Exact θ point and exponents for two models of polymer chains in two dimensions

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(Received 30 August 1989)

The collapse transition of a self-avoiding walk (SAW) on a two-dimensional lattice with directed bonds, the Manhattan lattice, is shown to occur at temperature $T_\theta = 2\varepsilon/\ln 2$, where ε is the attractive energy between nearest-neighbor pairs of monomers. The exact tricritical exponents are $\nu_t = \frac{4}{7}$ and $\gamma_t = \frac{6}{7}$. The latter result differs from the value for undirected two-dimensional lattices $\gamma_t = \frac{8}{7}$ because self-trapping configurations do not occur on the Manhattan lattice. The exact tricritical temperature and exponents for a constrained self-avoiding trail (SAT) on the square lattice are obtained by mapping the problem onto the self-avoiding walk on the Manhattan lattice. The mapping also shows that these SAT and SAW collapse transitions are in the same universality class. Finally, it is argued that the kinetic self-avoiding trail must be compact on the square lattice.

I. INTRODUCTION

At high temperatures a polymer chain in a good solvent behaves essentially as if it were a self-avoiding walk (SAW): its mean radius of gyration grows as $\langle R \rangle \sim N^\nu$, where ν has the same value as for the SAW and N is the molecular weight.[1] As the temperature T is reduced, however, the short-range van der Waals attraction between monomers becomes increasingly important. At a certain temperature T_θ the chain collapses. The exponent ν is $1/d$ in d dimensions for all $T < T_\theta$. Finally, the θ point $T = T_\theta$ is a tricritical point.[1-3]

Considerable progress has been made recently in understanding the nature of the collapse transition in two dimensions (2D). Coniglio *et al.*[4] have shown that a polymer ring on the hexagonal lattice at its collapse transition can be mapped onto the external perimeter or "hull" of a percolation cluster at threshold. Since it has been proven[5] that the radius-of-gyration exponent ν is $\frac{4}{7}$ for the perimeter of a percolation cluster at threshold in 2D, Coniglio *et al.* argued that the value of the size exponent at the tricritical point ν_t must also be $\frac{4}{7}$. This argument is not rigorous, however, since a subset of next-nearest-neighbor interactions appears in the polymer chain's Hamiltonian. Similarly, Duplantier and Saleur[6] have shown that $\nu_t = \frac{4}{7}$ for a tricritical SAW on the honeycomb lattice with vacancies. This SAW also has a subclass of next-nearest-neighbor interactions, so the collapse transition in this model is more properly referred to as a θ' point rather than a θ point. It is currently a matter of intense debate whether these additional interactions are relevant or not.[4,7-14]

A second question being investigated is whether the nature of the collapse transition is affected by the presence of loops. To address this issue, the collapse transition in self-attracting self-avoiding trails (SAT's) has been studied.[15-21] SAT's are paths on regular lattices in which sites may be revisited but bonds may not be.[22] It has been suggested recently that the collapse transition in self-attracting SAT's may be in a different universality class than the θ point.[16] A number of exact enumeration studies of trails in two and three dimensions support this view,[17-20] but these studies have been criticized[21] on the grounds that the trails constructed were all quite short. More convincing support comes from a scanning simulation on the square lattice in which trails of length $N \leq 300$ were generated.[21] The resulting estimate of the crossover exponent $\phi_t = 0.805 \pm 0.004$ differs significantly from the various values obtained for self-attracting SAW's in two dimensions.[6,8,9,11,12,23-27] (For example, analytical work[6] yielded $\phi_t = \frac{3}{7} = 0.428\ldots$ for the 2D SAW θ point.) In contrast, the values of ν_t and the entropy exponent γ_t appear to be the same for self-attracting SAT's and SAW's.[6,21]

In this paper I establish a rigorous correspondence between the statistics of a polymer ring on the Manhattan lattice at the θ point and the perimeter of a percolation cluster at threshold in bond percolation on the square lattice.[28] This mapping has three important consequences. First, it is shown that $\nu_t = \frac{4}{7}$ for SAW's on the Manhattan lattice with nearest-neighbor interactions only. Secondly, I demonstrate that the θ temperature is *exactly* $T_\theta = 2\varepsilon/\ln 2$, where ε is the attractive energy between nearest-neighbor pairs of monomers. Previously, the collapse transition temperature was known exactly only for the rather nonstandard problem of Ref. 6 which included next-nearest-neighbor interactions. This result should be quite useful in Monte Carlo studies of the tricritical point, since critical exponents can be computed much more precisely when the transition temperature is known. The third and final consequence is that the exponent γ_t is exactly $\frac{6}{7}$ for tricritical SAW's on the Manhattan lattice. Since Duplantier and Saleur[6] have shown that $\gamma_t = \frac{8}{7}$ for their tricritical SAW, we conclude that the θ' point is in a different universality class than the θ point for polymer chains on the Manhattan lattice. The conjecture[9,10] that the θ point is a $C = \frac{1}{2}$ superconformal theory leads to $\gamma_t = \frac{15}{14}$, which differs from both our result and that of Duplantier and Saleur.

I also demonstrate that the self-attracting SAT on the square lattice in which consecutive bonds are restricted to be at right angles can be mapped onto the self-

attracting SAW on the Manhattan lattice. This bond-to-site mapping[29] between the two problems is valid for all temperatures T, and so yields the exact tricritical point and the exponents ν_t and γ_t for the SAT. The mapping also shows that these two problems are in the same universality class. In particular, they share the same value of ϕ_t.

