Models of polymer collapse in three dimensions: Evidence from kinetic growth simulations

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We present simulational evidence that kinetically grown tricolor walks and kinetically grown trails on selected lattices in three dimensions are equivalent to interacting walks and trails at their respective collapse temperatures, all of which model polymers in dilute solution at the θ point. We discuss the relation of these models to the canonical model of a single self-attracting polymer in dilute solution: the self-avoiding walk with nearest-neighbor interactions. The main results concern the divergence of the specific heat and these differ from the predictions of the (three-parameter) Edwards model. The behavior of the kinetic trail simulations also raises doubts about the current field theoretic description of collapse in interacting trails.

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I. INTRODUCTION

There has been continuing interest in statistical mechanical models of the conformations of linear polymers in dilute solution in two and three dimensions [1]. One aim of these studies is to extract the universal (critical) scaling properties of these models, since they should hold exactly for a range of physical systems. It is expected that the models display three distinct behaviors. At high temperatures they should mimic polymers in a "good" solvent, where the excluded volume effect is dominant. Opposing this, at low temperatures the model should describe a collapsed, internally dense, state caused by the attractive interactions of different sections of a polymer mediated by a solvent. At one temperature, known as the θ point, the excluded volume and attractive forces "balance" to give a third, intermediate behavior. This third behavior is often approximated by a simple random walk model. However, it was realized some time ago that the real situation is more complex. In two dimensions, the θ state does not share the scaling features of a random walk [2,3]. In three dimensions the two equivalent descriptions of the θ state are given by the continuum Edwards model with two and three body forces [4,5] and $n \to 0$ limit of the magnetic (tricritical) $(\phi^2)^2-(\phi^2)^3$ O(n) field theory [6–8]. The analysis of these theories is subtle and predicts that $d=3$ is the upper critical dimension of the θ state, and therefore that the critical behavior of this state is given by mean-field theory predictions modified by logarithmic factors. On the other hand, the canonical model of polymer collapse in lattice statistical mechanics has been self-avoiding walks (SAW) on a regular lattice interacting via nearest-neighbor attraction. This model manifestly includes the "excluded volume" condition of real polymers as well as the attraction necessary for collapse. There has not been a direct demonstration that the behavior of this model around its collapse point is given by the Edwards model, although it is widely accepted as such [9].

The partition function of the self-interacting self-avoiding walk model (ISAW) is given by

$$Z_N(\omega)=\sum_{\varphi_N} \omega^m , \tag{1}$$

where the sum is over the set of all self-avoiding walks φ_N of length N with one end at some fixed origin. The Boltzmann weight $\omega=e^{\beta\varepsilon}$ is associated with a nearest-neighbor contact of energy $-\varepsilon$ (which we fix to be -1 without loss of generality). The average of any quantity Q over the ensemble set of allowed paths φ_N of length N is given generically as

$$\langle Q \rangle = \frac{\sum_{\varphi_N} Q(\varphi_N)\omega^m}{\sum_{\varphi_N} \omega^m} . \tag{2}$$

We define a normalized finite-size internal energy per step by

$$U_N=\frac{\langle m \rangle}{N} \tag{3}$$

and a normalized finite-size specific heat per step by

$$C_N=\frac{\langle m^2 \rangle-\langle m \rangle^2}{N} . \tag{4}$$

The limiting values of these are related in the usual way to the reduced free energy, given by

$$f(\omega)=\lim_{N\to\infty} -\frac{1}{N}\ln Z_n(\omega) . \tag{5}$$

Specifying a walk by the sequence of position vectors $\mathbf{r}_0 \equiv 0, \mathbf{r}_1, \ldots, \mathbf{r}_N$ the average mean-square end-to-end distance is

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$$\langle R_e^2 \rangle_N = \langle \mathbf{r}_N \cdot \mathbf{r}_N \rangle \ . \tag{6}$$

The scaling behavior of the above quantities as N becomes large defines the phase of the system. As the temperature is varied there should be a tricritical collapse transition at some $\omega=\omega_t$. Hence, as expounded above, there are three distinct asymptotic behaviors expected. For high temperatures ($\omega<\omega_t$) the excluded volume interaction is the dominant effect and the behavior is universally the same as the noninteracting SAW problem. Therefore the partition function and average root-mean-square end-to-end distance are expected to scale as

$$Z_N(\omega) \sim A\mu^N N^{\gamma_+ - 1} \tag{7}$$

and

$$\sqrt{\langle R_e^2 \rangle_N} \sim B N^{\nu_+} \ , \tag{8}$$

with A, B, and μ expected to vary with temperature and be nonuniversal, while the exponents γ_+ and ν_+ are expected to be constant and universal. The current best Monte Carlo estimate of ν_+ in three dimensions is 0.5877(6) [10]. The connective "constant" $\mu(\omega)$ is related to the reduced free energy $f(\omega)$ of the system as

