between polymers and the magnetic system, we will briefly outline how this analogy is obtained since the final result derived here is different from one available in literature.^{5,8-10} As was remarked in the Introduction, we will consider the lattice version of the magnetic system. There is an n -component classical spin $\vec{S}_i = \{S_i^{(\alpha)}, \alpha = 1, \dots, n\}$ at each site i . The length of each spin is constrained to be equal to \sqrt{n} :

$$\vec{S}_i^2 = \sum_{\alpha=1}^n (S_i^{(\alpha)})^2 = n. \quad (1)$$

The Hamiltonian of the constrained magnetic system is given by

$$\mathcal{H} = \sum_{\langle ij \rangle} K_{ij} \vec{S}_i \cdot \vec{S}_j + \sum_i H_i S_i^{(1)}, \quad (2)$$

where K_{ij} is the ferromagnetic coupling constant between spins at sites i and j , and H_i is the magnetic field in the $\alpha = 1$ direction at site i . The sum over $\langle ij \rangle$ is over distinct nearest-neighbor pairs. We have also absorbed a factor of $-1/kT$ in the definition of the Hamiltonian \mathcal{H} .

Because of the constraint (1), the partition function $Z_n(\{K_{ij}\}, \{H_i\})$ involves integration over angu-

lar variables $d\Omega_i$ of each spin \vec{S}_i :

$$Z_n(\{K_{ij}\}, \{H_i\}) = \frac{\int \left(\prod_{i=1}^N d\Omega_i \right) e^{\mathcal{H}}}{\int \left(\prod_{i=1}^N d\Omega_i \right)}. \quad (3)$$

Here N is the total number of sites. Let O_i stand for any product of the components $S_i^{(\alpha)}$, $\alpha = 1, \dots, n$ of any single spin \vec{S}_i , and define its angular average as follows:

$$\langle O_i \rangle_\Omega = \frac{\int d\Omega_i O_i}{\int d\Omega_i}.$$

It can be shown^{5,14} that

$$\langle 1 \rangle_\Omega = 1, \quad (4)$$

$$\langle (S_i^{(\alpha)})^2 \rangle_\Omega = 1, \quad \alpha = 1, \dots, n$$

are the *only* nonvanishing angular averages in the limit $n \rightarrow 0$. All other moments O_i have angular averages that vanish in the $n \rightarrow 0$ limit.

We are now in a position to calculate Z_0 , the $n \rightarrow 0$ limit of Z_n . For this purpose, we expand the exponential in (3) in a power series to obtain

$$Z_n = \left\langle \prod_{\langle ij \rangle} \left(1 + K_{ij} \vec{S}_i \cdot \vec{S}_j + \frac{K_{ij}^2}{2} (\vec{S}_i \cdot \vec{S}_j)^2 + \dots \right) \times \prod_k \left(1 + H_k S_k^{(1)} + \frac{H_k^2}{2} (S_k^{(1)})^2 + \dots \right) \right\rangle_\Omega. \quad (5)$$

Every term in (5) can be represented as a diagram on the lattice (Fig. 1). A term $K_{ij} S_i^{(\alpha)} S_j^{(\alpha)}$ for nearest-neighbor sites i and j is represented by a bond between i and j , which carries a "color index" α [Fig. 1(a)]. A term $\frac{1}{2} K_{ij}^2 (S_i^{(\alpha)} S_j^{(\alpha)})^2$ is represented as a "small" polygon made out of two α -colored bonds between nearest-neighbor sites i and j [Fig. 1(b)]. Each term $H_i S_i^{(1)}$ can be represented by a cross [Fig. 1(c)]. Each term $\frac{1}{2} H_i^2 (S_i^{(1)})^2$ can be represented by a filled circle [Fig. 1(d)]. It will be shown below that in the $n \rightarrow 0$ limit, we need not consider terms with higher powers of either K_{ij} or H_i .

Because of (4), we find that the only nonvanishing diagrams in the limit $n \rightarrow 0$ are those in which at each site i there appears only a *single* component α of S_i in the form $(S_i^{(\alpha)})^2$. Also, since a given bond $S_i^{(\alpha)} S_j^{(\alpha)}$ "transmits" the same index α from i to the neighboring site j , the color index α *must* be continuous along any connected piece of a diagram. Thus, terms with powers of K_{ij} or H_i higher than two can be omitted in the $n \rightarrow 0$ limit. We now observe that Figs. 1(b) and 1(e) can occur only as disconnected parts in a diagram. Each polygon [Figs. 1(b) and 1(e)] carries a definite color index α . When α varies from 1 to n , we

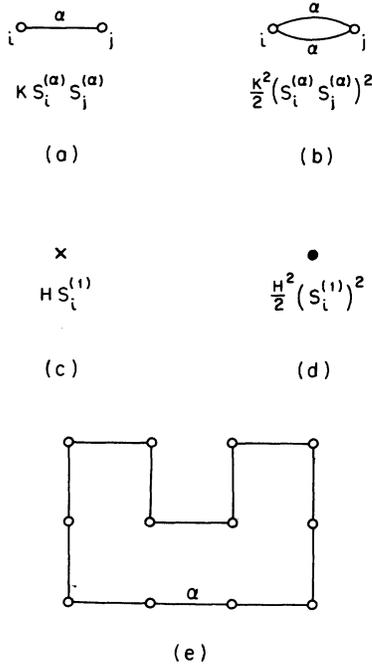


FIG. 1. Graphical representation of various terms in Z_n . (b) and (e) represent closed loops with color index α . These loops vanish in the limit $n \rightarrow 0$.

get n polygons each with different color, but having identical weight. When one sums over the color index α , these n polygons give a contribution proportional to n , which vanishes in the limit $n \rightarrow 0$. However, Fig. 1(d) contributes $\frac{1}{2} H^2$ in the limit $n \rightarrow 0$. Thus, it is only necessary to retain linear terms in the expansion of $\exp(K_{ij} \vec{S}_i \cdot \vec{S}_j)$ and quadratic terms in the expansion of $\exp(H_k S_k^{(1)})$, when $n=0$, and for this case (5) becomes

$$Z_0 = \left\langle \prod_{\langle ij \rangle} (1 + K_{ij} \vec{S}_i \cdot \vec{S}_j) \prod_k \left(1 + H_k S_k^{(1)} + \frac{H_k^2}{2} (S_k^{(1)})^2 \right) \right\rangle_{\Omega}.$$

As is evident, the only diagrams that contribute to Z_0 are those that contain any number of *non-intersecting* lines (consisting of bonds due to $K_{ij} S_i^{(1)} S_j^{(1)}$) such that each line terminates on two magnetic crosses at the two ends. There can also be any number of filled circles [Fig. 1(d)] at any of the sites *not* connected to these lines. One such diagram is shown in Fig. 2. This diagram contains six nonintersecting lines or *self-avoiding walks* (SAW) along with eight filled circles. Each bond of the SAW's gives a factor of K_{ij} , each SAW gives a factor $H_i H_j$, where i and j are the two end points of the SAW with magnetic crosses, and each filled circle gives a factor of $H_k^2/2$. It is tempting to consider a filled circle [Fig. 1(d)] as a SAW of *zero* length and this seems to have been the practice in the literature. How-

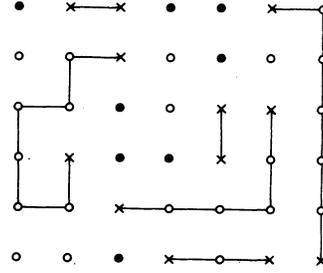


FIG. 2. Nonvanishing diagram appearing in Z_0 . There are six SAW's of total length $l = 22$. There are eight filled circles and six unfilled circles that are not connected with the SAW's.

ever, the weight of a SAW of zero length should be H_k^2 while the weight of the filled circle is $H_k^2/2$. Thus, a filled circle *cannot* be considered a SAW of zero length. In the following, a SAW is always assumed to be of *nonzero* length.

