Collapse transition of self-avoiding walks and trails by real-space renormalization

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Self-avoiding trails (SAT's) are paths on regular lattices that may revisit sites but not bonds. If each twice-visited site in a SAT is assigned an energy $-\varepsilon$, a collapse transition will occur at sufficiently low temperatures. Shapir and Oono [J. Phys. A: Math. Gen. **17**, L39 (1984)] have suggested that the collapse transition of a self-attracting SAT may be in a different universality class than the θ point of the self-avoiding walk (SAW). We present the results of a small-cell real-space renormalization-group study on a model that includes self-attracting SAW's and SAT's as special cases. We find distinct fixed points for the SAW and SAT collapse transitions, and so conclude that these transitions are indeed in different universality classes. We also find a tetracritical point characterizing the crossover between the two kinds of tricritical scaling behavior.

I. INTRODUCTION

A polymer in a good solvent can be treated as a self-avoiding walk[1] (SAW). As the temperature T is decreased or the solvent becomes poorer, the attractive long-range monomer-monomer interactions due to van der Waals forces become more important. At a certain temperature θ (the Flory θ temperature), the van der Waals forces cancel the excluded-volume repulsive interactions and the system undergoes a phase transition.[1,2] The θ point is a tricritical point.[1-4] For $T<\theta$, the attractive interactions prevail and the polymer collapses. Such polymer systems have been modeled by self-avoiding walks on a lattice with attractive nearest-neighbor interactions.[5,6]

It is currently being debated whether the presence of loops affects the large-scale behavior of polymer chains.[7-18] This work has centered on the properties of self-avoiding trails (SAT's), which are paths on regular lattices that may revisit sites but not bonds.[19] If each twice-visited site in a SAT is assigned an energy $-\varepsilon$, a collapse transition will occur for sufficiently low temperatures.[20] It is generally agreed that the low- and high-temperature phases of the self-attracting SAT have the same exponents as the corresponding phases of the self-attracting SAW.[21] However, Shapir and Oono[7] have suggested that the collapse transition of a self-attracting SAT may be in a different universality class than the usual SAW θ point. A number of exact enumeration studies of trails in two and three dimensions support this view,[8-11] but these studies have been criticized on the grounds that the trails constructed were all quite short.[13,15] More convincing support comes from a scanning simulation on the square lattice in which trails of length $N\leq 300$ were generated.[13,15] The resulting estimate of the crossover exponent, $\phi_t=0.805\pm0.004$, differs significantly from the various values obtained for self-attracting SAW's in two dimensions (2D).[22-31] In contrast, it has recently been shown that the collapse transitions of a self-attracting SAW on the Manhattan lattice and of the self-attracting SAT on the L lattice are in the same universality class.[17,18]

In this paper, we perform a small-cell real-space renormalization-group (RSRG) study of a self-attracting SAT in two dimensions (2D) with an energy $-\varepsilon$ assigned to each self-crossing and with an additional attractive interaction $-u$ between each nearest-neighbor pair of monomers. The usual self-attracting SAT and SAW problems are recovered in the $u\rightarrow 0$ and $\varepsilon\rightarrow-\infty$ limits, respectively. We find distinct fixed points for the collapse transitions in these two problems, indicating that these transitions belong to different universality classes. A tetracritical point characterizing the crossover between the two tricritical points also appears in our renormalization-group scheme.

This paper is organized as follows. In Sec. II we describe the model to be studied in greater detail. Our RSRG method is introduced in Sec. III by applying it to the $T=\infty$ behavior of a SAW in 2D. In Secs. IV and V the technique is applied to self-attracting SAW's and self-attracting SAT's, respectively. The self-attracting SAT with nearest-neighbor interactions is studied in Sec. VI. Section VII contains our conclusions.

II. THE MODEL

Consider a SAT of length N on the square lattice. In our model, an energy $-\varepsilon$ is assigned to each twice-visited site and each nearest-neighbor pair of monomers has an energy $-u$. The partition function is

$$Z_N(T)=\sum_{l=0}^{\infty}\sum_{m=0}^{\infty}C_N(l,m)e^{\beta(l\varepsilon+mu)},$$

where l is the number of self-crossings, m is the number of nearest-neighbor pairs of monomers in the polymer, and $\beta\equiv 1/k_BT$. $C_N(l,m)$ is the number of different configurations of the polymer with the given values of N, l, and m. The grand-canonical partition function is

$$Z(\mu,T)=\sum_{N=0}^{\infty}Z_N(T)e^{\beta\mu N},$$

where μ is the chemical potential. For convenience, we let $p=\exp(\beta\mu)$, $q=\exp(\beta\varepsilon)$, and $r=(\exp(\beta u)$. Note that self-attracting SAW's occur for $q=0$, while self-attracting SAT's are obtained for $r=1$.