$$\mu(\omega) = \exp[-f(\omega)] \ , \tag{9}$$

and this holds at all temperatures. One can also consider the partition function for closed walks (loops), which is expected to scale as

$$Z_N^{\text{loops}}(\omega) \sim D\mu^N N^{\alpha_+ - 2} \ , \tag{10}$$

where the (three-dimensional) hyperscaling relation

$$2-\alpha_+ = 3\nu_+ \tag{11}$$

is expected to hold. The finite-size internal energy U_N and specific heat C_N should converge to (temperature dependent) constants $U_\infty(\omega)$ and $C_\infty(\omega)$, respectively.

For low temperatures ($\omega>\omega_t$) it is accepted that the partition sum is dominated by configurations that are internally dense and the average root-mean-square end-to-end distance scales as

$$\sqrt{\langle R_e^2 \rangle_N} \sim B N^{\nu_-} \ , \tag{12}$$

with $\nu_- = \frac{1}{3}$. The partition function should scale differently [11] to that at high temperatures since a collapsed polymer should have a well defined surface (and associated surface free energy). Therefore

$$Z_N(\omega) \sim A\mu^N \mu_s^{N^{2/3}} N^{\gamma_- - 1} \ , \tag{13}$$

with $\mu_s<1$. Note that A, B, μ, and μ_s are temperature dependent. Again the internal energy U_N and specific heat C_N should converge to $U_\infty(\omega)$ and $C_\infty(\omega)$, respectively.

The collapse transition at $\omega=\omega_t$ is expected to be tricritical in nature and so should conform to a crossover scaling theory [12]. The crossover from high and low temperature behavior to that exactly at the collapse point is controlled by a crossover exponent ϕ. For example, for temperatures close to ω_t and large lengths N, the root-mean-square end-to-end distance is expected to behave as

$$\sqrt{\langle R_e^2 \rangle_N} \sim B_1 N^{\nu_t} \mathcal{R}(B_2 y) \ , \tag{14}$$

where $y=tN^\phi$ is the scaling variable with $t=(\omega_t-\omega)/\omega_t$, while B_1 and B_2 are nonuniversal constants. The function $\mathcal{R}$ has asymptotic properties for large arguments (positive and negative) so as to asymptotically match the high and low temperature behaviors:

$$\mathcal{R}(gy) \sim \begin{cases} E_+ y^{(\nu_+ - \nu_t)/\phi} & \text{as } y \to \infty \\ E_0 \quad \text{as } y \to 0 \\ E_- |y|^{(\nu_- - \nu_t)/\phi} & \text{as } y \to -\infty \ . \end{cases} \tag{15}$$

In three dimensions $\nu_t = \frac{1}{2}$ and there may be confluent and/or additive logarithmic corrections to these power laws. Exactly at the θ point the scaling of the partition function should be

$$Z_N(\omega) \sim A\mu^N N^{\gamma_t - 1} \ . \tag{16}$$

The mean-field value $\gamma_t=1$ is expected to hold in three dimensions. Similarly, the loop partition function has the same form as at high temperatures with α_t substituted for α_+, and hyperscaling should hold with

$$2-\alpha_t = 3\nu_t \ , \tag{17}$$

implying that $\alpha_t = \frac{1}{2}$. The thermodynamic limit specific heat $C_\infty(\omega)$ has a singularity at $\omega=\omega_t$ and its singular part behaves as

$$C_\infty^{\text{sing}}(\omega) \sim C_s t^{-\alpha} \ . \tag{18}$$

Note that this specific heat exponent is different from the exponent α_t which is defined in terms of the loop partition function. There is a tricritical scaling relation connecting α to the crossover exponent ϕ as

$$2-\alpha = 1/\phi \ . \tag{19}$$

At fixed Boltzmann weight $\omega=\omega_t$ the singular part of the internal energy and specific heat scale as

$$U_N^{\text{sing}} \sim U_t N^{(\alpha-1)\phi} \tag{20}$$

and

$$C_N^{\text{sing}} \sim C_t N^{\alpha\phi} \ . \tag{21}$$

Of course, U_N always approaches a constant so that the singular part is a finite-size correction. However, C_N may diverge, in which case the singular part will dominate the behavior in the large N limit. In three dimensions it is expected that $\alpha=0$ and so three dimensions is a marginal scenario. Therefore let us define a new "exponent" ζ characterizing the logarithmic divergence of C_N if $\alpha=0$:

$$C_N \sim C_t (\ln N)^\zeta \ . \tag{22}$$

The canonical (power law) exponents in three dimensions are believed to take on mean-field values, as mentioned, and these are collected in Table I.

