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Polymerization on the Diamond Hierarchical Lattice: The Migdal-Kadanoff Renormalization-Group Scheme

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Polymerization on the diamond hierarchical lattice: The Migdal-Kadanoff renormalization-group scheme

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The thermodynamics of the equilibrium polymerization model (grand-canonical ensemble of self-avoiding walks) in two dimensions is worked out by means of the Migdal-Kadanoff renormalization-group technique. This method involves renormalization-group flows in an eight-dimensional parameter space. At the critical point the number of relevant fields (positive exponents) is four. The leading exponent value differs by less than 1% from the (presumed) exact value. The results are exact for the polymerization problem defined on the diamond hierarchical lattice. Some results are peculiar to this lattice and are not expected to hold for Bravais lattices. For instance, the polymerized phase (infinite polymerization index) is dilute (zero density of chemical bonds).

I. INTRODUCTION

The equilibrium polymerization process in a grand-canonical ensemble of self-avoiding walks is solved exactly on an extremely inhomogeneous lattice, the diamond hierarchical lattice. Previous exact solutions of the polymerization process were obtained for the one-dimensional and for the Bethe lattices[1] and for the equivalent-neighbor lattice.[2] Unlike these and Bravais lattices, where all vertices are equivalent to each other, the vertices of the diamond hierarchical lattice can be classified[3] in an infinity of equivalence classes, with each class containing a vanishingly small fraction of all vertices. Hierarchical lattices are in general inhomogeneous, and this feature makes them crude models for disordered systems.[4] Hierarchical structures have been used to model the dynamics of glassy materials,[5] spin glasses in equilibrium,[6] and the backbone of the percolating cluster.[7] It is our hope that this study will provide insights into a subject of considerable current interest:[8] polymers in an inhomogeneous medium (such as the percolating cluster).

The recursion equations which exactly solve a statistical model on the diamond hierarchical lattice constitute the Migdal-Kadanoff renormalization-group approximation[9] for the same model defined now on a two-dimensional (2D) Bravais lattice, as first observed by Berker and Ostlund.[10] The drastic geometric differences between hierarchical and Bravais lattices cause important differences[11] in the thermodynamics of a given model when defined on these lattices. Other features, however, do not differ qualitatively. For example, the phase diagram for the polymerization problem on the diamond hierarchical lattice is the same as the expected phase diagram for regular lattices. We develop in this paper a computational framework for quantities such as the number of polymers, length of polymers, and their fluctuations, which can be used in the whole parameter space. By contrast, previous studies, such as ϵ expansion,[12] scaling theory,[13] and conformal invariance for two dimensions[14] have focused on the thermodynamic behavior in the vicinity of the polymerization critical point.

The diamond hierarchical lattice can accommodate no Hamilton walk (a self-avoiding walk covering a unit fraction of all vertices). In fact, the longest single self-avoiding walk occupies a vanishingly small fraction of all vertices in the thermodynamic limit. The maximum coverage (largest possible fraction of vertices on polymers) is achieved only with a nonzero density of polymers (macroscopically large numbers of polymers). The polymerization index (average number of bonds per polymer) lies in this case between 2 and 4; i.e., the maximum coverage is achieved mainly with small polymers. These features, unexpected from our experience with homogeneous lattices, which can accommodate Hamilton walks, are rooted in the geometry of the diamond hierarchical lattice. For the latter lattice all long self-avoiding paths are funneled through some high-coordinated vertices whose occupation by a polymer blocks all other paths through these vertices. We expect this *bottleneck* effect to also hold on the hierarchical lattice which serves as a model for the percolating backbone.[7] In the polymerized phase the polymerization index (average size of a polymer), as expected, is infinite. However, unlike expectations based on homogeneous lattices such as the one-dimensional (1D) and the equivalent-neighbor lattices, the bond density is zero in the thermodynamic limit.

Close to the critical polymerization point, the critical amplitude of the singular part of the free energy is equal to a constant plus an oscillatory contribution. Such oscillations are rooted in the self-similar character of the lattice, and have been studied before for other models.[15] Unlike those previous studies we find the oscillations to

have a relatively large amplitude.

The remainder of this paper is organized as follows. In Sec. II the salient geometric features of the diamond lattice which influence the statistics of self-avoiding walks are described. In Sec. III the recursion equations are derived after mapping the polymerization process into an Ising-Potts model (equivalent to the Hillhorst model[16]). Numerical results for the dependence of the number of bonds, the number of polymers, etc., on the model fields (two fugacities) are also presented here. The singular behavior of the thermodynamic quantities in the vicinity of the polymerized phase is discussed in Sec. IV. Section V contains our conclusions.

II. GEOMETRY OF THE DIAMOND LATTICE AND SELF-AVOIDING WALKS

The diamond hierarchical lattice is constructed iteratively as shown in Fig. 1. Four bonds of order zero are assembled into a diamond (or bond of order 1). Four diamonds are then put together into a diamond of diamonds (or bond of order 2). This process is continued indefinitely.

