The Collapse Point of Interacting Trails in Two Dimensions from Kinetic Growth Simulations

A. L. Owczarek[1] and T. Prellberg[1,2]

We present simulational evidence that kinetic growth trails on the square lattice are equivalent to interacting trails at their collapse temperature. As a consequence we give values for most of the canonical exponents of the trail collapse transition: these are significantly different from those proposed for interacting walks. We can also interpret our results in terms of the equivalent Lorentz lattice gas and find that this model does not display diffusion, as has been previously thought. Rather, the mean square displacement grows as $t \log t$ in time t.

1. INTRODUCTION

The canonical model in statistical mechanics of polymer conformations in solution has been self-avoiding walks on a regular lattice. This model manifestly includes the "excluded volume" condition of real polymers. Another model of polymer configurations studied extensively, and defined on a lattice, is that of trails.[1-4] These are paths on a lattice which have no two steps on the same bond of that lattice but may occupy the same site (for the square lattice see Fig. 1). This restriction is sometimes referred to as bond avoiding, in contrast to self-avoiding walks (SAW), 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 both these models, without further embellishment, should describe the universal properties of polymer conformations in a so-called 'good' solvent (that is, one that does not induce

---

[1] Department of Mathematics, University of Melbourne, Parkville, Victoria 3052, Australia.
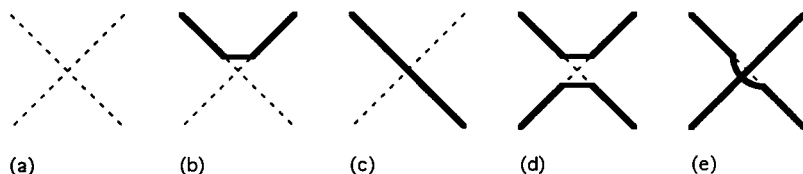[2] email: aleks,prel@mundoe.maths.mu.oz.au.

Fig. 1. The allowed vertex configurations (that do not differ by rotation) on the square lattice, with the heavy bold lines representing sections of the loop. Configurations (d) and (e) do not occur in walks and are those that are weighted in the ISAT problem. However, configuration (d) is topologically similar to a nearest-neigbor configuration that does occur in walks. On the other hand, configuration (e) has no counterpart in a walk system.

strong attractive interactions between sections of the polymer). It is believed that trails and SAW are in the same universality class[5, 6] which describes these good solvent polymers. In two dimensions the fractal dimension d_f of these objects is accepted to be 4/3, and so they are not compact, but rather swollen with respect to a random walk ($d_f = 2$). Moreover, the configurational properties of self-avoiding walks have been mapped formally to the statistics of the magnetic $O(n)$ model in the limit $n \rightarrow 0$[7-9] and so one can see directly that the long-length limit of SAW can be viewed as a critical phenomenon. This is clearer still in the grand ensemble of SAW (SAW of all lengths with a step fugacity) where the temperature of the $O(n)$ model is simply related to the step fugacity.

To model situations where the complex, solvent-mediated, monomer–monomer interactions affect a polymer's conformation, an attractive energy is associated with nonconsecutive nearest-neighbor sites on a SAW. For a trail the energy is usually associated with contact or multiply visited sites [configurations (d) and (e) of Fig. 1]. It is seen experimentally[10, 11] that as the temperature or solvent quality is decreased, a polymer in solution undergoes a rapid change in its size and collapses from an extended object (as compared to a random walk) to a compact one (fractal dimension equal to that of the space) at some value of these parameters. This is known as the θ-point[12] and is now believed to be a thermodynamic critical point. In the step-fugacity–polymer-temperature plane the θ-point is believed to be a tricritical point.[13]

The collapse transition of polymers in dilute solution has been the subject of intensive investigations in recent years, especially in two dimensions since the work of Duplantier and Saleur (DS)[14]. They predicted the exact values for the exponents at the tricritical point using the Coulomb gas method. Numerical evidence[15, 16] from studies of interacting self-avoiding walks (ISAW) has been ambiguous. However, an exact solution on the Manhattan lattice[17, 18] has lent weight to the DS values. In this

context, the collapse transition of interacting trails (ISAT) has also been studied. There is a prediction[2-4] that ISAT should be in a different universality class from ISAW. Again numerical results in two dimensions[19, 20, 16] have been inconclusive and results tend to show several of the exponent estimates to be similar for the two models (for a recent review see ref. 21).