TABLE I. The canonical values of the exponents for the collapse transition in three dimensions, the Edwards model, and the kinetic growth models simulated in this work. The logarithmic corrections to these power laws are, however, not all identical.

Exponent	Three-dimensional collapse
ν	$\frac{1}{2}$
γ_t	1
α_t	$\frac{1}{2}$
ϕ	$\frac{1}{2}$
α	0

In three dimensions fixed at the collapse temperature (equivalent to $\omega=\omega_t$ in the ISAW model) the Edwards model and tricritical O(n) field theory predict the following corrections to mean-field theory. The partition function for open configurations is given by

$$Z_N \sim A\mu^N \left[1-\frac{49}{484}\frac{1}{\ln N}\right] . \tag{23}$$

The mean-square end-to-end distance is predicted to behave like

$$\langle R_e^2 \rangle_N \sim BN \left[1-\frac{37}{363}\frac{1}{\ln N}\right] , \tag{24}$$

while the finite-size specific heat values asymptotically diverge as

$$C_N \sim C_t (\ln N)^{3/11} . \tag{25}$$

Monte Carlo studies [13,14] of ISAW and interacting trails (see below) have not verified these predictions. However, the lengths of walk/trails considered have been relatively short ($N<300$) due to the difficult nature of simulations of longer walks. Therefore it is desirable to look for models of collapsing polymers for which one can generate long configurations more easily.

Kinetic growth walks (KGW) [15–17] and smart kinetic growth walks (SKW) [18,19] were introduced a decade ago as dynamic models of polymerization. Kinetic growth walks [15–17] in two and three dimensions are defined simply as random walks which at each time step choose from the available sites keeping the self-avoidance condition strictly. On regular lattices these walks were found to eventually stop by entering self-made traps and their size scales in the same way as static noninteracting SAW. In contradiction to this behavior, smart kinetic growth walks [18] in two dimensions were explicitly constructed not to trap (configurations only close by loop formation). This was done by adding a "dressing" around the walk on the dual lattice that distinguishes the left- and right-hand sides of the walk as it is constructed, and forbidding steps that do not allow the further construction of the dressing. This effectively means that a walk can only enter places where there is at least one escape route. These SKW trace out the hulls of percolation clusters at threshold [18] and their size exponent has been later deduced to be the same as that of θ-point polymers. In fact, it was shown [19] that closed SKW defined on the honeycomb lattice are equivalent to static interacting self-avoiding loops with nearest-neighbor and next-nearest-neighbor attraction. Unfortunately SKW are difficult to generalize to three dimensions due to the nonlocal information that is required there.

However, a clever generalization *has* been recently found [20–22] and is known as tricolor walks (TCW). These are defined on the Wigner-Seitz cells of the body centered cubic (WS-bcc) lattice, and a three color dressing is added to the dual of this lattice to give the walk the "smart" property. The exact construction of this model is explained in great detail in [21]. We note that the WS-bcc lattice has coordination number 4. It was found that these tricolor walks have a fractal dimension close to 2 and map onto an interacting SAW model with nearest- and next-nearest neighbor interactions. It was then deduced that these kinetic walks may provide information about the collapse transition in three dimensions. In comparison, the SKW on the honeycomb lattice [23], KGW on the Manhattan lattice [24,25,3,26], which are smart by virtue of the lattice, and kinetic trails (see below) on the square lattice [27] have all provided information about the collapse of two-dimensional polymers. Since it has been argued [20–22] that tricolor walks might behave in an equivalent manner (that is, they might be related to collapsing polymers in three dimensions), it is of interest to investigate this matter further. In the two-dimensional cases the new ingredient in the most recent simulations has been the calculation of the internal energy and specific heat. This allows one to investigate whether the specific heat diverges or not: a sure sign of the existence of a transition. In this work, we simulate tricolor walks, calculating the specific heat, among other quantities, in an attempt to identify the critical nature of the static equivalent of TCW.