By construction this lattice is self-similar. There exists a "volume" scale, the so-called aggregation number,[3] which equals 4. In renormalization-group studies of models on d-dimensional Bravais lattices the aggregation number is written as l^d, with $l=d=2$ in this case, and l is the "length" scale. This scale is responsible for the modulation by oscillations of the power-law dependence of thermodynamic quantities close to criticality. This feature is peculiar to nonrandom hierarchical (fractal) structures. It does not occur for translationally invariant structures which do not possess a single scale l, e.g., for a one-dimensional lattice exact decimations can be performed with any integer $l \geq 2$, while for the diamond lattice exact decimations can be performed only with l equal to an integer power of 2: $2,4,8,\ldots$. A numerical study of the oscillations can be found in Sec. IV.

The diamond hierarchical lattice is an inhomogeneous structure. The primitive bonds can be divided into equivalence classes.[3] Each class is determined by a symmetry operation which maps the left branch into the right branch of the diamond shown in Fig. 1. In a lattice with 4^n primitive bonds there are 2^n equivalence classes, with each class containing 2^n primitive bonds. Hence in the thermodynamic limit, $n \to \infty$, the fraction of equivalent bonds out of the total number of bonds is vanishingly small, $2^{-n} \to 0$. By contrast, for a translationally invariant lattice (e.g., the square lattice) all bonds, except the surface ones which constitute a vanishingly small fraction of the total, are equivalent. Not all hierarchical lattices are as inhomogeneous as the diamond one. For example, in the case of the Cayley tree (Bethe lattice with surface) each equivalence class possesses a finite fraction of the total number of bonds. In this sense the diamond lattice is an *extremely* inhomogeneous structure, a property it shares with multifractals.[7]

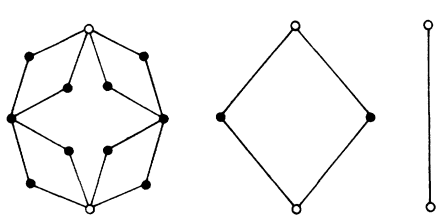

FIG. 1. Construction of the diamond hierarchical lattice.

We now focus on self-avoiding walks grown on the diamond lattice. First we consider a single walk covering the largest possible number of bonds. On the nth generation lattice with 4^n primitive bonds, this walk covers $2^{(n+1)}-1$ primitive bonds; i.e., it covers a vanishingly small fraction of all bonds: $2^{-n} \to 0$ as $n \to \infty$. This situation sets aside the diamond hierarchical lattice from Bravais lattices where Hamilton walks can be accommodated. It is rooted in the *bottleneck* effect: in order to cover as many primitive bonds as possible the polymer grows in a single direction (the vertical direction of Fig. 1). In fact, as it will be shown in Sec. IV, that the fractal dimension of this walk is 1. This is also the case with the hierarchical lattice which serves as a model for the percolating backbone.[7]

We next determine the maximum coverage of the diamond lattice with many self-avoiding walks. The vertices of coordination numbers $4,8,16,\ldots$, are all internal sites on polymers. Indeed, if this is not true, i.e., such a vertex is either the end of a polymer or is empty (not on any polymer), then we could draw from this vertex one or two more bonds, respectively. This means that we did not start with a maximum coverage configuration. Since for each vertex of coordination number larger than 2 there are two bonds, the fraction of bonds out of the total 4^n lattice edges is $b=2(S-S_2)/4^n$, where $S=\frac{2}{3}(4^n-1)$ is the total number of vertices and $S_2=\frac{1}{2}4^n$ is the number of vertices of coordination number 2. In the thermodynamic limit $n \to \infty$, the largest value for the fraction of bonds on polymers is $b=\frac{1}{3}$.

To determine the number of polymers for a maximum coverage configuration, we note that

$$b+p+\Phi_0=\tfrac{2}{3} , \tag{1}$$

where b,p, and Φ_0 are, respectively, the density of bonds on polymers, the density of polymers, and the density of uncovered sites (sites not on polymers). The densities are obtained by dividing the corresponding numbers by the number of lattice edges 4^n. Since $b=\frac{1}{3}$ it follows that

$$p+\Phi_0=\tfrac{1}{3} . \tag{2}$$

On the other hand, vertices of coordination number 2 either are not on polymers (Φ_0), or are at ends of polymers ($2p$), or are internal sites on polymers (x). Then

$$\Phi_0+2p+x=\tfrac{1}{2} , \tag{3}$$

where x is the ratio of the number of internal polymer sites of coordination number 2 to 4^n and $\frac{1}{2}$ is the ratio of the total number of vertices of coordination number 2 to 4^n. After subtracting Eq. (2) from Eq. (3) we find

$$p+x=\tfrac{1}{6}\ . \tag{4}$$

Since $x \geq 0$, the largest $p=\frac{1}{6}$ and this maximum coverage is achieved with trimers (polymerization index $b/p=2$ bonds per polymer). To compute the smallest p compatible with maximum coverage, we note that this situation arises when the polymers are as long as possible. We find a recursion equation: $P_{n+1}=4P_n+1$, $P_2=1$, where P_n is the number of polymers on the nth generation lattice. By iterating this equation we find, in the limit $n\rightarrow\infty$, $p=\frac{1}{12}$, which corresponds to the polymerization index $b/p=4$.