Let us now consider a diagram that has p SAW's and contains l bonds. The number of sites covered by these SAW's is $p+l$. There are $N - (p+l)$ uncovered sites. Let us consider one such uncovered site k . This site may or may not be covered by the filled circle. The generating function for this is given by

$$z_k = z(H_k) = 1 + H_k^2/2. \tag{6a}$$

The partition function $Z_0(\{K_{ij}\}, \{H_i\})$ can now be written as follows:

$$Z_0(\{K_{ij}\}, \{H_i\}) = \left(\prod_{k=1}^N z_k \right) + \sum_{\Gamma} \omega(\Gamma), \tag{7a}$$

where the first term is the contribution from configurations with no SAW, and the sum over Γ is over all possible distinct configurations Γ of SAW's, and $\omega(\Gamma)$ is the contribution of a configuration Γ :

$$\omega(\Gamma) = \left(\prod_k H_k \right) \left(\prod_{\langle ij \rangle} K_{ij} \right) \left(\prod_u z_u \right).$$

Here Γ represents some configuration of $p \geq 1$ SAW's of total length l , k represents one of the $2p$ end points of the SAW's in Γ , $\langle ij \rangle$ represents one of the l bonds in Γ , and u represents one of the $N - (p+l)$ sites of the lattice not covered by Γ .

We will now write down the form of Z_0 for the case of a homogeneous system for which all K_{ij} and H_i are constant and equal to K and H , respectively. The weight $\omega(\Gamma)$ takes a simple form: $\omega(\Gamma) = H^{2p} K^l z^{N-(p+l)}$. In the usual derivation available in the literature,⁵ the last factor, i.e., $z^{N-(p+l)}$ has been *overlooked* in the calculation of $\omega(\Gamma)$. Thus, the final form of the partition function $Z_0(K, H)$ given below is also different from the expression given in the literature⁵:

$$Z_0(K, H) = z^N + \sum_{p=1}^{\infty} \sum_{l \geq p} H^{2p} K^l U_{p,l} z^{N-(p+1)}, \quad (7b)$$

where

$$z = 1 + H^2/2 \quad (6b)$$

and $U_{p,l}$ is the number of ways of drawing p non-intersecting SAW's of total length l on the lattice. Each SAW contributes a factor of H^2 and each bond gives a factor of K . We will show in Sec. III that the above correction somewhat *restricts* the analogy between the polymer system and the magnetic system in the limit $n \rightarrow 0$. It should be remarked at this point that it is *not* clear what happens to the last factor of $(\prod_u z_u)$ in $\omega(\Gamma)$ or $z^{N-(p+1)}$ in (7b) if one considers a continuum version of the magnetic system.

III. POLYMER ANALOGY

Let us now identify a SAW with a polymer chain as was intended at the beginning of the Introduction. Let us also introduce the following two activities: η_k is the activity for a chain end to be located at site k and κ_{ij} is the activity for a bond $\langle ij \rangle$ of a polymer chain. Let Γ be some configuration of p polymer chains of total length l . We now introduce a grand canonical partition function for the polymer chains (or SAW's) as follows:

$$\hat{Z}(\{\kappa_{ij}\}, \{\eta_i\}) = 1 + \sum_{(\Gamma)} \hat{\omega}(\Gamma), \quad (8a)$$

where

$$\hat{\omega}(\Gamma) = \left(\prod_k \eta_k \right) \left(\prod_{\langle ij \rangle} \kappa_{ij} \right)$$

is the contribution of Γ . Here, k represents one of the $2p$ end points and $\langle ij \rangle$ one of the l bonds of the chains. A comparison of (7a) and (8a) shows that, in fact,

$$Z_0(\{K_{ij}\}, \{H_i\}) = \left(\prod_{i=1}^N z_i \right) \hat{Z}(\{\kappa_{ij}\}, \{\eta_i\}) \quad (9a)$$

provided we make the following identifications:

$$\begin{aligned} \kappa_{ij} &= \frac{K_{ij}}{\sqrt{z_i z_j}}, \\ \eta_i &= \frac{H_i}{\sqrt{z_i}}. \end{aligned} \quad (10a)$$

For a homogeneous system where all η_i and κ_{ij} are constant and equal to η and κ , respectively, we define the grand canonical partition function by

$$\hat{Z}(\kappa, \eta) = 1 + \sum_{p=1}^{\infty} \sum_{l \geq p} \eta^{2p} \kappa^l U_{p,l}, \quad (8b)$$

where we have used the quantity $U_{p,l}$ introduced in (7b). A comparison of (7b) and (8b) shows that

$$Z_0(K, H) = z^N \hat{Z}(\kappa, \eta) \quad (9b)$$

provided we have

$$\begin{aligned} \kappa &= \frac{K}{z(H)} = \frac{K}{1 + H^2/2}, \\ \eta &= \frac{H}{\sqrt{z(H)}} = \frac{H}{(1 + H^2/2)^{1/2}}. \end{aligned} \quad (10b)$$

A few remarks regarding the mappings (10a) or (10b) are in order. For the sake of clarity, we will consider the mappings given in (10b). We note that

$$\forall K < \infty, \quad \kappa \rightarrow 0 \text{ and } \eta \rightarrow \sqrt{2} \text{ as } H \rightarrow \infty. \quad (11a)$$

However, in the case $K \rightarrow \infty$ along with $H \rightarrow \infty$, the limiting value of κ can take any value between zero and infinity depending on the trajectories ($K = H^{2+\epsilon}$, any ϵ) along which K and H tend to infinity. The limit of η is always $\sqrt{2}$. Since η must never be negative in the polymer case, the mapping between η and H is physically meaningful only when $H \geq 0$. Also, the correspondence between \hat{Z} and Z_0 , the polymer system and the magnetic system, *only* works when η is small, i.e., $\eta \leq \sqrt{2}$. Finally, when H is very small

$$\begin{aligned} \kappa &\simeq K, \\ \eta &\simeq H. \end{aligned} \quad (11b)$$

For the homogeneous system, an alternative approach is to let

$$s = p + l, \quad (12)$$

denote the number of monomers, i.e., the number of sites covered by the SAW's and to define

$$\bar{U}_{p,s} = U_{p,s-p} \quad (13)$$

as the number of configurations of p polymer chains covering a total of s sites on the lattice. The analog of (8b) is

$$\bar{Z}(\kappa, \bar{\eta}) = 1 + \sum_{p=1}^{\infty} \sum_{s=2p}^{\infty} \bar{\eta}^{2p} \kappa^s \bar{U}_{p,s}, \quad (14)$$

where $\bar{\eta}$ is the activity for the chain ends and κ is now the activity for a monomer. If

$$\bar{\eta} = \eta / \sqrt{\kappa} \quad (15)$$

we find that $\bar{Z}(\kappa, \bar{\eta}) = \hat{Z}(\kappa, \eta)$. Moreover, we note that

$$Z_0(K, H) = z^N \bar{Z}(\kappa, \bar{\eta}) \quad (16)$$

provided we set

$$\bar{\eta} = H / \sqrt{K}, \quad (17)$$

and where κ is related via (10b). The mapping from (K, H) to $(\kappa, \bar{\eta})$ again has certain peculiarities. For any *finite* value of K , $\kappa \rightarrow 0$ and $\bar{\eta} \rightarrow \infty$

as $H \rightarrow \infty$. As K and H both tend to infinity simultaneously, the limiting values of κ and $\tilde{\eta}$ depend upon the trajectories along which K and H go to infinity. The same is true when K and H both tend to zero.

Thus, because of the peculiarities of the mappings mentioned above, we conclude that the correspondence between the polymer system and the magnetic system in the limit $n=0$ is *not* an isomorphism.