Another lattice model of polymer configurations studied extensively is that of trails [28–31]. These are paths on a lattice which have no two steps on the same bond of that lattice but may occupy the same site. This restriction is sometimes referred to as bond-avoiding, in contrast to self-avoiding walks which are site avoiding (that is, no two vertices of the walk may occupy the same site on the lattice). Clearly walks are, by default, also bond avoiding. Trails possess an excluded volume effect and it is believed that trails and SAW are in the same universality class [32,33] which describes good solvent polymers. It has been shown [29] that there should exist a collapse transition when contact attraction is added to the trail model. Moreover, Shapir and Oono [29] have argued that this point should be tricritical in nature, as it is at the ISAW collapse point. However, they predict that ISAW and interacting self-avoiding trails (ISAT) are in different universality classes. Importantly, while the upper critical dimension for ISAW is expected to be $d_u=3$, the Shapir-Oono field theory gives $d_u=4$ for ISAT. Therefore they expect generically that in three dimensions $\nu_t \neq \frac{1}{2}$ and $\gamma_t \neq 1$ (that is, the exponents do not take on mean-field values—of course it is always possible that some exponents fortuitously take on a mean-field

value below an upper critical dimension but this should not be the case with all exponents if hyperscaling is obeyed).

We define a general ISAT model in the following way. Consider a regular lattice of coordination number $2q$ and configurations φ_N of trails of length N starting from a fixed origin. Let m_k, $k=2,\ldots,q$ be the number of sites of the lattice that has been visited k times by the trail. The partition function of the general model is

$$Z_N(\omega_2,\ldots,\omega_q)=\sum_{\varphi_N}\omega_2^{m_2}\cdots\omega_q^{m_q}\ , \tag{26}$$

where ω_k is the Boltzmann weight associated with k-visited sites. The canonical model is one where every segment of the trail at some contact site interacts with every other segment at that site, so that

$$\omega_k=\omega^{\binom{k}{2}} \quad \text{for } k=2,\ldots,q\ , \tag{27}$$

with $\omega\equiv\omega_2$. Now, two other reasonably natural models are defined by

$$\omega_k=\omega^{k-1} \quad \text{for } k=2,\ldots,q \tag{28}$$

and

$$\omega_k=\omega \quad \text{for } k=2,\ldots,q\ . \tag{29}$$

It would be expected that each model possesses a collapse transition at some value of ω and that the transition falls into the same universality class. Of course, if the coordination number of the lattice is $2q=4$ then the only possibility is a single contact and all three models are isomorphic. The canonical model has been investigated in two and three dimensions using exact enumeration [30,34,31] and Monte Carlo techniques [35,14,36]. In two dimensions recent work [27] provides a body of evidence that reinforces the hypothesis that ISAT and ISAW are truly in different universality classes. This work was accomplished using a kinetic growth algorithm. It would be desirable, of course, to consider three-dimensional trail collapse since the topological difference between walks and trails only occurs in two dimensions. A path in two dimensions separates different areas of space so the crossings of trails make them topologically different. This property only occurs in two dimensions.

The growth model of kinetic trails (KGT) was introduced by Lyklema [37] for reasons similar to those that led to the introduction of kinetic walks. It is defined as follows: choose a starting site on a coordination $2q$ lattice and dynamically construct a trail by adding steps at integer time intervals, choosing at each time step equally from the available nearest-neighbor sites that do not violate the bond-avoiding condition. This produces trails of any length with a particular distribution different to that of noninteracting (static) trails. Except for the first step, if the kinetic trail is not on a site that has been visited previously, there are $2q-1$ choices and the probability of each is simply $1/(2q-1)$. If the trail has previously visited the site j times the choice is restricted to $2q-2j-1$ possibilities and the probability is $1/(2q-2j-1)$. One can see a step that has been visited k times in total has an associated probability of

$$P_{q,k}=\frac{1}{(2q-1)(2q-3)(2q-5)\cdots(2q-2k+1)}\ . \tag{30}$$

Lyklema [37] found estimates of the analogs of the exponents ν and γ for the square ($q=2$) and cubic ($q=3$) lattices. A kinetic trail on a regular lattice of coordination number $2q$ can be mapped onto a static interacting SAT model with fixed weights

$$\omega_k=(2q-1)^k P_{q,k}=\frac{(q-\frac{1}{2})^k}{(q-\frac{1}{2})_k}\ . \tag{31}$$

The connective constant of the partition function is then $\mu=2q-1$. As opposed to SKW and TCW every static open trail configuration occurs as a kinetic trail. Moreover, if we choose a coordination number $2q=4$ lattice so that a site can only be visited once or twice, the KGT maps precisely onto the canonical static trail problem described above.