To summarize, the maximum coverage configurations have $b=\frac{1}{3}$ and $\frac{1}{12}\leq p\leq\frac{1}{6}$. We have used these results to check the correctness of our numerical scheme (Sec. III) in this limit. The fact that a macroscopically large number of polymers $p\geq\frac{1}{12}>0$ is needed to achieve maximum coverage sets aside the diamond hierarchical lattice from Bravais lattices where Hamilton walks are possible and thus maximum coverage can be achieved even with a single walk ($p=0$). It also suggests, but does not prove, that the polymerized phase (polymerization index $b/p=\infty$), where $p=0$, is dilute ($b=0$). This result is proved in Sec. IV by using the recursion equations.

III. SOLUTION OF THE POLYMERIZATION MODEL

A. Recursion equations

The partition function of the grand-canonical ensemble of self-avoiding walks (polymerization model) is

$$Z=\sum k^B\pi^P\ . \tag{5}$$

The summation is over all possible graphs of self-avoiding walks that can be drawn on the edges of the diamond hierarchical lattice. B is the total number of bonds on polymers and P is the total number of polymers. The two positive parameters k and π are fugacities controlling, respectively, the amount of material polymerized and the number of polymers. In the language of the chemical reaction theory k is the activity for chain propagation and $\pi=\eta^2$, where η is the activity for the initiation or termination of a chain propagation.

Our solution of the model is based on its equivalence to a discrete version[16] of the n-vector model with $n\rightarrow 0$.[17] This discrete vector model can also be written as an Ising-Potts model:[2] at each lattice vertex i there is an Ising spin $S_i=\pm 1$ and a Potts spin $\sigma_i=1,2,\ldots,q$. The Hamiltonian is

$$-H/k_BT=qJ\sum_{\langle i,j\rangle}\delta(\sigma_i,\sigma_j)S_iS_j+\sqrt{q}\,H\sum_i\delta(\sigma_i,1)\ , \tag{6}$$

where δ is the Kronecker delta. The partition function Z_0 of this model with $q\rightarrow 0$, the analog of $n\rightarrow 0$, is related to the polymer problem partition function[18] Z:

$$Z=Z_0[2q(1+\tfrac{1}{2}H^2)]^{-N}\ , \tag{7}$$

where N is the number of lattice vertices. The fugacities k and π depend on the magnetic problem parameters J and H as follows:[18]

$$\begin{aligned} k&=J/(1+\tfrac{1}{2}H^2)\ ,\\ \pi&=H^2/(1+\tfrac{1}{2}H^2)\ . \end{aligned} \tag{8}$$

The Boltzmann weight associated with a primitive (zeroth-order) bond ij is

$$\begin{aligned} Z_{ij}&=\exp[qJ\delta(\sigma_i,\sigma_j)S_iS_j]\\ &\approx 1+qJ\delta(\sigma_i,\sigma_j)S_iS_j+\tfrac{1}{2}q^2J^2\delta(\sigma_i,\sigma_j) \end{aligned} \tag{9}$$

and the Boltzmann weight associated with a vertex k is

$$\begin{aligned} Z_k&=\exp[\sqrt{q}\,H\delta(\sigma_k,1)S_k]\\ &\approx 1+\sqrt{q}\,H\delta(\sigma_k,1)S_k+\tfrac{1}{2}qH^2\delta(\sigma_k,1)\ . \end{aligned} \tag{10}$$

Since we are eventually interested in the $q\rightarrow 0$, higher-order terms are not exhibited in Eqs. (9) and (10) as they make no contribution in that limit. The Migdal-Kadanoff renormalization group for d dimensions and with a linear scale factor $l=2$ is

$$Z'_{ij}=\left[\sum_{S_k,\sigma_k}Z_{ik}Z_kZ_{kj}\right]^{2^{d-1}}\ , \tag{11}$$

where Z_{ik} is the Boltzmann weight for an nth order bond, and Z'_{ij} is the Boltzmann weight for an $(n+1)$th-order bond. The single site weight Z_k does not renormalize. For $d=1$ and $d=2$, Eq. (11) provides the exact solution for the one-dimensional lattice and for the diamond hierarchical lattice of Fig. 1, respectively. Though only two parameters J and H determine the polymer problem studied here, the recursion equation (11) generates six more parameters. The Boltzmann weight for an nth order bond, $n\geq 1$, is

$$\begin{aligned} Z_{ij}=&1+\tfrac{1}{2}q^{1/2}h[\delta(\sigma_i,1)S_i+\delta(\sigma_j,1)S_j]+qJ\delta(\sigma_i,\sigma_j)S_iS_j+\tfrac{1}{2}qL[\delta(\sigma_i,1)+\delta(\sigma_j,1)]\\ &+qD\delta(\sigma_i,1)\delta(\sigma_j,1)S_iS_j+\tfrac{1}{2}q^{3/2}M\delta(\sigma_i,1)\delta(\sigma_j,1)(S_i+S_j)+q^2K\delta(\sigma_i,1)\delta(\sigma_j,1)+q^2R\delta(\sigma_i,\sigma_j)\ . \end{aligned} \tag{12}$$

The field h appearing above creates a magnetic field at each lattice vertex proportional to the vertex coordination number. It must be distinguished from H which is a uniform field.