Finally, I consider the usual self-attracting SAT on the square lattice in which there are no restrictions, so consecutive steps may be parallel. Let -2ε be the energy assigned to each self-intersection of this trail. I show that for $2\varepsilon/T=\ln 3=1.098\ldots$ the SAT is equivalent to the kinetic self-avoiding trail (KSAT) introduced by Lyklema.[30] Recently Meirovitch and Lim[21] have used the scanning simulation method to obtain the estimate $2\varepsilon/T_\theta=1.086\pm0.002$ for the θ temperature of this self-attracting SAT. This strongly suggests that the self-attracting SAT equivalent to the KSAT is in the collapsed phase, so the KSAT should have $\nu=\frac{1}{2}$. Although Lyklema concludes that $\nu=0.535$ from his Monte Carlo study of the KSAT in 2D,[30] his data are consistent with a very slow crossover to an asymptotic value of $\nu=\frac{1}{2}$.

The paper is organized as follows. The self-attracting SAW on the Manhattan lattice is studied in Sec. II. To be specific, in Sec. II A I determine the exact θ point and the value of ν_t. The entropy exponent γ_t is obtained in Sec. II B. In Sec. II C, I show that the problem is equivalent to two recently introduced random walks which were studied by Monte Carlo. The Monte Carlo work on these models provides additional support for our identification of ν_t and γ_t. The exact tricritical point and exponents for the constrained self-attracting SAT on the square lattice are found in Sec. III. I consider the unconstrained self-attracting SAT in Sec. IV. Finally, Sec. V summarizes the results obtained in the paper.

II. EXACT TRICRITICAL POINT AND EXPONENTS FOR POLYMER CHAINS ON THE MANHATTAN LATTICE

A. Tricritical point and exponent ν_t

Consider the equilibrium statistical mechanics of a self-avoiding loop of length N on the Manhattan lattice (Fig. 1). For simplicity, we take the loop to be anchored at a point. Each nearest-neighbor pair of monomers which is not bonded will be assigned an energy $-\varepsilon$. Thus, if $n(C)$ is the number of such monomer pairs in a loop configuration C, the loop's energy is $-\varepsilon n(C)$. The loop partition function is

$$Z_N^{\text{loop}}(T)=\sum_{C'}\exp[\beta\varepsilon n(C')] , \tag{1}$$

where $\beta\equiv T^{-1}$ is the inverse temperature and the sum runs over all allowed loop configurations. The Boltzmann weight of a particular configuration C is

$$w(C,N,T)=\exp[\beta\varepsilon n(C)]/Z_n^{\text{loop}} . \tag{2}$$

Our first step will be to show that for $T=T_0\equiv 2\varepsilon/\ln 2$, the problem is equivalent to the kinetic growth walk[31] (KGW) on the Manhattan lattice. The KGW is a growing SAW in which all self-avoiding moves are weighted equally at each step. On undirected lattices, the walk terminates if a closed loop is formed or if no self-avoiding moves are available. The second type of termination does not occur on the Manhattan lattice, since if the walk enters a cul-de-sac, an exit always exists.[32] This has the interesting consequence that the KGW and the indefinitely growing[33,34] SAW (IGSAW) coincide on the Manhattan lattice.

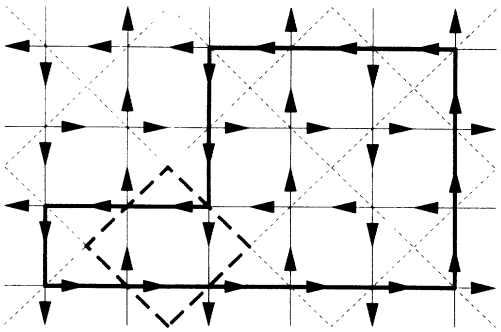

FIG. 1. Manhattan lattice (solid directed lines) and the underlying square lattice (undirected dashed lines). A SAW on the Manhattan lattice is shown in bold lines. The plaquette in the underlying lattice which this walk visits twice is delineated by bold dashed lines. There are two nearest-neighbor pairs in this SAW.

To see the equivalence between the polymer loop and the KGW, consider the ensemble of all KGW's which begin at a given point and which form closed loops after N steps. For an arbitrary loop configuration C, the number of twice-visited plaquettes in the underlying square lattice is $\frac{1}{2}n(C)$ (see Fig. 1). The probability that a loop of length N is formed is therefore

$$P(N)=\sum_{C'}2^{-N}\exp\left[\frac{\ln 2}{2}n(C')\right] , \tag{3}$$

where the sum runs over all possible self-avoiding configurations of the loop. The probability of a particular loop configuration C (given that the walk closes in N steps) is

$$p(C,N)=P^{-1}(N)2^{-N}\exp\left[\frac{\ln 2}{2}n(C)\right] . \tag{4}$$

Comparing Eqs. (1) and (3), we see that

$$Z_N^{\text{loop}}(T_0)=2^N P(N) , \tag{5}$$

while from Eqs. (2) and (4) we obtain

$$w(C,N,T_0)=p(C,N) . \tag{6}$$

Equation (6) shows that the fractal dimension of a polymer loop at $T=T_0$ is equal to that of the KGW.