In the remainder of this section, we will focus our attention on the homogeneous system. Let $\langle p \rangle$ denote the thermodynamic average of the number of chains:

$$2\langle p \rangle = \frac{\partial \ln \tilde{Z}}{\partial \ln \eta} \quad \text{or} \quad \frac{\partial \ln \tilde{Z}}{\partial \ln \tilde{\eta}}.$$

We find from, for example, (9b), that the fraction of chains per site

$$\begin{aligned} \phi_p &= \frac{\langle p \rangle}{N} = \frac{\eta}{2N} \left(\frac{\partial K}{\partial \eta} \frac{\partial}{\partial K} + \frac{\partial H}{\partial \eta} \frac{\partial}{\partial H} \right) (\ln Z_0 - N \ln z) \\ &= \frac{1}{2} H z m + \frac{1}{2} H^2 (K\epsilon - 1), \end{aligned} \quad (18a)$$

where

$$m = \frac{1}{N} \frac{\partial \ln Z_0}{\partial H}, \quad (19)$$

$$\epsilon = \frac{1}{N} \frac{\partial \ln Z_0}{\partial K}.$$

Here m is the magnetization per particle and ϵ is the energy per particle of the magnetic system ($n=0$). Incidentally, since $\phi_p \geq 0$ by definition, we have the following inequality satisfied by m :

$$m \geq H(1 - K\epsilon)/z. \quad (20)$$

For $K=0$, m is the magnetization of a single spin in a magnetic field and it can be shown¹⁴ that it is given by H/z . Also, we will see below that $K\epsilon \leq 1$ [see (23)]. Thus, we prove the important property of m (Ref. 14):

$$m \geq 0. \quad (21)$$

Let $\langle l \rangle$ be the average number of bonds:

$$\langle l \rangle = \frac{\partial \ln \tilde{Z}}{\partial \ln \kappa}. \quad (22)$$

It is easily seen that the bond density $\phi_l = \langle l \rangle / N$ is related to ϵ through

$$\phi_l = K\epsilon. \quad (18b)$$

It should be obvious on physical grounds that ϕ_l is bounded above by one and below by zero. Thus,

$$0 \leq K\epsilon \leq 1, \quad (23)$$

which was used to prove (21). For the density of monomers $\phi_s = \phi_l + \phi_p$, we have from (18a) and

(18b) that

$$\phi_s = K\epsilon + \frac{Hz}{2} \left(m - \frac{H}{z} + \frac{HK\epsilon}{z} \right). \quad (18c)$$

One can easily check that if one uses instead the following definition of ϕ_s ,

$$\phi_s = \frac{1}{N} \frac{\partial \ln \tilde{Z}(\kappa, \tilde{\eta})}{\partial \kappa},$$

one obtains the same expression as (18c) relating ϕ_s with magnetic quantities. Thus, we have expressed ϕ_l , ϕ_p , and ϕ_s in terms of m and ϵ , quantities characterizing the magnetic system. This completes part of the polymer-magnet dictionary. In Sec. IV we will relate the polymer correlation functions with magnetic quantities. That will complete our dictionary.

Before we leave this section, we would like to point out that it is not clear what happens to (9) and (10) in the continuum version of the problem. If one is interested in the limit $H \rightarrow 0$,⁹ i.e., $z \rightarrow 1$, the correction factors due to z in (9) and (10) are unimportant and one gets back the old mapping $\kappa \simeq K$ and $\eta \simeq H$.^{5,9} Thus, it is *conceivable* that the constrained lattice version considered here and the continuum-field-theory version are not very different at least for the case $H \rightarrow 0$.

IV. CORRELATION FUNCTIONS

des Cloizeaux⁹ has remarked that there is a correspondence between the longitudinal (transverse) correlation function of the magnetic system in the $n=0$ limit and the end-to-end correlation function between polymer ends belonging to the same chain or different chains (belonging to the same chain), and has been described in detail by Schäfer and Witten.¹¹ The above correspondence is presumably based on the comparison of diagrams obtained in the high-temperature expansion of the magnetic correlation function in the $n=0$ limit and the polymer diagrams in the grand canonical ensemble. For example, consider the connected part of the longitudinal correlation function (the angular brackets without the subscript Ω denote thermodynamic averages)

$$\begin{aligned} \chi_{ij} &= \langle S_i^{(1)} S_j^{(1)} \rangle_{c, n=0} \\ &= \langle S_i^{(1)} S_j^{(1)} \rangle_{n=0} - \langle S_i^{(1)} \rangle_{n=0} \langle S_j^{(1)} \rangle_{n=0} \end{aligned} \quad (24a)$$

and the diagrams that appear in its high-temperature expansion (Fig. 3). The spin components $S_i^{(1)}$ and $S_j^{(1)}$ may now replace magnetic crosses at sites i and j [Fig. 1(c)]. Thus we get two kinds of diagrams shown in Figs. 3(a) and 3(b). In Fig. 3(a), the two sites i and j are the end points of the same chain, while in Fig. 3(b) they represent the end points of different chains. Thus, it would seem⁹ that χ_{ij} describes the correlation between

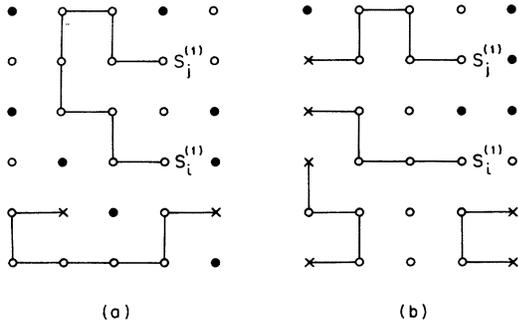


FIG. 3. Two kinds of diagrams that appear in $\langle S_i^{(1)} S_j^{(1)} \rangle_{c,n=0}$. The two sites i and j belong to the same chain in (a), while they belong to different chains in (b).

two chain ends located at sites i and j and belonging to either the same chain [Fig. 3(a)] or different chains [Fig. 3(b)]. Similarly, if we consider the diagrams that appear in the high-temperature series expansion of the connected transverse correlation function, for example, $\langle S_i^{(2)} S_j^{(2)} \rangle_{c,n=0}$ we find that the diagrams are such that the two sites i and j are the chain ends of the same chain (Fig. 4) with the color index $\alpha=2$ running along this chain. Schäfer and Witten¹¹ have argued that the correlation between any two monomers of the polymer chains also has a magnetic analog. This correlation function analog (for a magnetic system on a lattice) is given by the correlation between $\sum_k \tilde{S}_i \cdot \tilde{S}_k$ and $\sum_l \tilde{S}_j \cdot \tilde{S}_l$, where k and l are the nearest-neighbor sites of i and j , respectively:

$$C_{ij} = \frac{K^2}{4} \left\langle \sum_k \tilde{S}_i \cdot \tilde{S}_k \sum_l \tilde{S}_j \cdot \tilde{S}_l \right\rangle_{c,n=0}. \quad (24b)$$

However, we will see that one cannot justify that χ_{ij} (24a) and C_{ij} (24b) describe the end-end and monomer-monomer correlations, respectively. First consider χ_{ij} . If χ_{ij} describes the end-end correlation function as proposed by des Cloizeaux,⁹ then the total intensity of scattering in the forward direction from various chain ends must be proportional to the long-wavelength limit of χ_{ij} , i.e.,

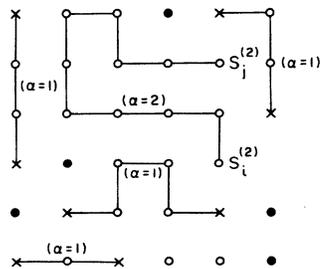


FIG. 4. Diagram appearing in $\langle S_i^{(2)} S_j^{(2)} \rangle_{c,n=0}$. This can also be thought of as a diagram with four red chains ($\alpha=1$) and one blue chain ($\alpha=2$).

the magnetic susceptibility χ . This necessarily implies that χ must be non-negative. However, we will establish elsewhere¹⁴ that χ can indeed become *negative*. This is also in *contradiction* with the assertion of Moore and Wilson¹² that χ must be non-negative. Therefore, χ_{ij} *cannot* describe the correlation between two chain ends located at i and j . Moreover, it can also be established¹⁴ that the magnetic specific heat $C = \partial \epsilon / \partial K$, where ϵ is the energy per site [see (20)], can also become negative for $n=0$. This should also be evident from (18b) and (23): For finite H , as $K \rightarrow \infty$, the bond activity κ (10b) also tends to infinity. On physical grounds, we expect that as $\kappa \rightarrow \infty$, $\phi_i \rightarrow 1$. This means that $\epsilon \sim 1/K$ for large K , and therefore, $\partial \epsilon / \partial K \sim -1/K^2$. Thus, the specific heat can indeed become *negative*. Something must be wrong since if C_{ij} were to describe the polymer monomer-monomer correlations, the intensity of scattering from various monomers in the forward direction must be proportional to C and could become negative. This is obviously absurd. Therefore, C_{ij} *cannot* be taken to describe the monomer-monomer correlation function as was proposed by Schäfer and Witten.¹¹