In this paper we tackle the question of the universality class of collapsing trails by arguing that one can map kinetic growth trails[22] (see below for a definition) onto ISAT at their collapse temperature. Thereby, we deduce the scaling of the important quantities in the ISAT model. These are markedly different from those predicted for the DS model[14, 23, 24] for walks and numerically confirmed for a related model[25] and those recently shown to be exact for ISAW on the Manhatten lattice.[17, 18] We therefore argue that the universality classes of ISAW and ISAT are indeed different, despite noninteracting SAW and trails belonging to the same universality class. (Our evidence, while strong, being numerical, does not constitute a proof.)

The model of interacting trails on the square lattice is defined as follows. Consider all different bond-avoiding paths of length N that can be formed on the square lattice with one end fixed at a particular site (the set $\mathscr{C}$). Associate an energy $-\varepsilon$ with each doubly visited site. For each configuration count the number m of doubly visited sites of the lattice and give that configuration a Boltzmann weight $w^m = \exp(\beta \varepsilon m)$. The partition function of the ISAT model is then given by

$$Z_N(w) = \sum_{\mathscr{C}} \exp(\beta \varepsilon m) \tag{1}$$

The average root-mean-square end-to-end distance $R_N(w)$ is defined similarly on this distribution.

For high temperatures the partition function and average root-mean-square end-to-end distance are expected to scale as

$$Z_N(w) \sim A\mu^N N^{\gamma - 1} \tag{2}$$

and

$$R_N(w) \sim BN^\nu \tag{3}$$

with A, B, and μ expected to vary with temperature and be nonuniversal, while γ and ν are expected to be constant, universal, and take on the values for noninteracting trails (and hence SAW). The connective 'constant' μ is related to the free energy $f(\beta)$ of the system as

$$\mu = \exp[-\beta f(\beta)] \tag{4}$$

The exact exponent values in two dimensions, from the work of Nienhuis on SAW,[26] are believed to be $v = 3/4$ and $\gamma = 43/32$.

For low enough temperatures 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

$$R_N \sim BN^{1/2} \tag{5}$$

The partition function should scale differently[27] from that at high temperatures, since a compact polymer should have a well-defined surface (and associated surface free energy). Hence

$$Z_N(w) \sim A\mu^N \mu_s^{N^{1/2}} N^{\gamma_c - 1} \tag{6}$$

with $\mu_s < 1$. Note that A, B, μ, and μ_s are temperature dependent.

It has been shown[2] that there should exist a collapse temperature β_t such that v takes on a value v_t between the high and low-temperature ones. For the sake of comparison the value[14] of v_t for ISAW is believed to be 4/7, which is also the exponent related to the size of the hulls of percolation cluster[28, 29] at threshold. Moreover, Shapir and Oono[2] showed that this point should be tricritical in nature, as it is at the ISAW collapse point. As mentioned above, it is an open question whether the ISAW and ISAT collapse points are in the same universality class. For ISAT at an estimated collapse point it has been further estimated that $v_t = 0.569 \pm 0.008$,[30] which includes the value $4/7 \approx 0.571$. (However, the estimates of v_t are known to be very sensitive to the assumed value of the critical temperature.) The scaling of the partition function should be of the high-temperature mathematical form with a different value of the exponent γ, denoted γ_t. For tricritical (θ-like) points there exists a scaling theory[31] defining the behavior of physical quantities around this point in the temperature–length (or step fugacity) plane. The crossover from high- and low-temperature behavior to that right at the collapse point is controlled by a crossover exponent ϕ. For example, for temperatures close to β_t and large lengths N the root-mean-square end-to-end distance is expected to behave as

$$R_N \sim B_t N^{v_t} \mathcal{R}(etN^\phi) \tag{7}$$

where $t = (\beta_t - \beta)/\beta_t$, while B_t and e 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.