The second step in establishing our correspondence between the tricritical polymer loop and the percolation hull will be to show that the KGW on the Manhattan lat-

tice traces out the perimeter of a bond percolation cluster on the square lattice at the percolation threshold $p=p_c=\frac{1}{2}$.[35] To see this, each time the walker in the KGW traverses a new plaquette in the underlying lattice, we place a bond along the main diagonal of the plaquette parallel to the walker's step, provided the diagonal is to the *right* of the walk (Fig. 2). In this way, each time the KGW enters a new plaquette a bond is placed on the plaquette diagonal with probability $\frac{1}{2}$. No new bond is added if the walker returns to a plaquette. The bonds on the main diagonals of the plaquettes are then the perimeter bonds of a percolation cluster on the square lattice at $p=p_c=1/2$, and the KGW walks around this perimeter, as claimed.

If the KGW closes in a clockwise fashion, it traces out the external perimeter of a percolation cluster (as in Fig. 2). In the trivial case of a clockwise loop of four steps, the KGW is the hull of a null cluster. Conversely, the KGW walks around an internal perimeter of a percolation cluster if it closes in a counterclockwise fashion. A counterclockwise loop of four steps walks around the inside of a square of four occupied bonds.

Clearly, the fractal dimension of KGW's that close in a clockwise fashion is the same as the fractal dimension of KGW's which close in the opposite way. Thus, polymer loops at $T=T_0$ have the same fractal dimension as KGW's that close in a clockwise fashion. A walk of this kind traces out the external perimeter of a percolation cluster at threshold, as we have just seen. We conclude that a polymer loop at $T=T_0$ has the same fractal dimension as the external perimeter of a bond percolation cluster on the square lattice at threshold.

Recently, Saleur and Duplantier[5] proved that the fractal dimension of the external perimeter of a percolation cluster at threshold is exactly $D=\frac{7}{4}$ for bond percolation on the square lattice. This result is consistent with a wide range of analytical and Monte Carlo work.[36] Thus, a polymer loop on the Manhattan lattice at temperature $T=T_0$ has radius of gyration exponent $\nu=\frac{4}{7}$. Now in 2D, the exponent ν is $\frac{1}{2}$ for polymer loops at temperatures $T<T_\theta$, while ν takes on the equilibrium SAW value[37] $\frac{3}{4}$ for $T>T_\theta$. Since $\nu=\frac{4}{7}$ at $T=T_0$, we conclude that $T_\theta=T_0$. The exact θ temperature is therefore $T_\theta=2\varepsilon/\ln 2$. In addition, the value of ν at the tricritical point is $\nu_t=\frac{4}{7}$.

A minor technical point in this last step of our argument must now be dealt with: the external perimeter formed by a KGW that closes in a clockwise fashion is not the same as the perimeter studied by Saleur and Duplantier (SD).[5] These authors define the "hull of a cluster Γ as the set of empty bonds that touch Γ and can be linked to infinity by a path (not restricted to the lattice) without touching Γ." The cluster shown in Fig. 2, for example, has a KGW hull of length $N=24$, while the SD hull contains 13 empty bonds. To avoid confusion with N, the number of bonds in the SD hull will be denoted by s'.

Our identification of T_θ and ν_t hinges on the assumption that the KGW hull has the same fractal dimension as the SD hull, $D=\frac{7}{4}$. I will now show that this assumption is correct.

There is no functional relationship between the values of N and s'. However, given the values of s', it is a simple matter to obtain upper and lower bounds on N. A step in the KGW crosses each empty bond in the SD hull, so $N\geq s'$ (Fig. 2). To get an upper bound on N, we construct a "dual hull" by placing bonds on the diagonals of those plaquettes in the underlying lattice which contain the empty bonds of the SD hull. The bonds of the dual hull are oriented at right angles to the empty bonds in the SD hull (Fig. 3). Clearly, the number of bonds in the dual

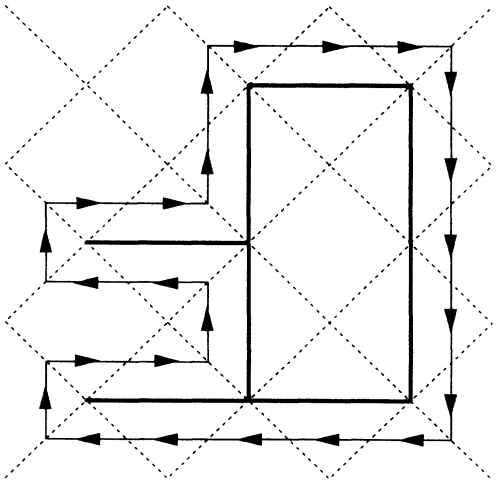

FIG. 2. A KGW on the Manhattan lattice (directed solid lines) walks around the perimeter of a bond percolation cluster on the square lattice (bold lines). The underlying lattice is shown with dashed lines. For clarity, the Manhattan lattice itself has not been shown.