In the following we will calculate various polymer correlation functions of interest, viz., the end-end correlation function $\hat{\chi}_{ij}$, the auto-end correlation function $\hat{\chi}_{ij}^a$, and the monomer-monomer correlation function \hat{C}_{ij} (see below for their exact definitions). Our calculation will show that the above identifications $\hat{\chi}_{ij} = H^2 \chi_{ij}$ and $\hat{C}_{ij} = C_{ij}$ need to be modified. These corrections are crucial. For example, it will be established that $\ln Z$ satisfies the proper convexity property, even though $\ln Z_0$ lacks this (i.e., the magnetic system may have negative susceptibility or specific heat in the $n \rightarrow 0$ limit¹⁴). We should point out that the corrections obtained below are *independent* of the corrections appearing in (9) and (10), and amount to realizing that $\ln \eta_i$ and $\ln \kappa_{ij}$ are the appropriate chemical potentials for the polymer system.

We start our discussion by first considering the correlation function between any two chain ends, whether they belong to the same chain or different chains. For the sake of brevity, we will call this simply end-to-end correlation function. We introduce the following two variables X_i and Y_{ij} :

$$X_i = \begin{cases} 1, & \text{if site is a chain end} \\ 0, & \text{otherwise.} \end{cases} \quad (25)$$

$$Y_{ij} = \begin{cases} 1, & \text{if } \langle ij \rangle \text{ is a bond belonging to some} \\ & \text{polymer chain} \\ 0, & \text{otherwise.} \end{cases}$$

Using these variables, we can rewrite $\hat{Z}(\{\kappa_{ij}\}, \{\eta_i\})$ in the following form:

$$\hat{Z}(\{\kappa_{ij}\}, \{\eta_i\}) = \sum \exp\left(\sum_i \zeta_i X_i + \sum_{\langle ij \rangle} \lambda_{ij} Y_{ij}\right), \quad (26)$$

where

$$\begin{aligned} \zeta_i &= \ln \eta_i, \\ \lambda_{ij} &= \ln \kappa_{ij}. \end{aligned} \quad (27)$$

The first sum in (26) is over all possible configurations of polymer chains, including one with no chains. The sum over i in the exponent is over all sites and over $\langle ij \rangle$ is over all distinct nearest-neighbor pairs.

From the definitions of X_i and Y_{ij} (25), it is evident that

$$\begin{aligned} \langle p \rangle &= \frac{1}{2} \left\langle \sum_i X_i \right\rangle, \\ \langle q \rangle &= \frac{1}{2} \left\langle \sum_{\langle ij \rangle} Y_{ij} \right\rangle, \\ \langle s \rangle &= \frac{1}{2} \left\langle \sum_i X_i + \sum_{\langle ij \rangle} Y_{ij} \right\rangle. \end{aligned} \quad (28)$$

$$\begin{aligned} \hat{\chi}_{ij} &= \delta_{ij} \left[H_i z_i \left(1 + \frac{3}{2} H_i^2\right) \left(m_i - \frac{H_i}{z_i}\right) + H_i^2 z_i \sum_k K_{ik} \epsilon_{ik} \right] + \frac{1}{2} H_i H_j \left(H_i z_j \sum_k K_{ik} \frac{\partial \epsilon_{ik}}{\partial H_j} + H_j z_i \sum_k K_{jk} \frac{\partial \epsilon_{jk}}{\partial H_i} \right) \\ &\quad + \frac{1}{4} H_i^2 H_j^2 \left(\sum_{k,l} K_{ik} \epsilon_{jl} \delta_{ik,jl} + \sum_{k,l} K_{ik} K_{jl} \frac{\partial \epsilon_{ik}}{\partial K_{jl}} \right) + H_i H_j z_i z_j \chi_{ij}, \end{aligned} \quad (34)$$

where

$$\begin{aligned} m_i &= \frac{\partial W_0}{\partial H_i}, \\ \chi_{ij} &= \frac{\partial^2 W_0}{\partial H_i \partial H_j}, \\ \epsilon_{ik} &= \frac{\partial W_0}{\partial K_{ik}}, \end{aligned} \quad (35)$$

and $\delta_{ik,jl}$ is one if the (ik) and (jl) pairs are identical, and zero otherwise. The quantities appearing in (35) and therefore, in the right-hand side of (34), characterize the magnetic system. Thus, (34) expresses the polymer correlation function $\hat{\chi}_{ij}$ in terms of quantities characterizing the magnetic system.

Let us now consider the long-wavelength limit of the polymer "susceptibility"

$$\hat{\chi} = \frac{1}{N} \sum_i \sum_j \hat{\chi}_{ij}. \quad (36)$$

For the homogeneous system, it is also given by

$$\hat{\chi} = \frac{1}{N} \frac{\partial^2 \hat{W}}{\partial \xi^2}. \quad (36')$$

It is easily seen from the form of \hat{W} [see (30) and

Now we are in a position to calculate the end-to-end correlation function (connected two-point correlation function)

$$\hat{X}_{ij} = \langle X_i X_j \rangle_c = \langle X_i X_j \rangle - \langle X_i \rangle \langle X_j \rangle. \quad (29)$$

Let us introduce the polymer free energy \hat{W} :

$$\hat{W} = \ln \hat{Z}. \quad (30)$$

In terms of \hat{W} , $\hat{\chi}_{ij}$ is given by

$$\begin{aligned} \hat{\chi}_{ij} &= \frac{\partial^2 \hat{W}}{\partial \zeta_i \partial \zeta_j} \\ &= \eta_i \frac{\partial \hat{W}}{\partial \eta_j} \delta_{ij} + \eta_i \eta_j \frac{\partial^2 \hat{W}}{\partial \eta_i \partial \eta_j}. \end{aligned} \quad (31)$$

We can express $\hat{\chi}_{ij}$ in terms of magnetic quantities by noting (A6) or (A7) (see Appendix A) and that

$$\hat{W} = W_0 - \sum_{i=1}^N \ln z_i, \quad (32)$$

where

$$W_0 = \ln Z_0 \quad (33)$$

is the magnetic free energy. It is easily seen (see Appendix A) that

(26)] that

$$\hat{\chi} = \frac{1}{N} \left\langle \left(\sum_i (X_i - \langle X_i \rangle) \right)^2 \right\rangle \geq 0.$$

Thus, the free energy \hat{W} satisfies the proper convexity condition, even though the corresponding magnetic system in the $n \rightarrow 0$ limit need not satisfy the convexity property with respect to the magnetic field H .¹⁴ We have also shown that the end-to-end correlation function $\hat{X}_{ij} = \langle X_i X_j \rangle_c$ is not identical with χ_{ij} , the magnetic longitudinal correlation function, but is related to it in a more complicated way than was previously assumed.^{9,11,12} These correction terms are very important and ensure the positivity of $\hat{\chi}$ even if the magnetic susceptibility χ is not positive.¹⁴ Using (34) in (36), we obtain the following expression for $\hat{\chi}$ relating it to χ (see Appendix A) for the homogeneous system:

$$\begin{aligned} \hat{\chi} &= H z \left(1 + \frac{3H^2}{2} \right) \left(m - \frac{H}{z} \right) + 2KH^2(1 + H^2)\epsilon \\ &\quad + 2zH^3K \frac{\partial \epsilon}{\partial H} + K^2H^4 \frac{\partial \epsilon}{\partial K} + H^2z^2\chi, \end{aligned} \quad (37)$$

where m , ϵ , and χ are the magnetization, the

energy, and the susceptibility of the magnetic system, and z is given in (6b). One can also obtain (37) by using (36') directly.