We first perform the decimation involved in the right-hand side of Eq. (11) and find

$$\begin{aligned} \sum_{S_k,\sigma_k}Z_{ik}Z_kZ_{kj}=&2qA\{1+\tfrac{1}{2}q^{1/2}\tilde{h}[\delta(\sigma_i,1)S_i+\delta(\sigma_j,1)S_j]+q\tilde{J}\delta(\sigma_i,\sigma_j)S_iS_j+\tfrac{1}{2}q\tilde{L}[\delta(\sigma_i,1)+\delta(\sigma_j,1)]\\ &+q\tilde{D}\delta(\sigma_i,1)\delta(\sigma_j,1)S_iS_j+\tfrac{1}{2}q^{3/2}\tilde{M}\delta(\sigma_i,1)\delta(\sigma_j,1)(S_i+S_j)+q^2\tilde{K}\delta(\sigma_i,1)\delta(\sigma_j,1)+q^2\tilde{R}\delta(\sigma_i,\sigma_j)\}\ , \end{aligned} \tag{13}$$

where

$$A=1+\tfrac{1}{2}H^2+hH+L+\tfrac{1}{4}h^2 ,$$

$$\tilde{h}=[(1+\tfrac{1}{2}H^2)h+2JH+2DH+M+\tfrac{1}{2}Hh^2+Jh+\tfrac{1}{2}Lh+Dh]/A ,$$

$$\tilde{J}=J^2/A ,$$

$$\tilde{L}=[(1+\tfrac{1}{2}H^2)L+MH+2K+\tfrac{1}{2}LHh+\tfrac{1}{2}Mh+\tfrac{1}{2}L^2]/A , \tag{14}$$

$$\tilde{D}=[(1+\tfrac{1}{2}H^2)\tfrac{1}{4}h^2+DHh+JHh+\tfrac{1}{2}Mh+2JD+D^2]/A ,$$

$$\tilde{M}=[(1+\tfrac{1}{2}H^2)\tfrac{1}{2}Lh+\tfrac{1}{2}MHh+Kh+JLH+JM+LDH+\tfrac{1}{2}LM+DM]/A ,$$

$$\tilde{K}=[(1+\tfrac{1}{2}H^2)\tfrac{1}{4}L^2+\tfrac{1}{2}LMH+LK+\tfrac{1}{4}M^2]/A ,$$

$$\tilde{R}=0 .$$

Since for $d=1$ the power in the right-hand side of Eq. (11) is 1, Eq. (14) provides an exact renormalization-group solution of the polymerization problem. The polymerization free energy per vertex $f=(\ln Z)/N$ is

$$f=\tfrac{1}{2}\sum_{n=0}^{\infty} C_n/2^n ,$$

where (15)

$$C_n=\ln[A_n/(1+\tfrac{1}{2}H^2)] .$$

We verified the correctness of Eqs. (14) and (15) and the accuracy of our numerics, by comparing the free energy obtained from (15) to the exact closed formula for 1D polymerization

$$f=\ln\{\tfrac{1}{2}(k+1)+[\tfrac{1}{4}(k-1)^2+k\pi]^{1/2}\} ,$$

where k and π are determined by J and H according to Eq. (8).

To obtain the recursion equations for the diamond hierarchical lattice we have to square Eq. (13) since the power on the right-hand side of Eq. (11) is two for $d=2$. We find

$$\begin{aligned} h'&=2\tilde{h} ,\\ J'&=2\tilde{J} ,\\ L'&=2\tilde{L}+\tfrac{1}{2}\tilde{h}^2 ,\\ D'&=2\tilde{D}+\tfrac{1}{2}\tilde{h}^2 ,\\ M'&=2\tilde{M}+2\tilde{J}\tilde{h}+2\tilde{D}\tilde{h}+\tilde{L}\tilde{h} ,\\ K'&=2\tilde{K}+\tilde{M}\tilde{h}+2\tilde{J}\tilde{D}+\tfrac{1}{2}\tilde{L}^2+\tilde{D}^2 ,\\ R'&=2\tilde{R}+\tilde{J}^2 . \end{aligned} \tag{16}$$

The polymerization free energy per primitive bond is

$$f=\tfrac{1}{4}\sum_{n=0}^{\infty} C_n/4^n ,$$

where (17)

$$C_n=2\ln[A_n/(1+\tfrac{1}{2}H^2)] .$$

B. Numerics

For given values of the fugacities k and π the free energy is computed as follows. First from Eq. (8) we determined the values of J and H. By comparing Eqs. (9) and (12) we find that the starting values of the other six fields are $h=L=D=M=K=0$ and $R=\tfrac{1}{2}J^2$. The free energy is then obtained from Eq. (17) by iterating Eqs. (14) and (16). The summation on the right-hand side of Eq. (17) is stopped after n terms if the $(n+1)$th term is less than 10^{-14}.