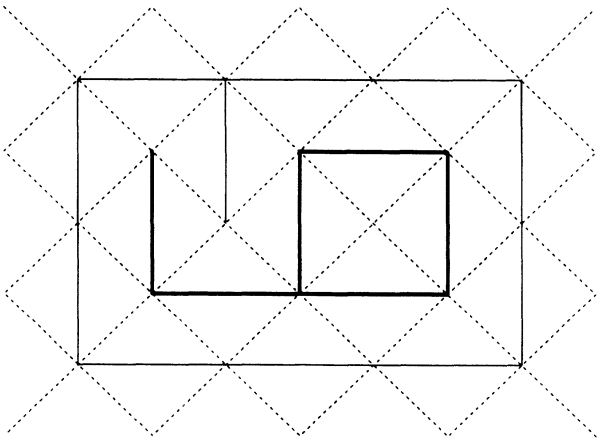

FIG. 3. The dual hull (solid lines) surrounds a percolation cluster (bold lines). The underlying lattice is shown with dashed lines.

hull is s'. If we take the lattice spacing of the Manhattan lattice to be unity, then each bond of the KGW hull is a distance $\frac{1}{2}$ from a bond in the dual hull. There are eight bonds in the Manhattan lattice which are a distance $\frac{1}{2}$ away from a particular bond in the dual hull. Therefore $N \leq 8s'$, and we conclude that

$$s' \leq N \leq 8s' \ . \tag{7}$$

It is not hard to obtain a better upper bound on N, but Eq. (7) is sufficient for our purposes.

Let L' be the side of the smallest square which completely contains the empty bonds in the SD hull. L' is a simple measure of the linear dimension of the SD hull. Since the fractal dimension of this hull is $\frac{7}{4}$,[5]

$$\langle s' \rangle \sim (L')^{7/4} \ \text{ as } L' \to \infty \ . \tag{8}$$

Now let L be the side of the smallest square which contains the KGW hull of the cluster. Clearly,

$$L' = L + 3 \ . \tag{9}$$

From Eq. (7) we have

$$\langle s \rangle \leq \langle N \rangle \leq 8 \langle s' \rangle \ . \tag{10}$$

Combining this with Eqs. (8) and (9) we find

$$\langle N \rangle \sim L^{7/4} \ \text{ as } L \to \infty \ . \tag{11}$$

Thus the fractal dimension of the KGW hull is $\frac{7}{4}$, as required.

B. Exponent γ_t

We next demonstrate that the tricritical exponent γ_t is exactly $\frac{6}{7}$. First, recall that γ_t is defined by

$$Z_N^{\text{open}}(T_\theta) \sim \mu^N N^{\gamma_t - 1} \ \text{ for } N \gg 1 \ , \tag{12}$$

where $Z_N^{\text{open}}(T_\theta)$ is the partition function of an open chain of length N at the θ point and the constant μ is the analog of the usual SAW connectivity constant. We shall first determine the value of μ. Since the free energy per monomer is the same for loops and open chains in the $N \to \infty$ limit,

$$\lim_{N \to \infty} \ln Z_N^{\text{loop}}(T_\theta)/N = \lim_{N \to \infty} \ln Z_N^{\text{open}}(T_\theta)/N = \ln \mu \ . \tag{13}$$

As shown above, $Z_N^{\text{loop}}(T_\theta) = 2^N P(N)$, where $P(N)$ is the probability that the KGW on the Manhattan lattice closes in N steps. Now every loop configuration formed by the KGW can be reflected in the x and y directions about the point of origin to yield another allowed loop configuration. This new loop has the same probability of occurrence as the original loop, but closes in the opposite way. Thus $P(N)$ is equal to the probability that the KGW closes in N steps given that it closes in a clockwise fashion. The latter probability is the probability that a percolation cluster at threshold has a KGW hull of length N.

Recently, Ziff[38] used scaling arguments and the exact fractal dimension of a percolation cluster hull at threshold to obtain exact values for other hull exponents. He found that the probability that a percolation cluster at threshold has a hull of length l decays as $l^{-\tau'+1}$ for large l, and that $\tau' = \frac{15}{7}$. This conclusion is supported by Ziff's Monte Carlo work on the hulls of site percolation clusters on the square lattice at threshold. If the result $\tau' = \frac{15}{7}$ is universal, then the probability that a bond percolation cluster on the square lattice has a KGW hull of length N must scale as

$$P(N) \sim N^{-8/7} \tag{14}$$

as $N \to \infty$. [Additional evidence corroborating Eq. (14) will be discussed in Sec. II C.] Combining Eq. (14) with (13), we conclude that $\mu = 2$.

Having obtained the leading-order asymptotic behavior of $Z_N^{\text{open}}(T_\theta)$, we turn to the first correction to this scaling behavior. We will compare $Z_N^{\text{open}}(T_\theta)$ with $P^{\text{open}}(N)$, the probability that the KGW on the Manhattan lattice performs an N-step walk without closing. To this end, let $\kappa(C)$ be the number of twice-traversed plaquettes in the underlying lattice in the chain conformation C. Then

$$P^{\text{open}}(N) = 2^{-N} \sum_C 2^{\kappa(C)} \ , \tag{15}$$

while

$$Z_N^{\text{open}}(T_\theta) = \sum_C 2^{n(C)/2} \ . \tag{16}$$

Both of these sums run over all open self-avoiding configurations of length N. For closed loops we have the equality $2\kappa(C) = n(C)$. For open chains this is replaced by the inequality $2\kappa(C) \leq n(C) \leq 2\kappa(C) + 2$, since each chain end can have a nearest-neighbor bond with energy $-\varepsilon$ which does not lie in a twice-traversed plaquette of the underlying lattice. Therefore

$$P^{\text{open}}(N) \leq 2^{-N} Z_N^{\text{open}}(T_\theta) \leq 2P^{\text{open}}(N) \ . \tag{17}$$

Monte Carlo work[32] strongly suggests that the KGW on the Manhattan lattice must ultimately form a closed loop, so

$$P^{\text{open}}(N) = \sum_{M=N+1}^{\infty} P(M) \sim N^{-\tau'+2}$$

for $N \gg 1$. Applying this to Eq. (17) and using the result $\mu = 2$, we have $\gamma_t = 3 - \tau' = \frac{6}{7}$.