III. RSRG FOR SAW'S

In the RSRG approach to critical phenomona in 2D polymer systems,[32–36] an $M\times M$ cell is renormalized onto an $L\times L$ cell, when L and M are integers and $1\leq L<M$. The correlation length is rescaled by a factor of L/M under this transformation. The parameters in the rescaled problem (p', q' and r') are given by the recursion relations

$$p'=p'(p,q,r),\ q'=q'(p,q,r)\ ,$$

and (3.1)

$$r'=r'(p,q,r)\ .$$

As usual, a critical point is a fixed point of the renormalization-group (RG) equations (3.1), and the corresponding critical exponents are found by linearizing about the fixed point.[37]

Numerous techniques have been employed to construct approximate recursion relations for the pure self-avoiding walk with no self-crossings and no nearest-neighbor interactions.[32,36] In this problem, q is fixed at zero and r is 1, so there is a single recursion relation $p'=p'(p)$. Here we study this problem using a RSRG method introduced by de Queiroz and Chaves (QC).[34,38] This method has the advantage that it is readily extended to arbitrary values of q and r.

To illustrate the QC method, we construct the recursion relation for p for $M=2$ and $L=1$. The recursion equation is shown symbolically in Fig. 1. Each occupied bond in the original cell is assigned a factor of p, while in the renormalized cell occupied bonds are given a weight p'. The symbolic equation in Fig. 1 means that all the paths that enter at one side and exit out the opposite side in the 2×2 cell are renormalized onto the single path that enters at one side and exists at the opposite side in the 1×1 cell. The corresponding recursion relation is

$$p'=2p^2+4p^3+2p^4\ . \tag{3.2}$$

We obtain a nontrivial fixed point at $p_c=0.2971$ and the radius-of-gyration exponent $\nu_{\rm SAW}\simeq\ln2/\ln2.459\simeq0.77$.[34]

Perhaps the simplest RSRG method is the corner rule.[32–34] The corner rule with $M=2$ and $L=1$ yields a nontrivial fixed point at $p_c=0.4656$ for the pure SAW in 2D, and the exponent $\nu_{\rm SAW}\simeq0.72$. The exact value of $\nu_{\rm SAW}$ is $\frac{3}{4}$.[39] We see that the QC method gives a value of p_c that differs substantially from that given by the corner rule. The two methods give values for $\nu_{\rm SAW}$ that are comparable in accuracy, however.

IV. RSRG FOR SELF-ATTRACTING SAW'S

For self-attracting SAW's, q is zero and we must construct recursion relations for p and r. We cannot obtain a closed set of recursion relations by carrying out $2\times2\rightarrow1\times1$ RSRG or $3\times3\rightarrow1\times1$ RSRG. The reason is that we cannot have nearest-neighbor pairs of monomers in a 1×1 cell, and so the recursion relations do not involve r'. We do obtain a closed set of recursion relations by performing $3\times3\rightarrow2\times2$ RSRG. For p, we renormalize all the paths that enter at one side and exit at the opposite side in the 3×3 cell onto the same kind of paths in the 2×2 cell. The recursion relation is shown symbolically in Fig. 2. Each bond contributes a factor of p and each nearest-neighbor pair of monomers gives a factor of r in the 3×3 cell. The same is true in the 2×2 cell, except that p and r are replaced by the renormalized parameters p' and r'.