We now turn our attention to the correlation function between two ends of the *same* chain. For the sake of brevity, we will call this auto-end correlation function, and use a superscript a to denote the quantity $\langle X_i X_j \rangle_c^a$. In order that we may calculate $\langle X_i X_j \rangle_c^a$, we introduce two kinds of chains, for example, "red" chains and "blue" chains. Later on we will associate red chains with SAW's with color index $\alpha=1$ and blue chains with SAW's with, for example, color index $\alpha=2$ that appear in the high-temperature expansion of the magnetic system described by (40) in the $n \rightarrow 0$ limit so that an analogy can be established between the two systems. Correspondingly, we define the following activities: η_i is the activity of a red chain end at site i , η'_i is the activity of a blue chain end, and κ_{ij} is the activity of a chain bond between nearest-neighbor sites i and j , regardless of the color of the chain. We also define the following chemical potentials: $\zeta'_i = \ln \eta'_i$, $\zeta_i = \ln \eta_i$, and $\lambda_{ij} = \ln \kappa_{ij}$. The grand canonical partition function is now given by

$$\hat{Z}'(\{\kappa_{ij}\}, \{\eta_i\}, \{\eta'_i\}) = \sum \exp \left(\sum_i \zeta'_i X'_i + \sum_i \zeta_i X_i + \sum_{\langle ij \rangle} \lambda_{ij} Y_{ij} \right), \quad (38)$$

where the sum is over all possible configurations and X'_i , X_i , and Y_{ij} are random variables defined below:

$$X'_i = \begin{cases} 1, & \text{if there is a blue chain end at } i \\ 0, & \text{otherwise.} \end{cases}$$

$$X_i = \begin{cases} 1, & \text{if there is a red chain end at } i \\ 0, & \text{otherwise.} \end{cases}$$

$$Y_{ij} = \begin{cases} 1, & \text{if there is a bond of any color between} \\ & \text{nearest-neighbor sites } i \text{ and } j \\ 0, & \text{otherwise.} \end{cases}$$

The form of (38) is self-explanatory [compare with (26)]. A possible configuration Γ_{ij} appearing in (38) is shown in Fig. 4. (The subscripts i and j indicate that the blue chain ends on i and j .) There are four red chains ($\alpha=1$). The remaining chain (the one ending on $S_i^{(2)}$ and $S_j^{(2)}$) should be thought of as a blue chain ($\alpha=2$). Let $\hat{\omega}_{ij}$ be the weight of this configuration. This weight includes η'_i and η'_j only linearly ($\eta'_i \eta'_j$ is the contribution to $\hat{\omega}$ due to the blue chain). Thus, $\partial \hat{\omega}_{ij} / \partial \eta'_i \partial \eta'_j$ is

independent of η'_i and η'_j . If Γ'_{ij} is another configuration with weight $\hat{\omega}'_{ij}$ so that there are more than one blue chain (and two blue chain ends are at i and j), then $\partial \hat{\omega}'_{ij} / \partial \eta'_i \partial \eta'_j$ depends on the activities of the blue chain ends not located at i and j . If we now take the limit $\{\eta'_i\} \rightarrow 0$, we notice that

$$\frac{\partial^2 \hat{\omega}'_{ij}}{\partial \eta'_i \partial \eta'_j} \rightarrow 0,$$

while $\partial^2 \hat{\omega}_{ij} / \partial \eta'_i \partial \eta'_j$, being independent of $\{\eta'_i\}$, remains finite. Thus, if one differentiates \hat{Z} in (38) with respect to η'_i and η'_j , and then sets all $\eta'_i = 0$, all configurations Γ'_{ij} with more than one blue chain disappear. The only remaining configurations are those Γ_{ij} which have only *one* blue chain with end points located at i and j . However, the weight of the blue chain ends $\eta'_i \eta'_j$ in these Γ_{ij} have been differentiated out. We also want to change this blue chain into a red chain. Therefore, we must multiply each configuration by $\eta_i \eta_j$. Thus, we obtain for $i \neq j$

$$\begin{aligned} \chi_{ij}^a &= \langle X_i X_j \rangle_c^a = \eta_i \eta_j \left. \frac{\partial \ln \hat{Z}'}{\partial \eta'_i \partial \eta'_j} \right|_{\{\eta'_i\} \rightarrow 0} \\ &= \left. \frac{\partial^2 \hat{W}'}{\partial \zeta'_i \partial \zeta'_j} \right|_{\{\eta'_i\} \rightarrow 0, \eta'_i \rightarrow \eta_i, \eta'_j \rightarrow \eta_j}, \end{aligned} \quad (39)$$

where $\hat{W}' = \ln \hat{Z}'(\{\kappa_{ij}\}, \{\eta_i\}, \{\eta'_i\})$ and $\{\eta'_i\}'$ means all η'_i except η'_i and η'_j , and $\zeta'_i = \ln \eta'_i$ as usual, and we have replaced $\langle X'_i X'_j \rangle_c$ by $\langle X_i X_j \rangle_c^a$.

We next wish to derive the magnetic analog of $\hat{\chi}_{ij}^a$. To do this, we introduce a transverse magnetic field, for example, in the 2 direction, so that the Hamiltonian of the magnetic system is now given by

$$\mathcal{H}' = \sum_{\langle ij \rangle} K_{ij} \vec{S}_i \cdot \vec{S}_j + \sum (H_i^{(1)} S_i^{(1)} + H_i^{(2)} S_i^{(2)}), \quad (40)$$

where we have introduced the superscripts one and two on the magnetic fields to indicate their directions. It can easily be checked that Z'_0 , the $n \rightarrow 0$ limit of the partition function for \mathcal{H}' given above, is related to Z' given in (38) via

$$\begin{aligned} Z'_0(\{K_{ij}\}, \{H_i^{(1)}\}, \{H_i^{(2)}\}) \\ = \left(\prod_{i=1}^N z'(H_i^{(1)}, H_i^{(2)}) \right) \hat{Z}'(\{\kappa_{ij}\}, \{\eta_i\}, \{\eta'_i\}), \end{aligned} \quad (41)$$

where

$$\begin{aligned} z'_i &= z'(H_i^{(1)}, H_i^{(2)}) = 1 + \frac{1}{2} [(H_i^{(1)})^2 + (H_i^{(2)})^2], \\ \eta_i &= H_i^{(1)} / (z'_i)^{1/2}, \\ \eta'_i &= H_i^{(2)} / (z'_i)^{1/2}, \\ \kappa_{ij} &= K_{ij} / (z'_i z'_j)^{1/2}. \end{aligned} \quad (42)$$

A configuration appearing in Z'_0 is shown in Fig. 4, where the chain (previously called a blue chain) ending on $S_i^{(2)}$ and $S_j^{(2)}$ should now be thought of as a chain ending on two blue crosses due to $H_i^{(2)}S_i^{(2)}$ and $H_j^{(2)}S_j^{(2)}$. The other four chains in Fig. 4 end on red crosses. Now, we identify a SAW with $\alpha=1$ with a red chain and a SAW with $\alpha=2$ with a blue chain, as was previously mentioned. Also, z'_i is the contribution of the site i uncovered by these SAW's. Again, the mapping in (42) is not a simple mapping (see comments in Sec. III).