Our exact result $\gamma_t = \frac{6}{7}$ differs from the value $\gamma_t = \frac{8}{7}$ Duplantier and Saleur[6] obtained for the θ' point in their model. Monte Carlo studies[9,11,12,24,27] of the square lattice θ point yielded the estimates $\gamma_t = 0.93 \pm 0.05$, $\gamma_t = 1.110 \pm 0.022$, and $\gamma_t = 1.075 \pm 0.040$, while transfer-matrix work[26] on this problem gave $\gamma_t = 1.00 \pm 0.05$. It therefore appears that the tricritical SAW on the Manhattan lattice is in a different universality class than both the square lattice θ point and the θ' point in the model studied by Duplantier and Saleur. To account for this, note that in the latter two problems the chain partition function includes contributions from self-trapping configurations. (A configuration is called self-trapping if growth must eventually lead to violation of the self-

avoidance constraint.) In contrast, self-trapping configurations do not occur on the Manhattan lattice.[32] This should have a significant effect on the asymptotic behavior of the KGW survival probability $P^{\text{open}}(N)$, and as Eq. (17) shows, this is what determines the value of γ_t.

We can understand why the IGSAW and the KGW have the same fractal dimension on the Manhattan lattice in much the same way. On undirected 2D lattices, the IGSAW has fractal dimension $D=\frac{7}{4}$,[5,34] while the KGW has $D=\frac{4}{3}$.[39–41] The two models differ on these lattices because in the KGW self-trapping produces a slow crossover to the asymptotic value of the fractal dimension $D=\frac{4}{3}$.[40] This crossover is absent in the KGW on the Manhattan lattice since self-trapping cannot occur.

C. Relation to two other models

We have shown that on the Manhattan lattice, the KGW is equivalent to a tricritical polymer loop. I will now demonstrate that the KGW on the Manhattan lattice is equivalent to two other models, one introduced by Gunn and Ortuno[42] (GO) and the other by Roux, Guyon, and Sornette[43] (RGS). Monte Carlo studies[42–45] of these models provide additional support for our identification of ν_t and γ_t.

In the GO model on the square lattice, a random walker turns left with probability $p(\pi/2)$, right with probability $p(-\pi/2)$, and goes straight with probability $p(0)$. The probability of a 180° turn is $p(\pi)=1-p(\pi/2)-p(-\pi/2)-p(0)$. If the walker returns to a site, it must make the same move (right, left, straight, or backwards) that it made on its first visit. Each walk begins by traversing the same bond in the same direction. I will show that the GO model with p's given by

$$p(\pi/2)=p(-\pi/2)=\tfrac{1}{2} \tag{18a}$$

and

$$p(0)=p(\pi)=0 \tag{18b}$$

is equivalent to the KGW on the Manhattan lattice.

To establish the correspondence, we perform a bond-to-site mapping[29] on the GO model with p's given by Eq. (18). Specifically, we place a site at the center of each bond of the GO walk and join consecutive sites (Fig. 4). The resulting walk is the KGW on the Manhattan lattice. Each KGW starts at a given site; correspondingly, each GO random walk initially traverses a particularly bond in a fixed direction.

Grassberger[44] performed a Monte Carlo simulation of the GO walk with $p(\pi/2)=p(-\pi/2)=\frac{1}{2}$ and found the fractal dimension $D=1.750\pm0.002$. This lends strong support to the assertion that D is exactly $\frac{7}{4}$ for the KGW on the Manhattan lattice, and hence for θ polymers on the Manhattan lattice. In addition, Salmeron, Ortuno, and Gunn[45] find that the probability that the GO walk closes in N steps, $P(N)$, decays as $P(N)\sim N^{-1.12}$ for large N, in good agreement with our Eq. (14).

Roux, Guyon, and Sornette[43] give two distinct formulations of their model. The formulation that generates a single loop by a random walk is most easily related to the KGW on the Manhattan lattice; for completeness we will describe the construction of the RGS walk in some detail. We start with a square lattice, which we call the underlying lattice, and construct a new square lattice—the covering lattice—by placing sites at the center of the bonds in the underlying lattice. The walker in the RGS model moves from site to site in the covering lattice. The initial position of the RGS walker is fixed (Fig. 5). The plaquette in the underlying lattice immediately above the initial position of the walker is now occupied with one of the tiles shown in Fig. 6, with the two possibilities being given equal weight. The walker moves along the tile diagonal leading from its current position, and so reaches the edge of a new plaquette. This plaquette is randomly occupied with one of the two types of tiles, and the walker again traverses the tile diagonal. The walk continues in this way, with a new tile being chosen each time a new

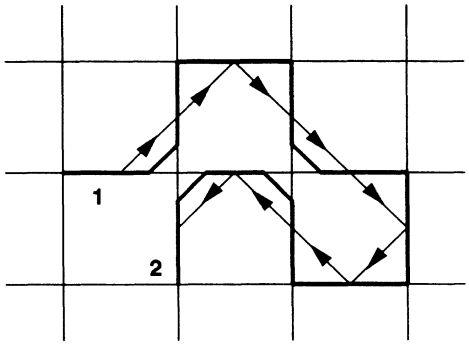

FIG. 4. Typical GO walk on the square lattice with $p(\pi/2)=p(-\pi/2)=\frac{1}{2}$ shown with bold lines. The first bond to be traversed is labeled 1, while the most recently visited bond is labeled 2. The corresponding KGW on the Manhattan lattice is shown with directed solid lines.