It is also interesting to consider polymer models in the presence of a boundary where an attractive surface potential is added in order to explore

a possible adsorption transition. One usually considers polymers attached at one or both ends to a surface and defines the respective partition functions $Z_N^{(1)}(w, w_s)$ and $Z_N^{(11)}(w, w_s)$. For example, defining the appropriate configurational set $\mathscr{C}^{(1)}$, one finds that the partition function of trails attached to an interactive surface is

$$Z_N^{(1)}(w, w_s) = \sum_{\mathscr{C}^{(1)}} w^m w_s^{m_s} \tag{8}$$

where m_s is the number of surface contacts. For fixed bulk weight w it is expected that an adsorption transition takes place as a function of w_s. The average number of surface contacts $M_{s,N} = \langle m_s \rangle$ is expected to be bounded as a function of N for all fixed w_s less than some value w_s^{ad}, while it is expected to scale linearly with N for $w_s > w_s^{ad}$. At this special value $w_s = w_s^{ad}$ the average number of surface contacts $M_{s,N}$ is expected to scale with some power of N between 0 and 1 indicative of the transition. Similarly, the partition functions $Z^{(1)}$ and $Z^{(11)}$ have associated exponents γ_1 and γ_{11} which take on different values depending on whether w_s is below, at, or above the adsorption point (also known as the special point). (The exponents for $w_s < w_s^{ad}$ are known as the ordinary values—these designations arise form a comparison to magnetic systems.) Importantly, all these exponents depend on whether the bulk temperature is above, at, or below the collapse point. Above bulk criticality the surface exponents should take on their SAW values, while below criticality the adsorption transition is expected to be first order.

The growth model of kinetic trails was introduced by Lyklema[22] as a description of polymerization. It is defined as follows. Choose a starting site on a square 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 from 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 three choices and the probability of each is simply 1/3. Otherwise, the choice is restricted to only one possibility, ignoring the effect of the start, and the probability is 1. One can easily see then that each 'probability 1' step is associated with a contact (doubly visited site). Lyklema[22] found estimates of the analogs of the exponents $\nu \approx 0.535$ and $\gamma \approx 1.025$ (this value for γ is a misprint which should have been quoted as 0.975 according to the data—in any case, it is close to 1).

Meirovitch *et al.*[19] and Bradley[32] carefully showed that the kinetic growth loops, with a modified starting position, could be mapped exactly

onto the static problem of interacting self-avoiding trails that are closed at a particular temperature (equivalent to Boltzmann weight $w_{KGT} = e^{\beta\varepsilon} = 3$). Meirovitch et al.[19] noted the proximity of the estimates of w_t to 3 and the possibility that they may coincide. Bradley rather noted that the work of Meirovitch and Lim[33, 30] gave $w_t = 2.962(6)$ and thus excluded $w = w_{KGT}$ as the possible collapse value. Given this estimate of the critical temperature, he tentatively concluded, not unreasonably, that $\beta\varepsilon = \log 3$ lay in the collapsed phase. This would indicate that Lyklema's exponent estimates should eventually cross over to the collapsed values.

In an extensive numerical study of the related Lorentz lattice gas,[34, 35] known as the Ruijgrok–Cohen mirror model,[36–38] Ziff et al.[38] apparently confirmed the prediction of Bradley when they found that ν was indeed 1/2. However, they found the presence of logaritmic corrections to some quantities.

As mentioned above, it was recently[27] illustrated that a different scaling form (6) was possible for the low-temperature polymer-problem partition function from that at high temperatures. The scaling form implied by the work of Ziff et al.[38] for the partition function is incompatible with the conjecture[27] for the collapsed phase and this led us to reexamine the problem of kinetic trails. Also recently, Bradley's work on kinetic walks on the Manhattan lattice[17] has been extended by the simulation of these walks keeping track of the internal energy and specific heat with a view to calculating the crossover exponent. This has proved successful,[17, 25] with the bonus that Bradley's mapping have been extended to surface properties. Here, we report on a similar study with kinetic growth trails.

2. SIMULATIONS OF KINETIC GROWTH TRAILS

We have generated kinetic growth trails of various lengths up to 10^6 steps. The occupied sites of the walk were stored by means of a hash table,[39] 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[40] we mention that we have used an implementation of a mixed linear congruential algorithm[41] 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 use finite-size approximations for the exponent estimations. For instance, if a quantity scales asymptotically with N as

$$X_N \sim CN^\lambda, \quad \lambda > 0 \qquad \text{or} \qquad X_N \sim A + CN^\lambda, \quad \lambda < 0 \qquad (9)$$

we use finite-size estimators λ_N defined as

$$\lambda_N = \log_2 \frac{X_N}{X_{N/2}} \qquad \text{or} \qquad \lambda_N = \log_2 \frac{X_N - X_{N/2}}{X_{N/2} - X_{N/4}} \qquad (10)$$

If justifiable, we then graphically extrapolate these estimations toward infinity. Using various different scales to do this gives a rather good idea about the type of finite-size corrections involved.