The transverse correlation function $\langle S_i^{(2)}S_j^{(2)} \rangle_{c,n=0}$ for the original system (2) is given in terms of Z'_0 (41) by

$$\langle S_i^{(2)}S_j^{(2)} \rangle_{c,n=0} = \frac{\partial^2 W'_0}{\partial H_i^{(2)} \partial H_j^{(2)}} \Big|_{\{H_i^{(2)}\} \rightarrow 0}, \quad (43)$$

$$\begin{aligned} \hat{\chi}^a &= \frac{1}{N} \sum_{ij} \hat{\chi}_{ij}^a \\ &= \frac{1}{N} \sum_i \hat{\chi}_{ii} + \frac{H^2}{N} \sum_{i \neq j} \langle S_i^{(2)}S_j^{(2)} \rangle_{c,n=0} \\ &= Hz(1 + 3H^2/2)(m - H/z) + 2KH^2(1 + 3H^2/4)\epsilon \\ &\quad + H^3zK(C^{(1)} - C^{(2)}) + (H^4K^2/4)(C^{(11)} - C^{(22)} + 2C^{(23)} - 2C^{(12)}) + H^2z^2S_c^{(1)} + H^2\chi^{(2)} - H^2S_c^{(2)}, \end{aligned} \quad (45)$$

where

$$\begin{aligned} C^{(\alpha)} &= \frac{1}{N} \sum_i \left\langle S_i^{(1)} \sum_k S_i^{(\alpha)} S_k^{(\alpha)} \right\rangle_{c,n=0} \\ &= \frac{1}{N} \sum_{i,k} (\langle S_i^{(1)} S_j^{(\alpha)} S_k^{(\alpha)} \rangle_{n=0} \delta_{\alpha 1} - \langle S_i^{(1)} \rangle_{n=0} \langle S_i^{(\alpha)} S_k^{(\alpha)} \rangle_{n=0}), \\ C^{(\alpha\beta)} &= \frac{1}{N} \sum_{i,k,l} \langle S_i^{(\alpha)} S_k^{(\alpha)} S_l^{(\beta)} S_l^{(\beta)} \rangle_{c,n=0} \\ &= \frac{1}{N} \sum_{i,k,l} (\langle S_i^{(\alpha)} S_k^{(\alpha)} S_l^{(\beta)} S_l^{(\beta)} \rangle_{n=0} \delta_{\alpha\beta} - \langle S_i^{(\alpha)} S_k^{(\alpha)} \rangle_{n=0} \langle S_l^{(\beta)} S_l^{(\beta)} \rangle_{n=0}), \\ S_c^{(\alpha)} &= \frac{1}{N} \sum_i \langle (S_i^{(\alpha)})^2 \rangle_{c,n=0} \\ &= \frac{1}{N} \sum_i [\langle (S_i^{(1)})^2 \rangle_{n=0} - \langle S_i^{(1)} \rangle_{n=0}^2 \delta_{\alpha 1}], \\ \chi^{(2)} &= \frac{1}{N} \sum_{i,j} \langle S_i^{(2)} S_j^{(2)} \rangle_{c,n=0}, \end{aligned} \quad (45')$$

and where we have used the fact that

$$\begin{aligned} \frac{1}{N} \sum_{i,k} \langle S_i^{(1)} \vec{S}_i \cdot \vec{S}_k \rangle_{c,n=0} &= C^{(1)} - C^{(2)}, \\ \frac{1}{N} \sum_{i,k,l} \langle \vec{S}_i \cdot \vec{S}_k \vec{S}_l \cdot \vec{S}_l \rangle_{c,n=0} &= C^{(11)} - C^{(22)} + 2C^{(23)} - 2C^{(12)}. \end{aligned}$$

We also note that for $n=0$, $\langle (S_i^{(2)})^2 \rangle_{n=0} = \langle (S_i^{(1)})^2 \rangle_{n=0}$. For the homogeneous system that we are considering, the meaning of $C^{(\alpha)}$ and $C^{(\alpha\beta)}$ are as follows: $C^{(\alpha)}$ is the correlation of $S_0^{(1)}$ located at the, for example, origin with any α -colored bond rooted at the origin. Similarly, $C^{(\alpha\beta)}$ is the correlation of any α -colored

with

$$W'_0 = \ln Z'_0(\{K_{ij}\}, \{H_i^{(1)}\}, \{H_i^{(2)}\}).$$

Using the relation (B4), given in Appendix B, we find that

$$\hat{\chi}_{ij}^a = H_i^{(1)} H_j^{(1)} \langle S_i^{(2)} S_j^{(2)} \rangle_{c,n=0}, \quad i \neq j. \quad (44)$$

Thus, the two correlations are proportional. It is evident that (39) is *not* valid for $i=j$. However, for $i=j$, one knows physically that $\hat{\chi}_{ij}^a$ is nothing but $\hat{\chi}_{ii}$ and can be obtained from (34). One can now compute the long-wavelength limit of the transverse polymer susceptibility $\hat{\chi}^a$ (in analogy with the magnetic terminology) which is given by (for the homogeneous case)

bond and any β -colored bond both rooted at a common point, for example, the origin. The quantity $\chi^{(2)}$ is the transverse susceptibility of the magnetic system. We again observe that the transverse polymer susceptibility $\hat{\chi}^a$ is related to the transverse magnetic susceptibility $\chi^{(2)}$ in a complicated way described by (45) and is different from the relation given previously.^{9,11}

Finally, we consider the monomer-monomer correlation function. From the last equation of (28) and from the definitions (25), we note that the following operator

$$W_i = \frac{1}{2} \left(X_i + \sum_j Y_{ij} \right) \quad (46)$$

is the monomer operator:

$$W_i = \begin{cases} 1, & \text{if } i \text{ is occupied by a monomer} \\ 0, & \text{otherwise.} \end{cases} \quad (47)$$

The monomer-monomer correlation function $\langle W_i W_j \rangle_c$ is therefore given by

$$\begin{aligned} \langle W_i W_j \rangle_c &= \frac{1}{4} \left[\left\langle \left(X_i + \sum_k Y_{ik} \right) \left(X_j + \sum_l Y_{jl} \right) \right\rangle - \left\langle X_i + \sum_k Y_{ik} \right\rangle \left\langle X_j + \sum_l Y_{jl} \right\rangle \right] \\ &= \frac{1}{4} \left(\langle X_i X_j \rangle_c + \sum_{kl} \langle Y_{ik} Y_{jl} \rangle_c + \sum_l \langle X_i Y_{jl} \rangle_c + \sum_k \langle X_j Y_{ik} \rangle_c \right). \end{aligned} \quad (48)$$

Let us calculate $\langle Y_{ik} Y_{jl} \rangle_c$:

$$\begin{aligned} \langle Y_{ik} Y_{jl} \rangle_c &= \frac{\partial^2 \hat{W}}{\partial \lambda_{ik} \partial \lambda_{jl}} \\ &= K_{ik} \frac{\partial \hat{W}}{\partial K_{jl}} \delta_{ik,jl} + K_{ij} K_{kl} \frac{\partial^2 \hat{W}}{\partial K_{ik} \partial K_{jl}}, \end{aligned}$$

where $\delta_{ik,jl} = 1$ if the (ik) pair is identical with (jl) ; otherwise it is zero. Using (A4), we find that

$$\langle Y_{ik} Y_{jl} \rangle_c = K_{ik} \epsilon_{jl} \delta_{ik,jl} + K_{ik} K_{jl} \frac{\partial \epsilon_{ik}}{\partial K_{jl}}. \quad (49)$$

Using (A5) and (A7), we find that

$$\langle X_i Y_{jl} \rangle_c = \frac{H_i^2}{2} \sum_k \left(K_{ik} \epsilon_{jl} \delta_{ik,jl} + K_{ik} K_{jl} \frac{\partial \epsilon_{il}}{\partial K_{ik}} \right) + H_i z_i K_{jl} \frac{\partial \epsilon_{jl}}{\partial H_i} \quad (50)$$

and a similar expression for $\langle X_j Y_{ik} \rangle_c$. Using these expressions in (48), we finally obtain

$$\begin{aligned} 4 \langle W_i W_j \rangle_c &= \delta_{ij} \left[H_i z_i \left(1 + \frac{3}{2} H_i^2 \right) \left(m_i - \frac{H_i}{z_i} \right) + H_i^2 z_i \sum_k K_{ik} \epsilon_{ik} \right] + z_i z_j \left(H_j \sum_k K_{ik} \frac{\partial \epsilon_{ik}}{\partial H_j} + H_i \sum_l K_{jl} \frac{\partial \epsilon_{jl}}{\partial H_i} \right) \\ &\quad + z_i z_j \sum_{kl} \left(K_{ik} \epsilon_{jl} \delta_{ik,jl} + K_{ik} K_{jl} \frac{\partial \epsilon_{ik}}{\partial K_{jl}} \right) + H_i H_j z_i z_j \chi_{ij}. \end{aligned} \quad (51)$$