In this work we utilize the mapping of the tricolor walk and kinetic trails onto static problems to investigate the properties of these static models in three dimensions. In addition to the tricolor walk which is defined on the Wigner-Seitz cells of the body-centered cubic lattice we consider kinetic trails on the diamond (coordination $2q=4$), cubic (coordination $2q=6$), and WS-bcc (coordination $2q=4$) lattices. This permits us to investigate the universality of interacting trails, in addition to the behavior of a kinetic trail that is isomorphic to a canonical static model on a coordination number $2q=4$ lattice. Our main results come from the calculation of the specific heat. While the TCW static model equivalent is not the canonical model, the length of the simulated walks allows the comparison of the logarithmic corrections of a lattice model of collapse to that of the Edwards model. Universality would suggest that the tricolor walk gives the behavior of the canonical ISAW as well. We realize that this is a debatable issue but point out that in two dimensions a similar debate seems to have resolved itself in favor of a wide universality of the collapse transition.

II. SIMULATIONS AND ANALYSIS TECHNIQUES

We have generated kinetic growth trails and tricolor walks of various lengths up to 2^{20} steps. The occupied sites of the walk were stored by means of a hash table [38], with the hash index being computed from the coordinates. This enables efficient testing of self-avoidance without having to store the whole lattice, so that the generation of a walk of length N requires time $O(N)$ only. The size of the hash table needs to exceed the maximal walk length only slightly, so that the memory requirement is also $O(N)$. When a walk reaches the desired maximal length or gets trapped, a new one gets generated, thereby ensuring the statistical independence of the walks sampled at fixed length.

We have calculated the proportion left open at various stages Q_N, the root-mean-square end-to-end distances R_N, and information on the number of contacts for the

calculation of the internal energy U_N and the specific heat C_N with estimates of statistical errors. With the recent focus on the reliability of random number generators [39] we mention that we have used an implementation of a mixed linear congruential algorithm [40] that has proved to be comparatively reliable.

Although the generated walks are independent of each other, we have highly correlated data between different lengths, as every walk of a given length has contributed to all data sets of shorter length. We notice that this can be effectively overcome by calculating quantities using an exponential spacing.

We simulated the model on an unbounded lattice to investigate the bulk behavior. For the sake of comparison, it took 30 CPU seconds to generate one walk of length 2^{20} on an IBM RISC 6000/560 computer. We have simulated 2.9×10^4 trails on the simple cubic lattice, 7.8×10^4 trails on the diamond lattice, 1.4×10^4 trails on the Wigner-Seitz bcc lattice, and 2.4×10^4 tricolor walks.

III. TRAILS

We now present the analysis of the simulations of the kinetic trails. These simulations were carried out on the simple cubic lattice (sc), the diamond lattice (diamond), and the lattice given by the Wigner-Seitz cells of the body-centered cubic lattice.

We first considered the behavior of the mean-squared end-to-end distance $R_N^2=\langle R_e^2\rangle_N$. For this we plotted in Fig. 1 R_N^2/N versus $N^{-1/2}$. One sees that this ratio approaches a constant as $N\to\infty$ with the finite-size corrections being of the order of some inverse power $\Delta\approx0.5$ of N, i.e.,

$$R_N^2\sim RN(1-R'N^{-\Delta}) . \tag{32}$$

The length scale exponent is therefore

$$\nu_{\mathrm{KGT}}=\tfrac{1}{2} . \tag{33}$$

The limiting value of the ratio R_N^2/N is correlated with the sparsity of the lattice, being smallest for the relatively dense bcc lattice and largest for the rather thin WS-bcc lattice. We note that in contrast to Eq. (23) the correction term is certainly not $O(1/\ln N)$.

Next, we considered the probability P_N of generation of trails of length N or larger. In Fig. 2 we plotted this quantity versus $N^{-1/2}$, resulting in straight lines. P_N does not decay to zero, but to a finite number P_∞ relatively close to one, showing that a kinetic trail grows indefinitely with a finite probability.

$$P_N\sim P_\infty+P'N^{-1/2} . \tag{34}$$

P_∞ decreases with the sparsity of the lattice. As the partition function for open configurations is related to P_N by

$$Z_N^{\mathrm{open}}\sim(2q-1)^N P_N , \tag{35}$$

where $2q$ is the coordination number of the lattice. This implies an exponent

$$\gamma_{\mathrm{KGT}}=1 \tag{36}$$

and a free energy equal to $\ln(2q-1)$. On the other hand, the linear behavior of the plot in Fig. 2 shows that the trapping rate

$$Q_N=P_N-P_{N+1} \tag{37}$$

decays as $N^{-3/2}$. Q_N is equal to the probability of loop formation, which is related to the loop partition function via

$$Z_N^{\mathrm{loops}}\sim(2q-1)^N Q_N . \tag{38}$$

Therefore open and closed trails have the same free energy and by equating the decay rate of Q_N with the power-law correction of Z_N^{loops} we get the