To get a recursion relation for r, we look at configurations in which one segment of the polymer enters at side A of the cell and exits at side B (Fig. 3), and a second segment enters at side C and exits at side D. We

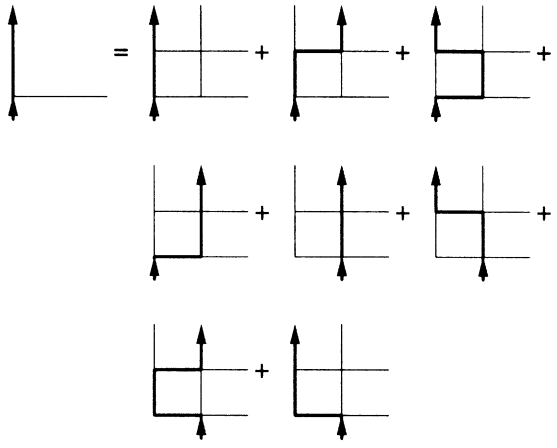

FIG. 1. Schematic representation of the recursion relation for p obtained by applying our $2\times2\rightarrow1\times1$ RSRG to the pure SAW on the square lattice.

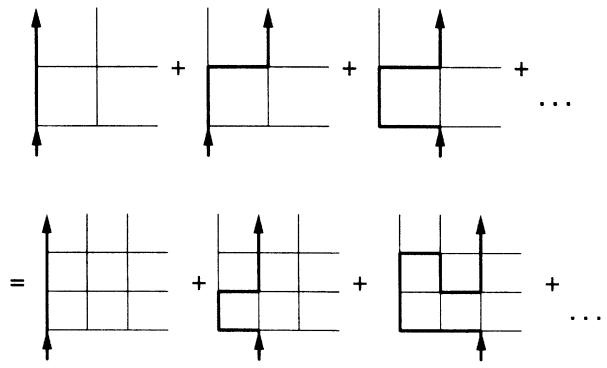

FIG. 2. The symbolic recursion relation for p obtained by applying our $3\times3\rightarrow2\times2$ RSRG technique to the self-attracting SAW on the square lattice. Only a few representative terms are shown for both the original and the renormalized cells.

also require the two segments to have at least one pair of monomers that are nearest neighbors, so the segments interact. The resultant recursion relation is shown schematically in Fig. 4.

A simple computer program was used to enumerate all configurations in the 3×3 cell that contribute to the recursion relations for p and r. We obtain the RG equations

$$2(p')^2+4(p')^3+2(p')^4r'=3p^3+12p^4+(16+8r)p^5+(4+12r+4r^2)p^6+(2+4r+14r^2)p^7+8r^3p^8+8r^4p^9 , \quad (4.1)$$

$$4r'(p')^3+4(r')^2(p')^4=12rp^5+(20r+32r^2)p^6+(12r+20r^2+56r^3)p^7+(4r^2+24r^3+42r^4)p^8+32r^5p^9 . \quad (4.2)$$

We find two nontrivial fixed points and a trivial fixed point located at $p_c=0$ and $r_c=0$. The first nontrivial fixed point has coordinates $p_c=0.3205$ and $r_c=1.4469$. The linearized RG equations have two eigenvalues greater than 1, so this fixed point is a tricritical point[3,4,37] for the self-attracting SAW. We find $\nu_t=0.689$ and $\phi_t=0.462$. Our values for the radius-of-gyration exponent ν_t and the crossover exponent ϕ_t should be compared with the values that Duplantier and Saleur[26] have argued are exact, $\nu_t=\frac{4}{7}$ and $\phi_t=\frac{3}{7}$. The second nontrivial fixed point is an ordinary critical point located at $p_c=0.3586$, $r_c=0$ with radius-of-gyration exponent $\nu_{\mathrm{SAW}}=0.826$. This corresponds to the $T=\infty$ critical point. The value of ν_{SAW} we obtain is within 10% of the exact value[39] $\nu_{\mathrm{SAW}}=\frac{3}{4}$.

The recursion relations (4.1) and (4.2) do not have a fixed point corresponding to the collapsed phase. The reason is that completely collapsed configurations cannot be accommodated in a finite cell. For example, at most two of the six bonds on sides B and D (Fig. 3) of the 3×3 cell may be occupied.

We should point out that Maritan *et al.* have studied this problem previously using a RSRG approach.[40,41] However, in our opinion two questionable approximations are made in their paper. First, the recursion relation for p was obtained by performing $2\times2\rightarrow1\times1$ RSRG, while $4\times2\rightarrow2\times1$ RSRG was used to get the recursion relation for r. We believe that it is preferable to obtain both recursion relations using the same original and renormalized cells. Second, Maritan *et al.* somewhat arbitrarily added some extra terms to their recursion relations. These terms were chosen to ensure the existence of a collapsed phase. Maritan *et al.* obtained the values $\nu_{\mathrm{SAW}}=0.69$ and $\nu_t=0.628$. They did not report a value for ϕ_t.