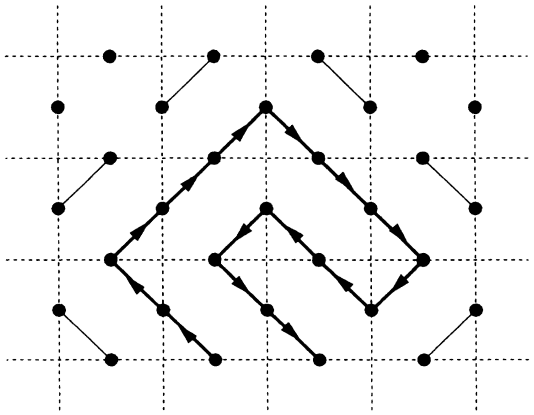

FIG. 5. Construction of the RGS walk. The underlying lattice is shown using dashed lines, while closed circles denote sites in the covering lattice. Bold directed lines indicate a representative RGS walk. Unvisited tile diagonals which lie in once-traversed plaquettes are shown with solid lines.

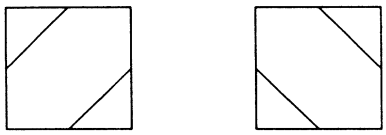

FIG. 6. Tiles used in the construction of the RGS walk.

plaquette is reached. If the walker revisits a plaquette, it follows the tile diagonal which it had not previously traversed. The walk ends if it returns to its initial position.

When defined in this way, the RGS model is obviously equivalent to the KGW on the Manhattan lattice. Roux, Guyon, and Sornette[43] find $D=1.73\pm0.02$ for their walk, in agreement with our exact result $D=\frac{7}{4}$. They also find that the probability of forming a loop with N steps decays as $P(N)\sim N^{-\tau'+1}$ for $N\gg1$, with $\tau'=2.16\pm0.10$. This agrees well with the exact result $\tau'=\frac{15}{7}$.

III. EXACT TRICRITICAL POINT AND EXPONENTS FOR A CONSTRAINED SAT

In the next two sections we will consider the equilibrium properties of two different types of self-avoiding trails (SAT's) on the square lattice. These SAT's have an energy -2ε coming from each twice-visited site, while each pair of parallel consecutive steps is assigned an energy u. Here we consider the limit $u=+\infty$. The opposite extreme $u=0$ will be studied in the next section.

Consecutive steps must be at right angles for the case $u=+\infty$. Thus, by assigning directions to the bonds of the square lattice appropriately, we may think of the SAT as residing on the anti-Manhattan (AM) lattice (Fig. 7). The directions of the bonds on the AM lattice automatically enforce the constraint on the angle between consecutive steps.

The covering lattice of the AM lattice is constructed by placing sites at the center of the bonds of the AM lattice. Nearest-neighbor sites in the covering lattice are connected by directed bonds oriented as shown in Fig. 7. Clearly, the covering lattice of the AM lattice is just the Manhattan lattice.

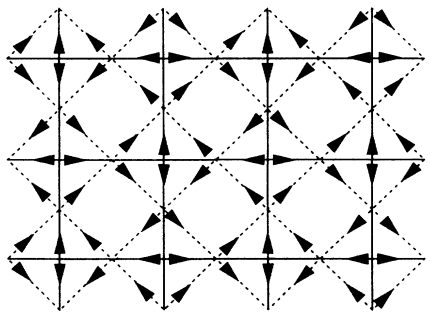

FIG. 7. The anti-Manhattan lattice (solid directed lines) and its covering lattice, the Manhattan lattice (dashed directed lines).

The closed self-attracting SAT with $u=+\infty$ is equivalent to the closed self-attracting SAW on the Manhattan lattice, as we now show using a bond-to-site mapping.[29] By placing sites at the center of the bonds of a SAT, each closed SAT with N steps on the AM lattice is associated with a closed SAW of length N on the Manhattan lattice. We require each SAT to traverse a particular bond in the AM lattice. This corresponds to the requirement that each SAW be anchored at a point on the Manhattan lattice. Finally, each self-intersection with energy -2ε in the SAT maps onto two nearest-neighbor pairs in the SAW with the same energy. The SAT and SAW are therefore equivalent for all temperatures T.[46]

We can now carry over the results of our studies on self-attracting SAW's on the Manhattan lattice to self-attracting SAT's on the AM lattice. In particular, the collapse transition must occur at the same temperature for both models, and both must have the same value of ν_t. The θ temperature for closed SAT's on the square lattice with $u=+\infty$ is therefore

$$T_\theta=2\varepsilon/\ln2\ , \tag{19}$$

and the tricritical radius of gyration exponent is

$$\nu_t=\tfrac{4}{7}\ . \tag{20}$$

The two models must also have the same crossover exponent ϕ_t, although I have not been able to determine its value.