$$\alpha_{\mathrm{KGT}}=\tfrac{1}{2} . \tag{39}$$

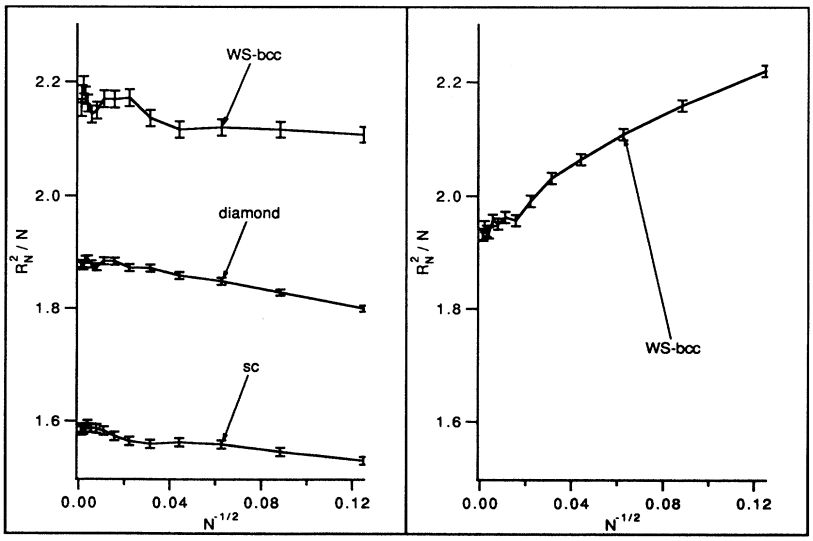

FIG. 1. For each of the three-dimensional (3D) simulations R_N^2/N is plotted against $N^{-1/2}$. For each of the kinetic trails the data are plotted on the left while the tricolor walk data are plotted on the right. Here, as in the next pictures, the error bars are indicated explicitly.

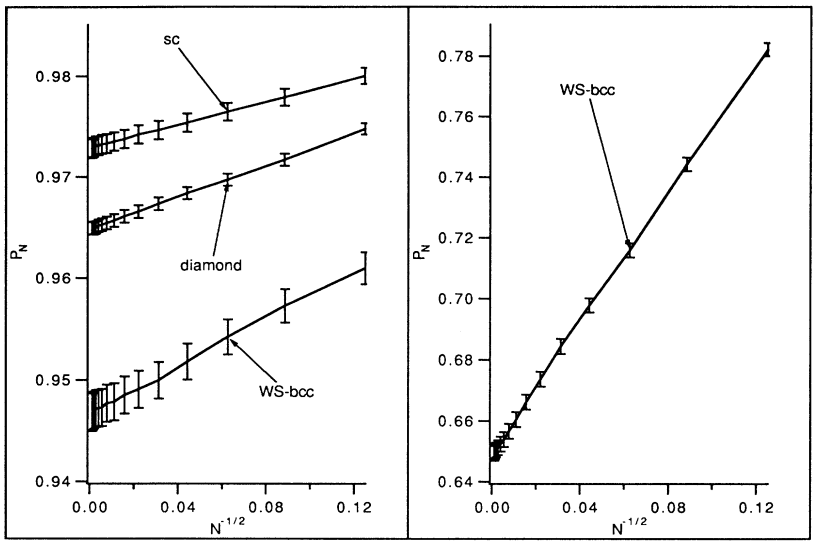

FIG. 2. For each of the 3D simulations the probability that a path has not yet trapped, Q_N, is plotted against $N^{-1/2}$. For each of the kinetic trails the data are plotted on the left while the tricolor walk data are plotted on the right.

The scaling of the internal energy U_N is depicted in Fig. 3. For the lattices with coordination number 4, U_N is directly related to the mean number of contacts per step, whereas for the simple cubic lattice it is some weighted combination of the mean number of two- and three-visited sites per step. We see that U_N behaves as

$$U_N \sim U_\infty - UN^{-1/2} , \tag{40}$$

with U_∞ increasing with the sparsity of the lattice.