V. RSRG FOR SELF-ATTRACTING SAT'S

We next study self-attracting SAT's in the absence of any nearest-neighbor interactions. In this case, r is fixed in value to 1 and we must find recursion relations for p and q. We can obtain complete recursion relations for the self-attracting SAT by performing either the $3\times3\rightarrow1\times1$ or the $3\times3\rightarrow2\times2$ RSRG, in contrast to the situation for the self-attracting SAW. First we do the $3\times3\rightarrow2\times2$ RSRG. The rule we use to obtain the recursion relation for p is similar to that used for the self-attracting SAW, but each self-crossing point contributes a factor of q. For example, the contribution coming from the diagram in Fig. 5 is p^9q^2. To get a recursion relation for q, we look at configurations in which one segment of the polymer enters at side A of the cell and exits at side D (Fig. 3), and a second segment enters at side C and exits at side B. For example, the diagram in Fig. 6 gives a term p^8q^2. Thus we get the the recursion relations

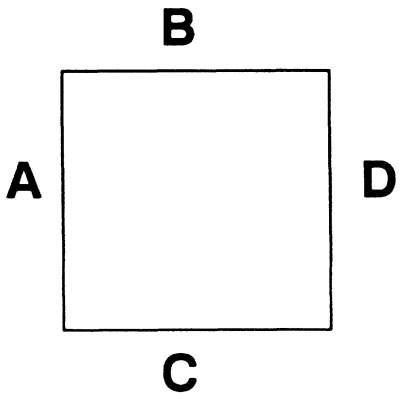

FIG. 3. A cell on the square lattice. The four sides of the cell are A, B, C, and D.

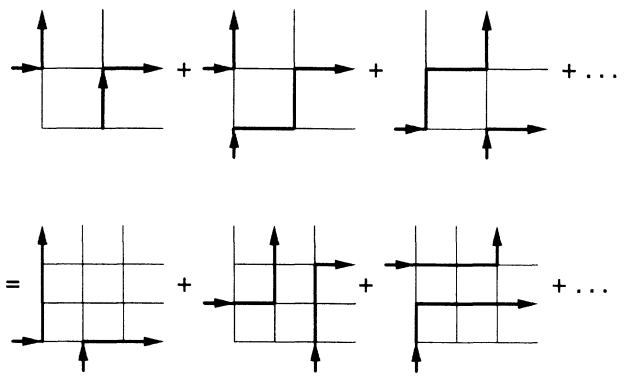

FIG. 4. Schematic representation of the recursion relation for r in our $3\times3\rightarrow2\times2$ RSRG approach to the self-attracting SAW on the square lattice.

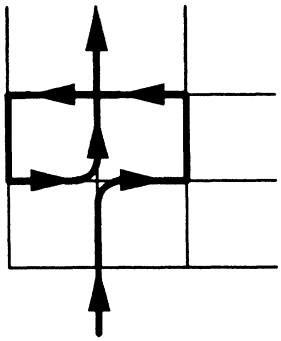

FIG. 5. One possible configuration of the self-attracting SAT on a 3×3 cell. This configuration contributes a term p^9q^2 to the recursion relation for p.

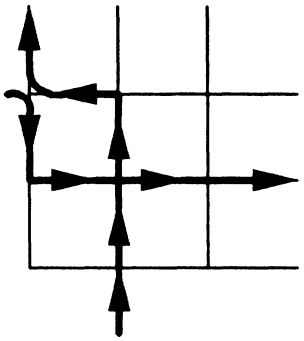

FIG. 6. A second possible configuration of the self-attracting SAT in a 3×3 cell. This configuration contributes a term p^8q^2 to the recursion relation for q.

$$2(p')^2+4(p')^3+2(p')^4=3p^3+12p^4+24p^5+20p^6+20p^7+(8+16q)p^8 +(8+24q+10q^2)p^9+(16q+20q^2)p^{10}+4q^2p^{11}\,, \tag{5.1}$$

$$4q'(p')^4+8q'(p')^5+4(q')^2(p')^6=9qp^6+48qp^7+(108q+16q^2)p^8+(104q+64q^2)p^9 +(56q+76q^2+8q^3)p^{10}+96q^2p^{11}+124q^3p^{12}+120q^4p^{13}+46q^5p^{14}\,. \tag{5.2}$$