Finally, let us determine the value of γ_t for constrained SAT's on the square lattice. As previously, the trails may be considered to be embedded in the AM lattice. The partition function for open SAT's with $N+1$ steps is

$$\Omega_{N+1}(T)=\sum_\Gamma \exp[2\beta\varepsilon\lambda(\Gamma)]\ , \tag{21}$$

where the sum runs over all open SAT's of this length which begin at a given bond, and $\lambda(\Gamma)$ denotes the number of twice-visited sites in one such trail Γ. In particular,

$$\Omega_{N+1}(T_\theta)=\sum_\Gamma 2^{\lambda(\Gamma)}\ . \tag{22}$$

We will compare this with Eq. (16) for $Z_N^{\rm open}(T_\theta)$. To accomplish this, let C be the open SAW of length N associated with Γ, an open SAT of length $N+1$. Each site which is visited twice by the SAT has two associated nearest-neighbor pairs in the SAW, except for twice-visited sites at the ends of the SAT. If sites of the latter kind are present, each has only one associated nearest-neighbor pair in the SAW. Thus

$$\tfrac{1}{2}n(C)\le\lambda(\Gamma)\le\tfrac{1}{2}n(C)+1\ . \tag{23}$$

Using this inequality and Eqs. (16) and (22), we obtain

$$Z_N^{\rm open}(T_\theta)\le\Omega_{N+1}(T_\theta)\le2Z_N^{\rm open}(T_\theta)\ . \tag{24}$$

Equation (24) shows that μ and γ_t have the same value for the SAT as for the SAW. Accordingly, the exponent γ_t for tricritical SAT's on the square lattice with $u=\infty$ is

$$\gamma_t=\tfrac{6}{7} . \tag{25}$$

Recently, Meirovitch and Lim[21] used the scanning simulation method to study the collapse transition of self-attracting SAT's with $u=0$ on the square lattice. Their results $\nu_t=0.569\pm0.008$ and $\gamma_t=1.133\pm0.024$ indicate that the SAT transition with $u=\infty$ is in a different universality class than the transition with $u=0$. Also, we have shown that the collapse transitions of the SAW on the Manhattan lattice and of the SAT on the AM lattice are isomorphic, so these transitions belong to the same universality class. This is in contrast to the situation for undirected lattices, since the SAT and SAW collapse transitions appear to belong to different universality classes in this case.[16–21] In particular, the current best estimate[21] of the crossover exponent for the SAT on the square lattice, $\phi_t=0.805\pm0.004$, is far removed from any of the values of ϕ_t obtained for the SAW on this lattice.[6,8,9,11,12,23–27]

IV. FRACTAL DIMENSION OF THE KINETIC SELF-AVOIDING TRAIL ON THE SQUARE LATTICE

The kinetic self-avoiding trail has been studied by Lyklema as a model of a θ polymer.[30] The KSAT is a growing self-avoiding trail, so no bond can be visited twice, though sites may be. In the square lattice version of the KSAT, a walker starts at a given site at time $t=0$. At each subsequent time step, the walker traverses one of the neighboring bonds which has not previously been visited. If there is more than one such bond, the alternatives are weighted equally. The walk terminates upon returning to its point of origin.

We will actually study a slightly modified version of the KSAT on the square lattice. This walk begins at an extra site which we place midway along a particular bond, and ends when it returns to this special site. The KSAT rules are otherwise unaltered. It seems clear that the large-scale properties of the KSAT are unchanged by this modification of the initial condition. We shall show that for the special temperature $T_1=2\varepsilon/\ln 3$, the self-attracting SAT on the square lattice with $u=0$ is equivalent to the modified KSAT.

For the modified KSAT, the probability that a loop of length N is formed is given by

$$P(N)=3^{-N}\sum_{C'}3^{\nu(C')} , \tag{26}$$

where the sum runs over all possible loop configurations C', and $\nu(C')$ is the number of twice-visited sites in the loop C'. Also, the lattice spacing in Eq. (26) has been taken to be unity, so the distance between the point of origin and its nearest neighbors is $\frac{1}{2}$. The probability of a particular loop configuration C (given that the walk closes when it reaches length N) is

$$p(C,N)=P^{-1}(N)3^{-N+\nu(C)} . \tag{27}$$

Now consider the self-attracting SAT on the square lattice with $u=0$. We shall consider only closed configurations of length N which contain a given bond. The partition function for this model is

$$Z_N^{\text{loop}}(T)=\sum_{C'}e^{2\beta\varepsilon\nu(C')} , \tag{28}$$

where the sum runs over all allowed loop configurations C'. The Boltzmann weight of a particular configuration C is

$$w(C,N,T)=\exp[2\beta\varepsilon\nu(C)]/Z_N^{\text{loop}}(T) . \tag{29}$$

For the temperature $T_1=2\varepsilon/\ln 3$, we have

$$Z_N^{\text{loop}}(T_1)=3^N P(N)$$

and

$$w(C,N,T_1)=p(C,N) .$$

The modified KSAT is therefore equivalent to the $u=0$ version of the self-attracting SAT at the temperature $T=T_1$.