This is the full form of the monomer-monomer correlation function and is different from the expression (24b) (Ref. 11). We will complete our dictionary by giving the result for

$$\begin{aligned} \hat{C} &= \frac{1}{N} \sum_{i,j} \langle W_i W_j \rangle_c \\ &= \frac{1}{4} H z \left(1 + \frac{3 H^2}{2} \right) \left(m - \frac{H}{z} \right) + z (1 + H^2) K \epsilon + H z^2 K \frac{\partial \epsilon}{\partial H} + z^2 K^2 \frac{\partial \epsilon}{\partial K} + \frac{1}{4} H^2 z^2 \chi \end{aligned} \quad (52)$$

for the homogeneous system. It should be obvious that

$$\hat{C} = \frac{1}{N} \left\langle \left(\sum_i (W_i - \langle W_i \rangle) \right)^2 \right\rangle \geq 0.$$

One can easily check that (52) can also be derived

for the homogeneous system by noting the following identity which is evident from (48):

$$\hat{C} = \frac{1}{N} \left(\frac{1}{4} \frac{\partial^2 \hat{W}}{\partial \zeta^2} + \frac{\partial^2 \hat{W}}{\partial \lambda^2} + \frac{\partial^2 \hat{W}}{\partial \zeta \partial \lambda} \right). \quad (53)$$

Thus, we have established that the polymer

monomer-monomer correlation is given by $\langle W_i W_j \rangle_\xi$ and is very different from (24b). Moreover, $\hat{C} \geq 0$ even though the corresponding long-wavelength limit C [see the paragraph after (24)] of the magnetic system may not be positive.

As has been pointed out by des Cloizeaux,⁹ one is interested in the situation where $H \rightarrow 0$. In this limit, we observe that $\kappa \approx K$ and $\eta \approx H$, i.e., the corrections due to $z \approx 1$ are not important. However, the right thing to do is to take the limits of various expressions obtained above as $H \rightarrow 0$. For example, we must look at the limit of (37) as $H \rightarrow 0$ in order to calculate $\hat{\chi}$ as $H \rightarrow 0$. One can appreciate the effect of the observation that, for example, the chemical potential for the chain end is given by $\xi = \ln \eta$ and which ensures the non-negativity of $\hat{\chi}$ by neglecting the difference between η and H , i.e., assuming $\eta = H$:

$$\hat{\chi} = \frac{1}{N} \frac{\partial^2 \hat{W}}{\partial \xi^2} = \frac{1}{N} H \frac{\partial}{\partial H} \left(H \frac{\partial W_0}{\partial H} \right) = mH + \chi^2 H. \quad (54)$$

This shows clearly that even if χ becomes negative, the presence of the first term in (54) ensures that $\hat{\chi} \geq 0$. However, since there are corrections to η due to z , one must look at the full expression (37). It is conceivable that the correction due to z in κ and η may not be important for $H \rightarrow 0$ even in the field-theory version of the problem. In that case, (54) [or (37)] shows clearly that $\hat{\chi}$ will *not* be given merely by $\chi^2 H$, but by the full expression (54) [or (37)] and will always remain non-negative. Moreover, it is possible to calculate m and χ and other quantities of interest using field-theoretical methods and calculate $\hat{\chi}$ using (54), or to be more precise, using (37). But this will be valid only if one can show that the constrained-lattice model considered here is not very different from the field-theory version. However, it should again be emphasized that the connection between the two versions is *not* very clear, and also lies beyond the scope of the present work. It is certainly possible that one can use field theory to calculate $\hat{\chi}$, \hat{C} , etc., without any noticeable effect by using (37), (52), etc., respectively.

V. CONCLUSIONS

In order that the analysis can be carried out explicitly, we have only considered the *constrained* version of the magnetic system by putting an n -component classical spin of fixed length \sqrt{n} at each site of a *lattice*. As has been expected, we find that as $n \rightarrow 0$, there appears a correspondence between the magnetic system in a magnetic field in this limit and a grand canonical ensemble of polymer chains (SAW's) of varying

lengths. However, the correspondence is *not isomorphic*, as has been assumed previously. We find that the activities κ_{ij} and η_i of the corresponding polymer system are not simply K_{ij} and H_i , respectively, as has been reported by other authors: These variables are related to each other via (10). The peculiarities of these mappings break down the isomorphism of the correspondence between the magnetic system in the presence of a magnetic field in the $n \rightarrow 0$ limit and the polymer chains in a solution. Moreover, the polymer free energy \hat{W} differs from the magnetic free energy W_0 in this limit by an amount equal to the free energy of a system of independent n -component classical spins (i.e., $K_{ij} = 0$ or $K = 0$) in a magnetic field as $n \rightarrow 0$. This is exhibited in (32). Here z_i represents the partition function in $n \rightarrow 0$ limit of the spin \vec{S}_i in a magnetic field H_i in the $\alpha = 1$ direction.

We have expressed the polymer variables ϕ_p , ϕ_i , and ϕ_s in terms of m , the magnetization per particle and ϵ , the energy per particle of the magnetic system in the $n \rightarrow 0$ limit [see (18)]. We have also calculated the polymer correlation functions $\hat{\chi}_{ij}$, $\hat{\chi}_{ij}^a$, and \hat{C}_{ij} [see (34), (44), and (51)]. It is found that these quantities are *not* the same as χ_{ij} , $\chi_{ij}^{(2)}$, and C_{ij} , respectively, describing the magnetic system as proposed by other authors.^{9,11} The relations expressing $\hat{\chi}_{ij}$, $\hat{\chi}_{ij}^a$, and \hat{C}_{ij} in terms of magnetic correlation functions are highly involved and unfortunately do not make transparent the analogy between the two systems. It is hoped that the correct correspondence given here might be eventually useful in the clarification of the physics underlying this correspondence.

It will be established elsewhere¹⁴ that the susceptibility χ and the specific heat C of the magnetic system can indeed become *negative* for $n \leq 1$, that is, the magnetic free energy W_0 does not necessarily satisfy the convexity properties with respect to H and K . However, as has been established here, this disease does not afflict the polymer system since the polymer free energy \hat{W} satisfies the proper convexity properties with respect to the chemical potentials ξ and λ , i.e., $\hat{\chi}$ and \hat{C} are *non-negative*. This is because the roles of chemical potentials are played by ξ and λ [see (27)] and not by K and H .

Before we end, we would like to emphasize the following two points: (i) We have considered the lattice version of the magnetic system. It is conceivable that there are some differences between this and its continuum version considered by des Cloizeaux⁹ and Schäfer and Witten.¹¹ But, it is also possible that one can use the continuum version for $H \rightarrow 0$ without any noticeable difference. (ii) The analogy between the polymer sys-

tem and the magnetic system is shown only in the high-temperature phase, where the series expansion makes sense. However, there are reasons to believe that the analogy *works* even when the temperature of the magnetic system is below its critical value. This will be the subject matter of a future publication. It would be shown there that the magnetization m is not a monotonic function of the temperature for $n < 1$. Moreover, the susceptibility χ seems to be a positive quantity just below T_c but becomes negative at lower temperatures.

Note added in proof. Recently, Wheeler and Pfeuty¹⁶ have also reported the correct form of $Z_0(K, H)$ [see (7b)]. However, their interpretation of $Z_0(K, H)$ and its relation to the polymer problem is very different from the one presented here: According to Wheeler and Pfeuty,¹⁶ the weight of any SAW of length $l \geq 1$ is $H^2 K^l$, while the weight of a SAW of zero length ($l=0$) is $H^2/2$ and not H^2 . They have given some plausibility arguments to justify this distinction between the two kinds of SAW's. We have insisted in the present work that the weight of any SAW be given by $\eta^2 \kappa^l$. This has required us to focus on SAW's of only nonzero lengths. However, it is possible to define another mapping between the magnetic variables K and H and the polymer variables $\bar{\kappa}$ and $\bar{\eta}$ [we have used bars to denote a different mapping than the one given in (10b)] that enables one to consider SAW's of all lengths including zero lengths with weight $\bar{\eta}^2 \bar{\kappa}^l$ ($l \geq 0$), as has been reported elsewhere.¹⁷

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APPENDIX A: SAW'S WITH COLOR INDEX $\alpha = 1$