First we simulated the model on an unbounded lattice to investigate the bulk behavior. For this, we generated 1.226×10^7 samples of trails up to a length $N = 10^4$; 2.66×10^6 of length 10^5; and 4.5×10^5 of length 10^6. For the sake of comparison, it took 66 CPU days to generate the trails of length 10^6 on a IBM RISC 6000/560.

In a fashion similar to the work on the Manhattan lattice,[17] one can extend Bradley's mapping to consider trails on the half-plane (see Fig. 2). In this way it is possible to explore a range of surface potentials and thereby consider nonattractive surfaces (the ordinary point) and look for the adsorption transition (special point). We generated 5.5×10^5 samples of trails of lengths up to 5×10^4 with adsorbing boundary conditions which gives boundary conditions that mimic the bulk, and hence no surface attraction, which is the ordinary point. We also generated 10^6 samples of maximum length 2.0×10^5 with completely reflecting boundary conditions, which is equivalent to a boundary weight of $w_s = 3$, and we argue this is the special point. We calculated the number of surface contacts in these simulations in addition to the survival rate.

Our first result from the bulk simulations is that not only is the specific heat at $w_{KGT} = 3$ diverging, but the local exponent estimates increase as a function of the trail length (see Fig. 3). The conclusion that the temperature given by $w_{KGT} = 3$ is the exact collapse temperature is in conflict with the above-mentioned Monte Carlo results.[30] To resolve this conflict, we note that these Monte Carlo results were extracted from trails
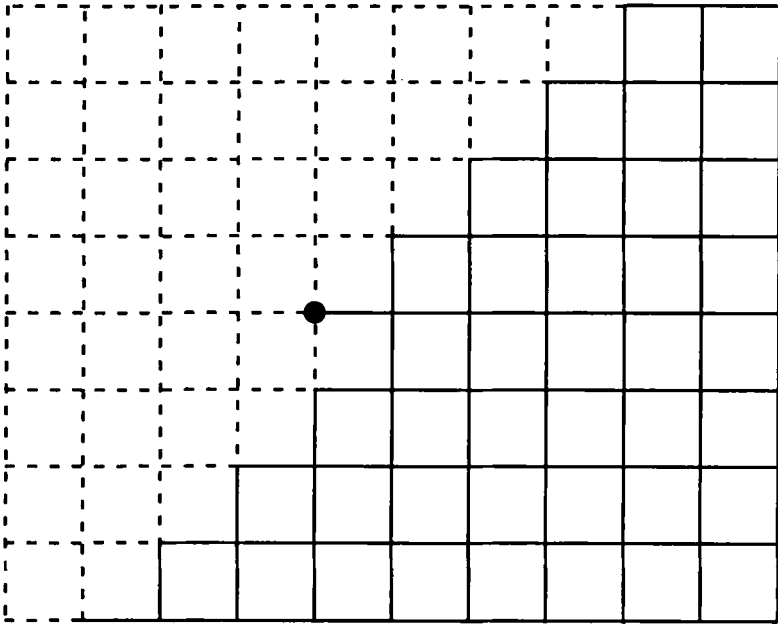
Fig. 2. The boundary shape of the lattice used in the surface simulations. The dashed part of the lattice indicates that part of the lattice unused by the trail. A trail can move along the surface freely and at every second site can choose with probability $1 - p_s$ to cross the boundary and enter the dashed section of the lattice. In this case the trail is terminated and a new configuration begun. For the ordinary point, absorbing boundary conditions, with $p_s = 2/3$, are used, while for the special point, reflecting boundary conditions, with $p_s = 1$, are utilized. Every trail begins at the site marked with the bullet.

of lengths around $N = 200$. However, in ref. 17 we showed for a similar model that one might have to consider much longer configurations to be able to eliminate the influence of finite-size corrections to scaling.