The derivatives of f with respect to $\ln k$ and $\ln\pi$ give the fraction of bonds on polymers to the total number of lattice bonds (denoted by b) and the ratio of the number of polymers to the total number of lattice bonds (denoted by p). The derivatives of b and p with respect to $\ln k$ and $\ln\pi$ determine the fluctuations of these quantities:

$$\begin{aligned} b&=\frac{\delta f}{\delta \ln k} , \quad p=\frac{\delta f}{\delta \ln\pi} ,\\ \mathcal{N}\langle \delta b^2\rangle&=\frac{\delta b}{\delta \ln k} ,\\ \mathcal{N}\langle \delta p^2\rangle&=\frac{\delta p}{\delta \ln\pi} , \quad \mathcal{N}\langle \delta b\,\delta p\rangle=\frac{\delta b}{\delta \ln\pi} , \end{aligned} \tag{18}$$

where $\mathcal{N}$ is the number of lattice edges (to be distinguished from N the number of lattice vertices). These quantities were computed by numerically differentiating f. The following inequalities constitute checks on the validity of the results:

$$f\ge 0, \quad b\ge 0, \quad p\ge 0, \quad \langle \delta b^2\rangle \ge 0 ,$$

$$\langle \delta b^2\rangle\langle \delta p^2\rangle \ge \langle \delta b\,\delta p\rangle^2 .$$

Figures 2–7 exhibit a few results concerning the dependence of various thermodynamic quantities on the two fugacities. In Figs. 2 and 3 we show the dependence of b and p on k for a few fixed values of π. For the small-

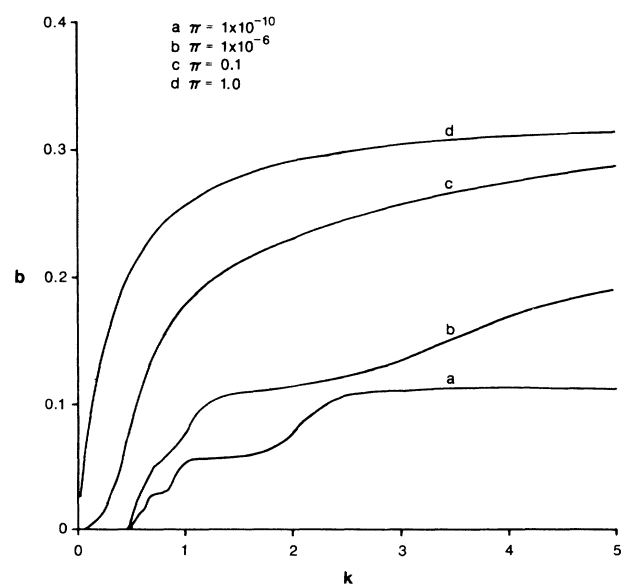

FIG. 2. Variation of b with k for the following π values: 10^{-10}, 10^{-6}, 10^{-1}, and 1.

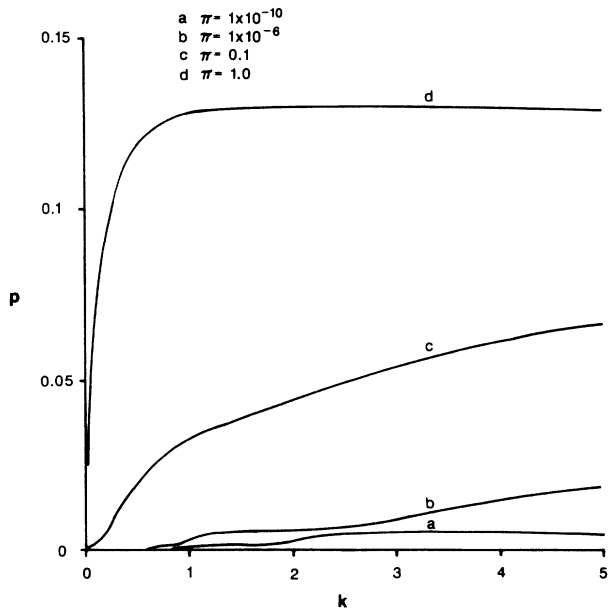

FIG. 3. Variation of p with k for the following π values: 10^{-10}, 10^{-6}, 10^{-1}, and 1.

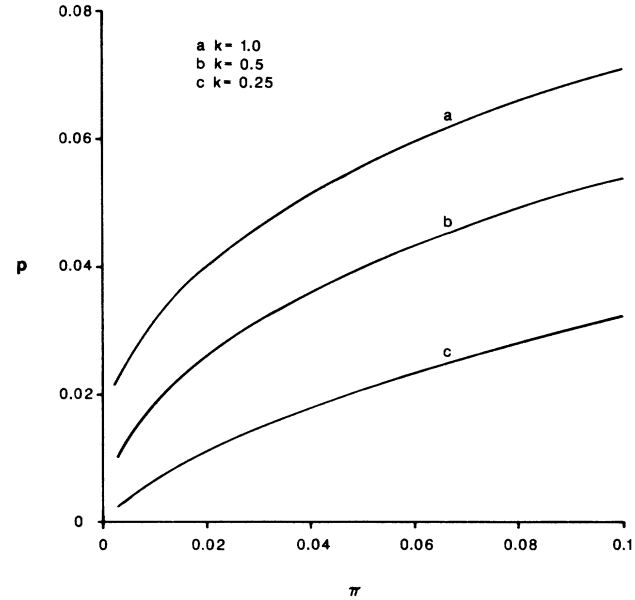

FIG. 5. Variation of p with π for the following k values: 0.25, 0.5, and 1.