Most importantly, the results for the specific heat C_N are given in the upper part of Fig. 4. (For coordination number 4, C_N is simply related to the fluctuation of the average number of contacts.) We see that for all three models the specific heat *diverges* as N increases. Moreover, the divergence is significantly weaker than a power law would suggest. On the other hand, C_N plotted versus the logarithm of N indicates a possible power-law dependence in $\ln N$. Assuming

$$C_N \sim C(\ln N)^{\zeta} \tag{41}$$

we calculated the local slopes ζ_N of $\ln C_N$ versus $\ln\ln N$, which are plotted versus $1/\ln N$ in the lower part of Fig. 4. The errors in the simulation of WS-bcc trails are too large to allow any exponent extrapolation, so that we restrict ourselves to the simple cubic and diamond lattices. It is evident that there is a strong drift in ζ_N (we point out that if there was a power-law dependence of N and not of $\ln N$, the estimators ζ_N would have to diverge and not decrease, as they do here). However, the exponent estimates for both models seem to coincide, and we estimate

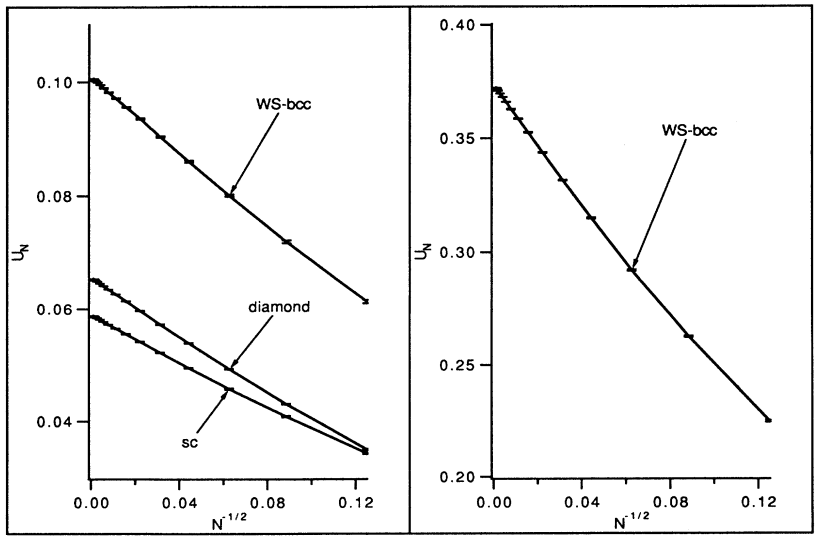

FIG. 3. For each of the 3D simulations the finite-size internal energy U_N is plotted against $N^{-1/2}$. For each of the kinetic trail simulations the data are plotted on the left while the tricolor walk data are plotted on the right.

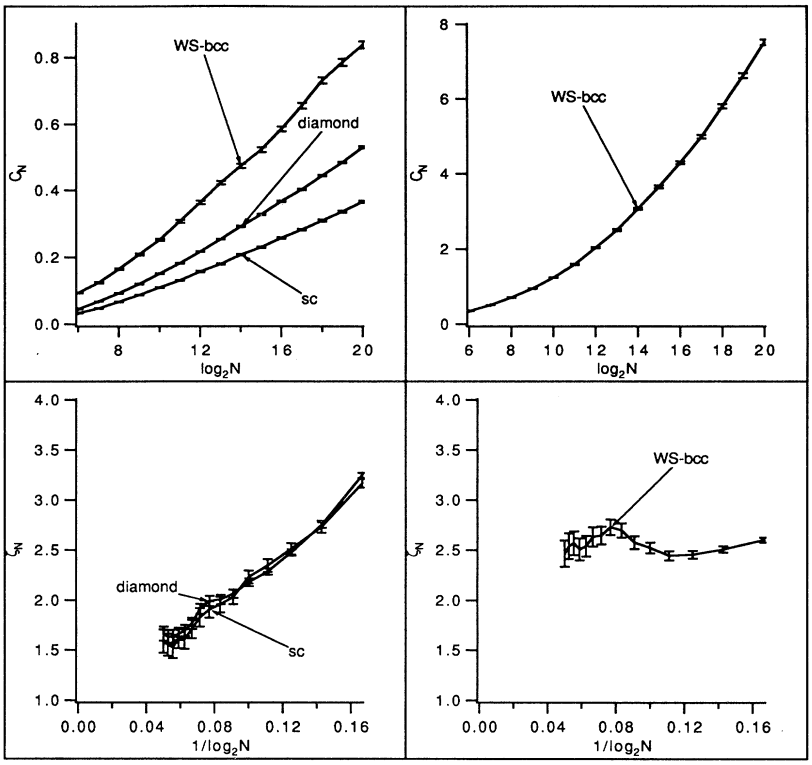

FIG. 4. The finite-size specific heat C_N for each of the 3D simulations plotted vs the $\log_2 N$ in the top two graphs. The slow increase indicates a power-law divergence in that variable. For each of the kinetic trail simulations data are plotted on the left while the tricolor walk data are plotted on the right. The bottom two graphs are local estimates ζ_N of the power law of the logarithmic divergence in each case (except for the trails on the WS-bcc lattice) plotted against $1/(\log_2 N)$.

$$\zeta_{\mathrm{KGT}}=1.0\pm0.5\ . \tag{42}$$

We are fairly confident that we are able to exclude the exponent $\zeta=\frac{3}{11}$ from the Edwards model [see Eq. (25)].