Using the scaling relation $2 - \alpha = 1/\phi$, we obtained local estimates of the exponents α and ϕ of the form[31]

$$C_N \sim CN^{\alpha\phi} \tag{11}$$

where C is a constant. We see that there is a weak drift of the exponent estimates as the walk length increases, and we extrapolate tentatively

$$\phi = 0.88 \, {}^{+0.07}_{-0.05} \tag{12}$$

Given the monotonic change of the exponent estimates, we are rather confident that the crossover exponent is larger than 0.8. However, as we have reason to expect the presence of logarithmic corrections, we cannot exclude with certainty that the crossover exponent might be equal to one.
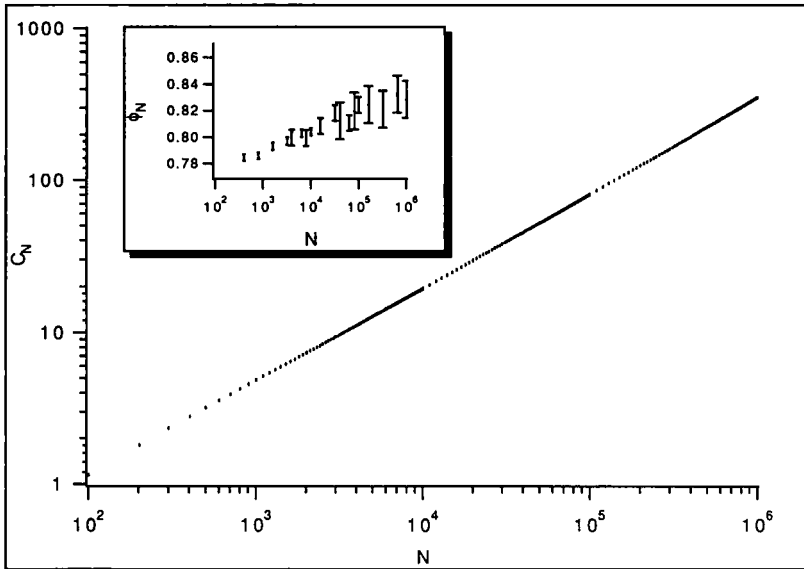
Fig. 3. The finite-size specific heat C_N plotted versus the length N in a double-logarithmic plot, indicating a power-law divergence. The inset shows local estimates ϕ_N of the crossover exponent ϕ from the specific heat data, indicating a strong drift of the estimates. Here, as in the next figures, either the error bars are indicated explicitly or the data converged within graphical accuracy.

The consistency of this approach has been checked by calculating estimates of the exponents α and ϕ from the internal energy, which is expected to scale as

$$U_N \sim U_\infty - UN^{(\alpha-1)\phi} \tag{13}$$

where U is a constant and again $2 - \alpha = 1/\phi$. We get comparable exponent estimates (see Fig. 4), providing reasonable evidence that the tricritical scaling relation holds and certain evidence that $w = w_{KGT}$ is the collapse transition point. Hence we are able to be far more confident that the collapse transition is at $w = w_{KGT}$ than we are about its nature. However, the evidence does still suggest a tricritical scaling.

Now we examine the partition function scaling. In Fig. 5 we plot the inverse of the probability Q_N that a trail has not trapped after N steps versus $\log N$. We find, in agreement with Ziff et al.,[38] a linear dependence, so that
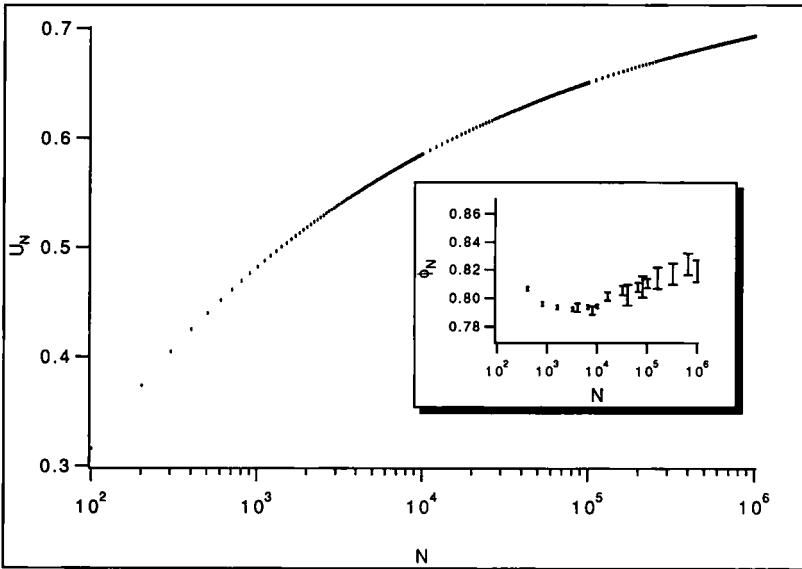
$$Q_N \sim \frac{Q}{\log N} \tag{14}$$