er π some structure develops, which is tied to oscillations peculiar to hierarchical models (see Sec. IV below). The dependence of b and p on π for three fixed values of k (below, at, and above the critical $k_c = \frac{1}{2}$) is shown in Figs. 4 and 5. As $\pi \to 0$, b and p tend to zero for all k. In Fig. 6 we show the polymerization index (average size of a polymer, b/p) as a function of k for a fixed small value of π. The sharp maximum occurs at $k \approx k_c = \frac{1}{2}$. In the limit $\pi \to 0$, for $k > k_c$, we expect $b/p \approx O(1/\ln\pi) \to \infty$ (see Sec. IV, below). The fluctuation of p is shown in Fig. 7 as a function of k for a fixed value of π. The positivity of this quantity is ensured in our computation by the fact that the Migdal-Kadanoff scheme is *realizable.*[10]

IV. SINGULAR BEHAVIOR

In the two-dimensional subspace determined by J and H, $R = \frac{1}{2}J^2$, $h = L = D = M = K = 0$, which corresponds to the polymerization problem defined in Eq. (5), we find

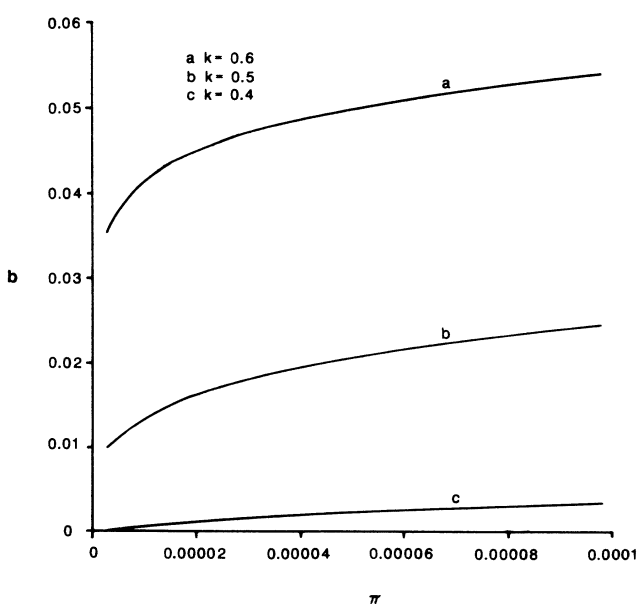

FIG. 4. Variation of b with π for the following k values: 0.4, 0.5, and 0.6.

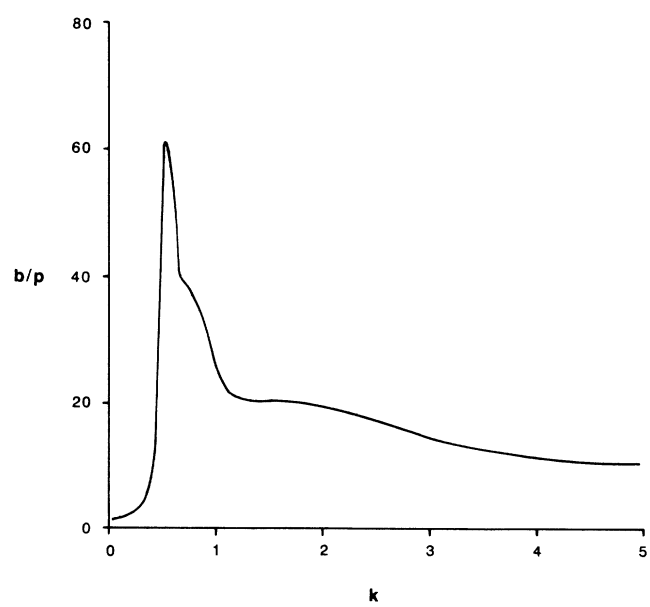

FIG. 6. Variation of the polymer index (b/p) with k for $\pi = 10^{-6}$.

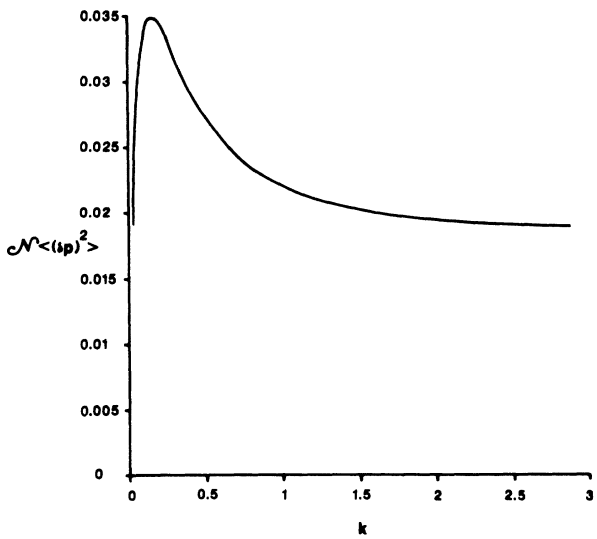

FIG. 7. Variation of the p fluctuation $\mathcal{N}\langle\delta p^2\rangle$ with k for $\pi=1$.