We find two nontrivial fixed points and one trivial fixed point that is located at $p_c=0$, $q_c=0$. One nontrivial fixed point is located at $p_c=0.3117$, $q_c=6.561$. The exponents at this tricritical point are $\nu_t=0.625$ and $\phi_t=0.741$. The other nontrivial fixed point is located at $p_c=0.3209$, $q_c=0$ and is an ordinary critical point. We find the radius-of-gyration exponent $\nu_{\rm SAT}=0.896$. This fixed point corresponds to the critical point at $T=\infty$. For the same reason as previously, the RG equations have no fixed point for the collapsed phase.

A great deal of analytical and numerical work in 2D suggests that at infinite temperature, $\nu_{\rm SAT}=\nu_{\rm SAW}=\frac{3}{4}$.[21] Our results for $\nu_{\rm SAT}$ is quite far from this value, which shows that our small-cell RSRG in general is not able to give accurate estimates for the exponents. However, the values we obtain for ν_t and ϕ_t are in reasonable agreement with the values $\nu_t=0.569\pm0.008$ and $\phi_t=0.807\pm0.005$ obtained for self-attracting SAT's on the square lattice using the scanning simulation method.[13,15] Our estimate of ϕ_t differs substantially from most values obtained for the crossover exponent of the self-attracting SAW,[22–31] including the value we found in Sec. IV. Our work, therefore, lends, support to the claim that the collapse transitions of the SAT and SAW are in different universality classes in 2D. Much more convincing support for this claim will be obtained in the following section, however.

For the $3\times3\rightarrow1\times1$ RSRG, the left-hand side of Eq. (5.1) is replaced by p', while the left-hand side of Eq. (5.2) becomes $(p')^2q'$. We again find two nontrivial fixed points. The fixed point for the tricritical point is located at $p_c=0.3013$, $q_c=8.778$. The corresponding exponents are $\nu_t=0.700$ and $\phi_t=0.464$. The fixed point corresponding to the critical point at $T=\infty$ is found at $p_c=0.3156$, $q_c=0$ and has $\nu_{\rm SAW}=0.774$.

Before concluding our discussion of the self-attracting SAT with no nearest-neighbor interactions, we should remark that Jug[42] has also studied this problem using a small-cell RSRG method. Jug's technique is not readily extended to deal with the more general problem with nearest-neighbor interactions, however. Jug finds $\nu_t=0.494$, $\phi_t=0.486$, and $\nu_{\rm SAT}=0.787$.

VI. RSRG FOR SELF-ATTRACTING SAT'S WITH NEAREST-NEIGHBOR INTERACTIONS

So far we have studied the pure self-attracting SAT and the pure self-attracting SAW. The question we now face is whether the tricritical point for pure self-attracting SAT's is in the same universality class as the tricritical point for pure self-attracting SAW's. To investigate this, we generalize the self-attracting SAT problem by introducing nearest-neighbor interactions. We combine the rules we used before for self-attracting SAW's and self-attracting SAT's. In the unrenormalized cell each occupied bond gives a factor of p, each self-crossing gives a factor of q, and each nearest-neighbor pair of monomers gives a factor of r. For example, the configuration in Fig. 7(a) contributes a term p^9qr^2 to the recursion relation for p, the configuration in Fig. 7(b) gives a term p^9q^2r in the recursion relation for q, and the configuration in Fig. 7(c) adds a term $p^{10}qr^4$ to the recursion relation for r. We get the following RG equations for the $3\times3\rightarrow2\times2$ RSRG:

$$2(p')^2+4(p')^3+2(p')^4r'=3p^3+12p^4+(16+8r)p^5+(4+12r+4r^2)p^6+(2+4r+14r^2)p^7+(8r^3+16qr)p^8$$
$$+(8r^4+24qr^2+10q^2)p^9+(16qr^3+20q^2r)p^{10}+4q^2r^2p^{11}\ , \tag{6.1}$$
$$4q'(p')^4+8q'r'(p')^5+4(q')^2(p')^6=9qp^6+(16q+32qr)p^7+(12q+16qr+80qr^2+16q^2)p^8$$
$$+(8qr+24qr^2+72qr^3+64q^2r)p^9+(56qr^4+4q^2+16q^2r+56q^2r^2+8q^3)p^{10}$$
$$+96q^2r^3p^{11}+124q^3r^2p^{12}+120q^4rp^{13}+46q^5p^{14}\ , \tag{6.2}$$
$$4r'(p')^3+4(r')^2(p')^4=12rp^5+(20r+32r^2)p^6+(12r+20r^2+56r^3+16qr)p^7$$
$$+(4r^2+24r^3+42r^4+36qr^2)p^8+(32r^5+16qr^2+24qr^3)p^9$$
$$+44qr^4p^{10}+36q^2r^3p^{11}+24q^3r^2p^{12}\ . \tag{6.3}$$

For the same reason as before, a fixed point for the collapsed phase does not appear in the above equations. We find that the equations have four nontrivial fixed points and a trivial fixed point located at $p_c=q_c=r_c=0$, none of which correspond to the collapsed phase.

The first fixed point is located at $p_c=0.3586$, $q_c=0$, $r_c=0$. There is one eigenvalue that is greater than 1, $\lambda_1=1.6340$. The exponent $\nu_{\rm SAW}$ is 0.826. This point is a critical point that corresponds to the high-temperature phase. The second fixed point is at $p_c=0.320$, $q_c=0$, $r_c=1.447$. There are two eigenvalues that are greater than 1, $\lambda_1=1.3129$ and $\lambda_2=1.8018$. This means that this fixed point is a tricritical point. It is obvious that this point is the tricritical point for self-attracting SAW's because $q_c=0$. The exponent ν_t is 0.689 and the crossover exponent $\phi_t=0.462$. These are the same exponents as we obtained for the pure self-attracting SAW in Sec. IV. The third fixed point is at $p_c=0.3365$, $q_c=7.9423$, $r_c=0$. There are two eigenvalues that are greater than 1, $\lambda_1=1.5849$ and $\lambda_2=2.1571$. This fixed point is the tricritical point of the self-attracting SAT. The reason is that, as we can see from the RG flows in p,q,r space shown in Fig. 8, any point near line II in the $r=1$ plane is renormalized towards this fixed point. We find that the radius-of-gyration exponent ν_t is 0.527 and the crossover exponent ϕ_t is 0.599. The last nontrivial fixed point is a tetracritical point that is located at $p_c=0.3336$, $q_c=7.9069$, $r_c=0.0929$. There are three eigenvalues that are greater than 1, namely $\lambda_1=1.0207$, $\lambda_2=1.6419$, and $\lambda_3=2.1183$. The tricritical radius-of-gyration exponent is $\nu_{\rm tetra}=0.540\,18$, and the two crossover exponents are $\phi_{\rm tetra1}=0.0273$ and $\phi_{\rm tetra2}=0.661$.

A sketch showing the position of these fixed points and the entire RSRG flow is given in Fig. 8. The lines I, II, and III are on the critical surface. Any system that is on the critical surface inside the area bounded by the lines I, II, and III flows to point A, the critical point for $T=\infty$. The fixed point B is the tricritical point for self-avoiding SAT's, while the fixed point C is the tricritical point for self-avoiding SAW's. We call line I a tricritical line because any system on this line flows onto one of the two tricritical points B and C. The tetracritical fixed point D separates the points on the tricritical line that flow toward B from those that flow onto C. It therefore describes the crossover between the two different types of tricritical scaling behavior.

Thus, we find distinct tricritical points for the SAW and SAT, in agreement with the analytical and numerical work that suggests that these θ points are in different universality classes.[7–13,15,16] The exponents we obtain for the self-attracting SAW θ point are the same as we found

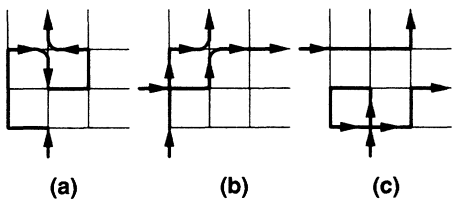

FIG. 7. Three allowed conformations to the self-attracting SAT with nearest-neighbor interactions within a 3×3 cell: (a) contributes a term p^9qr^2 to the recursion relation for p, (b) gives a term p^9q^2r in the recursion relation for q, and (c) adds a term $p^{10}qr^4$ to the recursion relation for r.