Fig. 4. The finite-size internal energy U_N plotted versus the length N in a double-logarithmic plot. The inset shows local estimates ϕ_N of the crossover exponent ϕ from the internal energy data. Again there is a strong drift of the estimates.

where Q is a constant. Inserting $Z_N \sim 3^N Q_N$, we get

$$Z_N \sim Q \frac{3^N}{\log N} \tag{15}$$

This partition function scaling is certainly different from the one in the extended phase. Since Q_N is bounded above, the high-temperature scaling can be ruled out. Moreover, the scaling (15) is inconsistent with the expected partition function scaling form in the collapsed phase (6).[27] This provides further evidence that $w_{KGT} = 3$ is the collapse transition point.

Next we consider the end-to-end distance scaling. Here we use the fact that the model of kinetic trails has a reinterpretation as a lattice gas. Following Ziff et al.,[38] the model of kinetic trails is isomorphic to paths in the Lorentz lattice gas[34, 35] model known as the Ruijgrok–Cohen mirror model[36–38] with a scatterer concentration $c = 2/3$. One original interest[36, 37] in the mirror model lay in the calculation of the diffusion coefficient D. From ref. 38, Eq. (19), it follows that this diffusion coefficient is bounded below (and is asymptotically dominated) by the product of the average
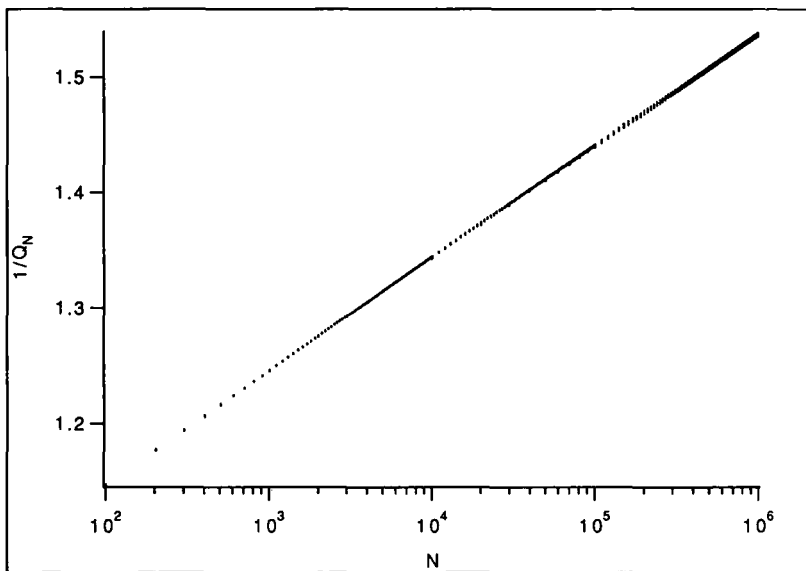
Fig. 5.   The inverse of the probability of open trails Q_N plotted versus the logarithm of the length N, indicating linear behavior.

mean-square end-to-end distance R_N^2 and the probability of open trails Q_N, normalised by $4N$; that is,

$$D > \frac{R_N^2 Q_N}{4N} \tag{16}$$

Originally, it was expected that this model exhibits diffusion,[36] which in turn implies that the length scale exponent is equal to $1/2$, and this view was supported by simulational evidence based on simulations of walks up to lengths of 4000 steps.[37] Using our data, we plot in Fig. 6 this lower bound, which now appears to diverge logarithmically. We therefore conclude that there is no diffusion constant and moreover that the system exhibits superdiffusive rather than the more usual subdiffusive behavior[42] that sometimes arises in these lattice gases.