an unstable fixed point at $J=\frac{1}{2}$ and $H=0$ (or $k=\frac{1}{2}$ and $\pi=0$). The recursion equations for $H=0$ are

$$J'=2J^2 \text{ and } R'=J^4 \ . \tag{19}$$

The field R does not affect the free energy in any way (it is redundant[19]) and can be ignored. Linearizing the recursion equation at the fixed point $J=\frac{1}{2}$ we find the thermal eigenvalue $\lambda_T=2$ and then the thermal exponent $y_T=\ln\lambda_T/\ln 2=1$. This exponent is the fractal dimension[20] of the infinite self-avoiding walk. The fractal dimension of the self-avoiding walk on the hierarchical lattice which models the percolating cluster[7] is also unity. This result differs from Flory's formula $y_T=(d+2)/3=\frac{4}{3}$ for $d=2$. In fact, for general d the recursion equation (19) becomes

$$J'=2^{d-1}J^2 \ , \tag{20}$$

which has the unstable fixed point at $J=2^{1-d}$ and the thermal exponent is $y_T=1$, independent of d. This result shows the great difference between d-dimensional Bravais lattices, $d\geq 2$, and the hierarchical lattices corresponding to the Migdal-Kadanoff renormalization-group scheme. On these hierarchical lattices the linear polymer grows only along the one direction, the vertical of Fig. 1, which explains why the polymer is one-dimensional. The "heat capacity" exponent, within the Migdal-Kadanoff renormalization group, is

$$a=2-d/y_T=2-d \ .$$

We estimate next the free energy f for small values of the field π (small H), for k (or J) greater than the critical value of $\frac{1}{2}$. Then Eq. (19) approximates the first n iterations until the other fields start to become nonnegligible because of the $HJ^{(n)}$ contribution in the second of Eq. (14):

$$HJ^{(n)}\approx u \ , \tag{21}$$

where u is a fixed small number, say 10^{-2}. Iterating n times Eq. (19) we find

$$J^{(n)}=(J/J_C)^{2^n} \ , \tag{22}$$

where $J_C=\frac{1}{2}$. We estimate n from Eqs. (21) and (22):

$$\begin{aligned} 2^n&=[\ln(u/H)]/[\ln(J/J_C)] \\ &=\tfrac{1}{2}[\ln(u^2/\pi)]/[\ln(k/k_C)] \ . \end{aligned} \tag{23}$$

Since, for the first n iterations $A\approx 1$, see Eq. (14),

$$f(J,H)\approx 4^{-n}f(J^{(n)},H) \ . \tag{24}$$

Now $J^{(n)}$ is large (since H is small) and consequently we use a "low-temperature," or maximum coverage, approximation:

$$f(J^{(n)},H)\approx\tfrac{1}{3}\ln J^{(n)}+\tfrac{1}{12}\ln H^2 \ , \tag{25}$$

where $\frac{1}{3}$ and $\frac{1}{12}$ are, respectively, the values of b and p at maximum coverage, (see Sec. II). A finite entropic contribution is neglected in Eq. (25), Combining Eqs. (23), (24), and (25) we find

$$f(k,\pi)\approx\tfrac{1}{3}[\ln(k/k_c)]^2/\ln(1/\pi) \qquad \text{for } \pi\to 0, \quad k>k_C=\tfrac{1}{2} \ . \tag{26}$$

By taking the logarithmic derivatives of f with respect to k and π [see Eq. (18)] we find that b and p vanish logarithmically slowly as π tends to zero. The polymerization index b/p, on the other hand, diverges logarithmically slowly. Similar conclusions hold for dimensions larger than 2, within the Migdal-Kadanoff scheme. For $d=1$, on the other hand, the same analysis yields the exact result $f=\ln k$ for $k\geq 1$ and $\pi\to o$.

The critical exponents y_i are obtained from $y_i=\ln\lambda_i/\ln 2$ where 2 is the change in scale factor and λ_i are the eigenvalues of the recursion equations at the critical fixed point. We find four positive exponents; i.e., there are four relevant fields associated with the polymerization critical point. It will be interesting to verify this Migdal-Kadanoff scheme prediction that the codimension[21] of the polymerization critical point is four by other methods (e.g., Nienhuis's Coulomb gas representation of 2D phase transitions[22]). The largest exponent is the "magnetic" one:

$$y_h=\ln[\tfrac{1}{4}(9+\sqrt{33})]/\ln 2\approx 1.8821 \ .$$

It differs by less than 1% from Nienhuis's[22] value $\frac{91}{48}\approx 1.8958$. The other three positive exponents are all equal to unity, and this includes the thermal exponent discussed at the beginning of this section.

Close to the critical polymerization point $k_C=\frac{1}{2}$, $\pi_C=0$, the singular contribution to the free energy can be written in a scaling form:

$$f_s\approx|k-k_C|^{2-\alpha}A_{\pm}(\pi/|k-k_C|^{\Delta}) \ , \tag{27}$$

where $\Delta=2y_h/y_T$ (the factor of 2 is due to the fact that $\pi\approx H^2$) and $2-\alpha=2/y_T$. The requirement that the critical manifold be an isolated point at $\pi=0$ and $k=k_C$ implies

$$A_{\pm}(x) \approx A_{\infty} x^{(2-\alpha)}/\Delta \quad \text{for } x \to \infty \ . \tag{28}$$

Hence along the critical isotherm close to the critical point

$$f_s \approx A_{\infty} \pi^{(2-\alpha)/\Delta} \ . \tag{29}$$

By computing f along the critical isotherm and fitting the numerical values to Eq. (29), we find that $A_{\infty} = 0.426\,80 \pm 0.000\,03$ and $(2-\alpha)/\Delta = 0.531\,25 \pm 0.000\,06$. This exponent value agrees with the exponent value determined by linearizing the recursion equations: $(2-\alpha)/\Delta = 1/y_h \approx 0.5313$.