Meirovitch and Lim[21] have recently performed very accurate simulations of the self-attracting SAT on the square lattice with $u=0$. They find $2\varepsilon/T_\theta=1.086\pm0.002$, where the error indicates a 95% confidence limit. In contrast, $2\varepsilon/T_1=\ln 3=1.098\ldots$, which is well outside this error. It therefore appears that T_1 is slightly below T_θ. If so, the asymptotic value of the radius of gyration exponent for the KSAT should be $\nu=\frac{1}{2}$.

To analyze his Monte Carlo results on the KSAT, Lyklema[30] assumed that the asymptotic behavior of the mean-square radius of gyration is given by a series of the form

$$\langle R^2(N)\rangle = AN^{2\nu}(1+BN^{-\Delta}+CN^{-1}+\cdots) \tag{30}$$

and defined a finite-size estimator of the exponent ν as follows:

$$\nu(N)\equiv\frac{1}{2}\frac{\ln[\langle R^2(N+i)\rangle/\langle R^2(N-i)\rangle]}{\ln[(N+i)/(N-i)]} . \tag{31}$$

Here i is a fixed positive integer. Inserting Eq. (30) into (31), we obtain

$$\nu(N)=\nu-\tfrac{1}{2}BN^{-\Delta}-\tfrac{1}{2}CN^{-1}+\cdots . \tag{32}$$

Lyklema then plotted $\nu(N)$ versus N^{-1} and extrapolated to $N=\infty$ by fitting to the form (32). The resulting estimate $\nu=0.535\pm0.003$ differs markedly from our value $\nu=\frac{1}{2}$.

This discrepancy can be explained by noting that our mapping between the KSAT and the self-attracting SAT shows that the mean-square radius of gyration of the KSAT must have the scaling behavior[1,2]

$$\langle R^2(N)\rangle = N^{2\nu_t}f(N\tau_1^{1/\phi_t}) , \tag{33}$$

where $\tau_1\equiv|T_1-T_\theta|/T_\theta$. The scaling function $f(x)$ is nonzero and finite for $x=0$, while

$$f(x)\sim x^{2(\nu-\nu_t)}$$

for $x \to \infty$. Since the KSAT is in the low-temperature phase, $\nu = \frac{1}{2}$. We expect the corrections to scaling to be given by an expression of the form

$$f(x) \sim x^{2(\nu - \nu_t)}(a + bx^{-\Delta} + cx^{-1} + \cdots) \quad (34)$$

for $x \gg 1$. When Eq. (34) is inserted in (33), Eq. (30) is reproduced exactly, so Eq. (30) can be used to extrapolate to the $N = \infty$ limit. Equation (30) is only valid for $x_1 \equiv N\tau_1^{1/\phi_t} \gg 1$, however. Using Meirovitch and Lim's value[21] $\phi_t = 0.807 \pm 0.005$, we find that for the largest value of N studied by Lyklema ($N = 2000$), x_1 is only 6.6, which is not large compared to 1. Chains much longer than Lyklema's must therefore be constructed before Eq. (30) can be used to perform the extrapolation. We conclude that the asymptotic value of ν for the KSAT is most likely $\frac{1}{2}$, although this will be difficult to confirm in a Monte Carlo study because an ensemble of trails—each of at least 10^5 steps long—must be generated to obtain the true asymptotic behavior.

V. SUMMARY

In this paper, the exact θ temperature $T_\theta = 2\varepsilon/\ln 2$ was determined for the self-attracting SAW on the Manhattan lattice. The tricritical exponents $\nu_t = \frac{4}{7}$ and $\gamma_t = \frac{6}{7}$ were also found. These results were obtained by mapping the problem onto the KGW on the Manhattan lattice, and hence onto the hull of a critical bond percolation cluster on the square lattice. Additional support for our conclusions was obtained by mapping the KGW on the Manhattan lattice onto the walk of Gunn and Ortuno[42] and the walk of Roux, Guyon, and Sornette,[43] and then comparing with Monte Carlo work on these models.[42–45]

Our value $\nu_t = \frac{4}{7}$ agrees with Duplantier and Saleur's result for the θ' point,[6] but γ_t differs in the two models: γ_t is $\frac{6}{7}$ for our model, while $\gamma_t = \frac{8}{7}$ for the θ' point. Moreover, numerical studies[8,9,11,12,24,26,27] of the θ point on undirected 2D lattices have all yielded values of γ_t which are considerably larger than $\frac{6}{7}$. The low value of γ_t in our problem is due to the absence of self-trapping configurations on the Manhattan lattice.

The second half of this paper was concerned with the properties of SAT's. A bond-to-site mapping was used to establish that the self-attracting SAT on the square lattice in which consecutive bonds are restricted to be at right angles is equivalent to the self-attracting SAW on the Manhattan lattice. This mapping shows that the collapse transitions in these two problems are in the same universality class. This is in contrast to recent work on undirected 2D lattices which suggests that the SAT and SAW θ points are in different universality classes.[16–21] The mapping also yields the exact collapse transition temperature and the exponents ν_t and γ_t for the restricted SAT. Finally, we mapped the unrestricted self-attracting SAT at a particular temperature T_1 onto the KSAT. The Monte Carlo results of Meirovitch and Lim[21] were then used to argue that the KSAT exponent ν must crossover to an asymptotic value of $\frac{1}{2}$.

ACKNOWLEDGMENTS

I would like to thank J.-M. Debierre and P. N. Strenski for valuable discussions. This work was supported by the IBM Research Division and the Polymeric Materials Center of the Colorado Advanced Materials Institute.

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