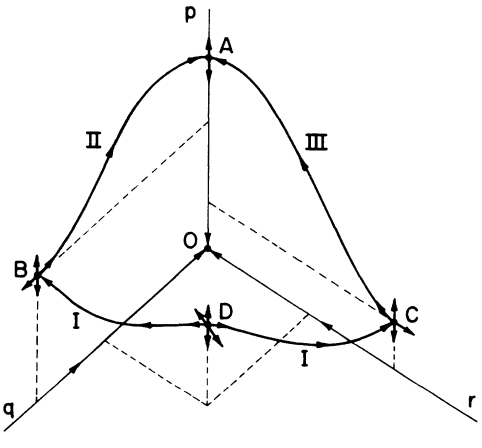

FIG. 8. Renormalization group flows for the self-attracting SAT with nearest-neighbor interactions. Point A is the $T=\infty$ critical point for SAW's and SAT's. Points B and C are the tricritical points for self-attracting SAT's and SAW's, respectively. Point D is a tetracritical point. The flow lines I, II, and III are on the critical surface.

in Sec. IV, since the recursion relations (6.1) and (6.3) reduce to Eqs. (4.1) and (4.2) when q and q' are set to zero. The exponents we find for the self-attracting SAT θ point ($\nu_t = 0.527$ and $\phi_t = 0.599$) should be compared to the values obtained by Meirovitch and Lim[13,15] for this problem, $\nu_t = 0.569 \pm 0.008$ and $\phi_t = 0.807 \pm 0.005$.

Bradley[17,18] has shown that the self-attracting SAW on the Manhattan lattice can be mapped onto the self-attracting SAT on the L lattice, so the collapse transitions in these two models are in the same universality class. This is not in conflict with our conclusion that the SAW and SAT θ points are in different universality classes on undirected lattices, since the Manhattan and L lattices are both directed. Indeed, the θ point of SAW's on the Manhattan lattice is known to be in a different universality class than the collapse transition of SAW's on the undirected square lattice.[18] Lattice directionality is therefore a relevant parameter at the θ point, and our conclusions on undirected lattices cannot be carried over to directed lattices.

Finally, we note that a single ordinary critical point appears in our RSRG, so the high-temperature phases of the SAW and SAT have the same critical exponents in the present approximation. This is in accord with a large body of evidence that suggests that the $T = \infty$ critical points of the SAW and the SAT are in the same universality class.[21]

VII. CONCLUSIONS

In this paper we carried out a small-cell RSRG study of self-attracting SAW's and SAT's in two dimensions. These two problems were first studied separately. For the pure self-attracting SAW, we found exponents for the tricritical point and for the high-temperature critical point that are within 10% of the values that Duplantier and Saleur[26] and Nienhuis[39] have argued to be exact. For the pure self-attracting SAT, the exponents we found for the tricritical point are in good agreement with the most recent numerical work.[13,15] The exponent ν_{SAT} for the high-temperature critical point differed markedly from the accepted value $\nu_{SAT} = \frac{3}{4}$, however.[21] Since our estimate $\phi_t = 0.462$ for the crossover exponent for the self-attracting SAW θ point is far removed from the value we obtained for the self-attracting SAT ($\phi_t = 0.741$), the two θ points are apparently in different universality classes.

To further investigate this issue, we performed a RSRG study of the self-attracting SAT with an additional nearest-neighbor interaction. This problem has the pure self-attracting SAW and SAT as limiting cases. We found two distinct tricritical points, and so again came to the conclusion that the SAW and SAT collapse transitions are in different universality classes. A tetracritical point characterizing the crossover between these two types of tricritical scaling behavior was also found. Finally, a single ordinary critical point appears in our RSRG, confirming that the SAW and SAT share the same high-temperature scaling behavior.

Our work supports the analytical and numerical studies that suggest that the SAW and the SAT θ points are in different universality classes.[7-13,15,16] It might be argued that this support is of limited value since our small-cell RSRG is only approximate. Certainly, if we chose larger cells, the location of the critical points and the values of the critical exponents would be obtained more precisely. However, we believe that the number and kind of the critical points would be unaltered. In particular, we believe that our conclusion that the SAW and the SAT collapse transitions belong to different universality classes would be unaffected by employing larger cells.

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