Equation (27) overlooks oscillating corrections to scaling characteristic of nonrandom self-similar models. The scaling function $A_{\pm}$ which is a function of $k-k_C$ also, satisfies the following equation:

$$A_{\pm}(\pi/|k-k_C|^{\Delta}, k-k_C) = A_{\pm}(\pi/|k-k_c|^{\Delta}, \lambda_T(k-k_C)) \ , \tag{30}$$

where λ_T is the thermal eigenvalue equal to 2 for this model. If the renormalization-group procedure describes a statistical model on a translationally invariant lattice (e.g., one-dimensional lattice) then $A_{\pm}$ must be independent of the scale factor 1 and implicitly of the thermal eigenvalue; i.e., $A_{\pm}$ is independent of the second argument in Eq. (30). However, for the hierarchical lattice there exists an intrinsic scale factor which produces oscillations as a function of $\ln|k-k_C|$ with a period $\ln\lambda_T = \ln 2$. The plot of $\mathcal{N}\langle \delta b^2 \rangle$ versus $\ln(k-k_C)$ for fixed $\pi/(k-k_C)^{\Delta} = 0.01$ (see Fig. 8) shows the oscillations with the expected period ln2. It is noteworthy that the amplitude of these oscillations is 25% of the uniform part, a much larger fraction than in previous studies[15] of oscillations for Potts models (typical fraction 10^{-5}).

At the high-temperature fixed point (all fields: $J, H, \ldots$ are zero) the magnetic exponent is positive, doubly degenerated, and equal to unity. Of course a positive exponent signals a singularity in the free energy on the locus of points in the parameter space which flow towards this fixed point. The exponent value is "dangerous" in Wegner's terminology,[19] i.e., it implies a logarithmic singularity:

$$f \approx -a\pi \ln\pi \quad \text{for } \pi \to 0, \quad k < \tfrac{1}{2} \ , \tag{31}$$

where a is a positive function of k. Singular behavior at "high temperatures" is peculiar[11] to the hierarchical lattices which possess vertices of unbounded coordination number. It does not occur on Bravais lattices, where f vanishes linearly with π.

V. CONCLUSIONS

We have studied the grand-canonical ensemble of self-avoiding walks (equilibrium polymerization model) by using the Migdal-Kadanoff position-space renormalization-group technique. A framework for computing quantities such as the number of chemical bonds and the number of polymers in the whole parameter space (as opposed to close to the critical point only as in previous works) was realized. This framework can be perfected by using more sophisticated position-space renormalization-group techniques to become trustworthy in comparing to and predicting experimental data. At the polymerization critical point we find four positive exponents (four relevant fields in the renormalization-group terminology). It will be interesting to verify whether this result is genuine or a mere artifact of the Migdal-Kadanoff scheme. The value of the leading exponent (the magnetic one) comes within 1% of the presumed exact value, while the thermal exponent value differs substantially (33%) from the exact value.

Our calculations, though only approximate for 2D Bravais lattices, constitute the exact solution of the polymerization model on the diamond hierarchical lattice. Viewed from this perspective, our work is a contribution to the field of polymers on fractals. The geometry of the diamond hierarchical lattice causes certain results which are not expected to hold on Bravais lattices. For example, no Hamilton walk can be accommodated by this lattice. Also the polymerized phase (infinite polymerization index) is dilute in the sense that the density of chemical bonds is zero. The critical amplitudes of various quantities close to the critical point exhibit oscillations produced by the self-similar character of the lattice. Quite surprisingly these oscillations are much more substantial than the (previously studied) oscillations for Potts models.

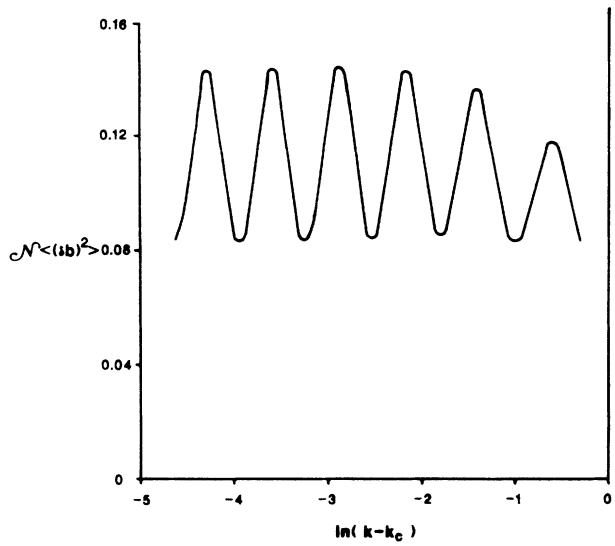

FIG. 8. The dependence of the b fluctuation $\mathcal{N}\langle \delta b^2 \rangle$ on $\ln(k-k_C)$ for $\pi/(k-k_C)^{\Delta} = 0.01$ showing oscillations with the period ln 2. The amplitude of the oscillations is about 25% of the uniform contribution.

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