Taking all of this together, we have compelling evidence that the model of kinetic trails is equivalent to a model of interacting trails at its collapse transition. The exponents associated with this transition have been shown to assume their mean-field values. Moreover, as C_N diverges logarithmically and the singular part of U_N decays with $N^{-1/2}$ (with possibly logarithmic corrections), we see that we indeed have tricritical behavior with an associated crossover exponent of

$$\phi_{\mathrm{trails}}=\tfrac{1}{2}\ . \tag{43}$$

However, the results are in contradiction with both the prediction for ISAW from the Edwards model and with the prediction that the upper critical dimension for ISAT is $d_u=4$.

IV. TRICOLOR WALKS

We perform an analysis analogous to that described in the preceding section on the data from the tricolor walk simulations.

The data for the mean-squared end-to-end distance, which is shown in Fig. 1, show that

$$\nu_{\mathrm{TCW}}=\tfrac{1}{2}\ , \tag{44}$$

and that we have a power-law correction with an exponent of $\Delta\approx0.5$. [If one simply estimates ν_{TCW} without assuming corrections to scaling one obtains $\nu_{\mathrm{TCW}}=0.498(5)$.] However, in contrast to both the behavior of kinetic trails and the predictions from the Edwards model, the asymptotic value is approached *from above.*

The probabilities P_N show the same behavior as for trails (see Fig. 2), except that P_∞ is significantly smaller than in all the trail models investigated. The free energy is ln3, and we obtain

$$\gamma_{\mathrm{TCW}}=1 \quad \text{and} \quad \alpha_{\mathrm{TCW}}=\tfrac{1}{2}\ . \tag{45}$$

The internal energy U_N scales also as for trails, and is significantly larger than in the simulated trail models. The specific heat C_N diverges and again shows a power-law dependence in $\ln N$. However, the plot of ζ_N shows that the finite-size corrections are rather small compared to the trail simulations. We also get a value for the exponent ζ which is significantly larger than for trails,

$$\zeta_{\mathrm{TCW}}=2.5\pm0.5\ . \tag{46}$$

The prediction $\zeta=\frac{3}{11}$ from the Edwards model is clearly outside the error range. Summarizing, we have strong evidence that the model of TCW is equivalent to a model of interacting walks at its collapse transition. The exponents associated with this transition have been shown to assume their mean-field values and we have tricritical behavior with a crossover exponent

$$\phi_{\mathrm{walks}}=\tfrac{1}{2}\ . \tag{47}$$

V. CONCLUSIONS

The conclusions from the mappings and simulations are various. We have found that the specific heat of the three-dimensional tricolor kinetic walk diverges logarithmically. This kinetic walk had already been shown to be equivalent to an interacting walk model in three dimensions at a particular temperature [20–22]. Hence we conclude that this temperature is indeed the collapse point, as had been tentatively suggested previously. Moreover, the power of the logarithmic divergence differs from that found from field theoretic methods applied to the (three-parameter) continuum Edwards model [4,5]. If this were indeed the case it may be explained by denying the universality of collapse in three dimensions (that is, the static model equivalent to TCW is not representative of the universality class of ISAW at the collapse point) or by the failure of the Edwards model.

We have studied kinetic trails [37] on three three-dimensional lattices and have found a divergent specific heat for these models also. We have pointed out that these kinetic trails can all be mapped onto interacting trail systems with particular attractive couplings. As expected, whether the model contains multiple contact interactions is irrelevant to the universality class. Hence for trails in three dimensions there is no $\theta-\theta'$ problem [41,42]. The divergence of the specific heat differs from that of the TCW model and the Edwards model. This is consistent with the two-dimensional confirmation that interacting walks and trails are in different universality classes. However, we have found that the exponent $\nu_t=\frac{1}{2}$ in contradiction to the predictions in [29,34,43].

Finally, we would like to point out that the particular advantage of the models investigated is that their structure permits one to generate configurations whose lengths are *three orders of magnitude* larger than is currently realizable with conventional Monte Carlo techniques. This advantage is clear for the model of interacting trails, where a direct comparison to Monte Carlo simulations is possible (see, e.g., [14]).

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