We note from (10a) that

$$z_i = 1 + H^2/2 = \frac{1}{1 - \eta_i^2/2}. \quad (\text{A1})$$

$$\begin{aligned} \frac{\partial^2}{\partial \eta_i \partial \eta_j} = & \delta_{ij} \left(\frac{3}{2} H_i z_i^2 \frac{\partial}{\partial H_i} + \frac{1}{2} z_i (1 + H_i^2) \sum_k K_{ik} \frac{\partial}{\partial K_{ik}} \right) + \frac{1}{2} H_i \sqrt{z_i} z_j^{3/2} \sum_k K_{ik} \frac{\partial^2}{\partial H_j \partial K_{ik}} + \frac{1}{2} H_j \sqrt{z_j} z_i^{3/2} \sum_k K_{jk} \frac{\partial^2}{\partial H_i \partial K_{jk}} \\ & + \frac{1}{4} H_i H_j \sqrt{z_i z_j} \sum_{k,l} \left(K_{ik} \delta_{ik,jl} \frac{\partial}{\partial K_{jl}} + K_{ik} K_{jl} \frac{\partial^2}{\partial K_{ik} \partial K_{jl}} \right) + z_i^{3/2} z_j^{3/2} \frac{\partial^2}{\partial H_i \partial H_j}. \end{aligned} \quad (\text{A9})$$

One obtains (34) by using (A7) and (A9) in (31). The following relations are easily proven for the homogeneous system:

Thus,

$$H_i = \eta_i / (1 - \eta_i^2/2)^{1/2}, \quad (\text{A2})$$

$$K_{ij} = \kappa_{ij} / [(1 + \eta_i^2/2)]^{1/2} [(1 + \eta_j^2/2)]^{1/2}.$$

From this we note that

$$\begin{aligned} \partial H_i / \partial \eta_i &= z_i^{3/2}, \\ \partial H_i / \partial \kappa_{ij} &= 0, \end{aligned} \quad (\text{A3})$$

$$\partial K_{ij} / \partial \eta_i = \frac{1}{2} K_{ij} H_i \sqrt{z_i},$$

$$\partial K_{ij} / \partial \kappa_{ij} = \sqrt{z_i z_j}.$$

We will now express the differential operators $\partial / \partial \kappa_{ij}$ and $\partial / \partial \eta_i$ in terms of $\partial / \partial K_{ij}$ and $\partial / \partial H_i$. Since

$$\frac{\partial}{\partial \kappa_{ij}} = \frac{\partial K_{ij}}{\partial \kappa_{ij}} \frac{\partial}{\partial K_{ij}} = \sqrt{z_i z_j} \frac{\partial}{\partial K_{ij}}, \quad (\text{A4})$$

we find that

$$\kappa_{ij} \frac{\partial}{\partial \kappa_{ij}} = K_{ij} \frac{\partial}{\partial K_{ij}}. \quad (\text{A5})$$

For $\partial / \partial \eta_i$ we have

$$\frac{\partial}{\partial \eta_i} = \sum_k \frac{\partial K_{ik}}{\partial \eta_i} \frac{\partial}{\partial K_{ik}} + \frac{\partial H_i}{\partial \eta_i} \frac{\partial}{\partial H_i},$$

where the sum over k is over the q nearest-neighbor sites k of i . Using (A3) we find that

$$\frac{\partial}{\partial \eta_i} = \frac{1}{2} H_i \sqrt{z_i} \sum_k K_{ik} \frac{\partial}{\partial K_{ik}} + z_i^{3/2} \frac{\partial}{\partial H_i}, \quad (\text{A6})$$

and

$$\frac{\partial}{\partial \xi_i} = \eta_i \frac{\partial}{\partial \eta_i} = \frac{H_i^2}{2} \sum_k K_{ik} \frac{\partial}{\partial K_{ik}} + H_i z_i \frac{\partial}{\partial H_i}. \quad (\text{A7})$$

Moreover, since $\hat{W} = W_0 - \sum_i \ln z_i$,

$$\frac{\partial \hat{W}}{\partial H_i} = \frac{\partial W_0}{\partial H_i} - \frac{H_i}{z_i}, \quad (\text{A8})$$

$$\frac{\partial \hat{W}}{\partial K_{ij}} = \frac{\partial W_0}{\partial K_{ij}}.$$

Now, it is easily seen that

$$\begin{aligned}
\frac{1}{N} \sum_{i,k} K_{ik} \epsilon_{ik} &= \frac{2}{N} \sum_{\langle ik \rangle} K_{ik} \epsilon_{ik} = 2K\epsilon, \\
\frac{1}{N} \sum_{ij,k} \frac{\partial \epsilon_{ik}}{\partial H_j} &= \frac{2}{N} \sum_{\langle ik \rangle, j} \frac{\partial \epsilon_{ik}}{\partial H_j} = 2 \frac{\partial \epsilon}{\partial H}, \\
\frac{1}{N} \sum_{ijk} K_{ik} \frac{\partial}{\partial K_{jl}} \delta_{ik,jl} &= \frac{4}{N} \sum_{\langle ik \rangle} \sum_{\langle jl \rangle} K_{ik} \frac{\partial}{\partial K_{jl}} \delta_{ik,jl} = 4K\epsilon, \\
\frac{1}{N} \sum_{ijkl} K_{ik} K_{jl} \frac{\partial^2}{\partial K_{ik} \partial K_{jl}} &= \frac{4}{N} \sum_{\langle ik \rangle, \langle jl \rangle} K_{ik} K_{jl} \frac{\partial^2}{\partial K_{ik} \partial K_{jl}} = 4K^2 \frac{\partial \epsilon}{\partial K},
\end{aligned} \tag{A10}$$

where $\sum_{\langle ik \rangle}$ is a sum over distinct pairs $\langle ik \rangle$ of sites. Using these relations in (36), one obtains the final expression (37) for $\hat{\chi}$.

APPENDIX B: SAW'S WITH COLOR INDEX $\alpha = 1$ AND 2

We notice from (42) that

$$1 - (\eta_i^2 + \eta'_i{}^2)/2 = \frac{1}{1 + (H_i^{(1)2} + H_i^{(2)2})/2}. \tag{B1}$$

Using this relation to express $H_i^{(1)}$, $H_i^{(2)}$, and K_{ij} in terms of κ_{ij} , η_i , and η'_i , we find that

$$\begin{aligned}
\partial H_i^{(1)}/\partial \eta'_i &= \frac{1}{2} H_i^{(1)} H_i^{(2)} (z'_i)^{1/2}, \\
\partial H_i^{(2)}/\partial \eta'_i &= z_i'^{3/2}/z_i, \\
\partial K_{ij}/\partial \eta'_i &= \frac{1}{2} K_{ij} H_i^{(2)} (z'_i)^{1/2}.
\end{aligned} \tag{B2}$$

Using these derivatives, we write $\partial/\partial \eta'_i$ in the following form:

$$\begin{aligned}
\partial/\partial \eta'_i &= \sum_k \frac{\partial K_{ik}}{\partial \eta'_i} \frac{\partial}{\partial K_{ik}} + \frac{\partial H_i^{(1)}}{\partial \eta'_i} \frac{\partial}{\partial H_i^{(1)}} + \frac{\partial H_i^{(2)}}{\partial \eta'_i} \frac{\partial}{\partial H_i^{(2)}} \\
&= \frac{1}{2} H_i^{(2)} (z'_i)^{1/2} \sum_k K_{ik} \frac{\partial}{\partial K_{ik}} + \frac{1}{2} H_i^{(1)} H_i^{(2)} (z'_i)^{1/2} \frac{\partial}{\partial H_i^{(1)}} \\
&\quad + \frac{z_i'^{3/2}}{z_i} \frac{\partial}{\partial H_i^{(2)}}.
\end{aligned} \tag{B3}$$

Thus for $i \neq j$

$$\frac{\partial^2}{\partial \eta'_i \partial \eta'_j} \Big|_{H_i^{(2)} \rightarrow 0} = \sqrt{z_i z_j} \frac{\partial^2}{\partial H_i^{(2)} \partial H_j^{(2)}} \Big|_{H_i^{(2)} \rightarrow 0}. \tag{B4}$$

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