Reinterpreting this result in connection with the partition function scaling, we see that $R_N^2 Q_N / 4N \sim C_1 \log N$ implies

$$R_N \sim R N^{1/2} \log N \tag{17}$$

Therefore, we have indeed $\nu = 1/2$, however, with a logarithmic correction. Note that even assuming the diffusion constant existed, R_N still would have
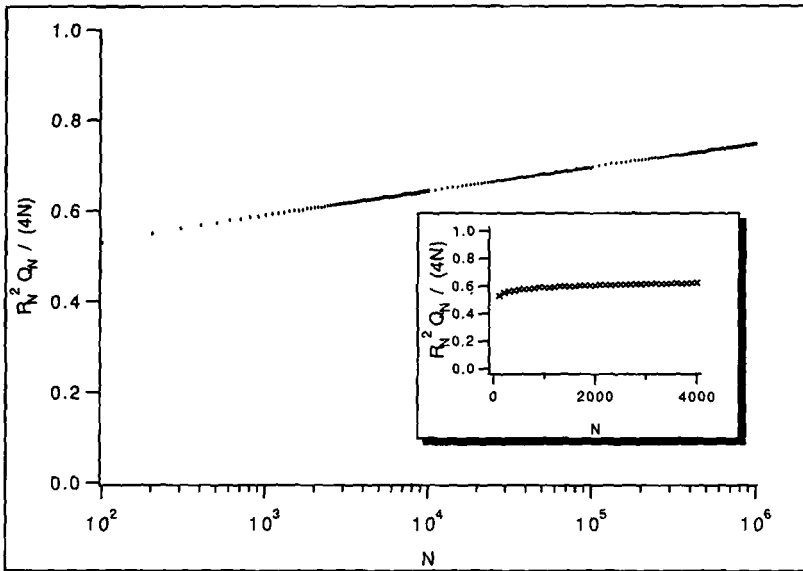
Fig. 6. A lower bound of the mean square displacement in the mirror model with $c = 2/3$ is given by the contributions $Q_N R_N^2$ from open trail configurations. This gives a lower bound $Q_N R_N^2/(4N)$ of the diffusion coefficient D. The deviation from diffusive behavior is shown by the linear increase of this bound in log N. The inset shows a plot of the same quantity on a linear scale for short walks for comparison with Fig. 2 in ref. 37, thereby highlighting the understandable difficulty in finding this logarithmic growth.

a confluent logarithmic correction.[38] Although we obtain the exponent value $\nu = 1/2$ expected in the collapsed phase, this does not imply that we are in the collapsed phase. Considering the density of the configurations $\rho_N \sim C_2 N/R_N^2$, we can conclude that

$$\rho_N \sim C_3(\log N)^{-2} \tag{18}$$

so that the density in fact decreases to zero logarithmically. Note again that Ziff et al.[38] could have come to a similar conclusion, albeit with different power to the logarithm. This zero-density conclusion is in contradiction to the definition of the collapsed phase, where a nonzero density is expected. We therefore conclude again that $w = w_{KGT}$ is the collapse transition point.

Let us now turn to the surface simulations. By considering the half-plane shown in part in Fig. 2 and our earlier ideas,[17] one can understand that the generation of kinetic growth trails on this half-plane can also lead to the statistics of ISAT interacting with a surface. This surface potential is controlled by choosing the probability of passing across the surface. When

a configuration passes across the surface the trail is stopped and a new configuration is begun. The usual partition functions $Z_N^{(1)}$ and $Z_N^{(11)}$ are then proportional to the probabilities Q_N of trails being open at a certain length N, and absorbing into the surface (as the site at which the walk starts cannot be revisited by construction, they cannot form loops), respectively.

Let us first consider completely absorbing boundary conditions, corresponding to $w_s = 1$. Here the probability P_N of adsorption at step N is related to the probabilities of survival Q_N via

$$P_N = Q_N - Q_{N+1} \tag{19}$$

Assuming a power law decay of Q_N, we can therefore deduce that

$$\gamma_{11}^{\text{ord}} = \gamma_1^{\text{ord}} + 1 \tag{20}$$

and using the Barber scaling relation
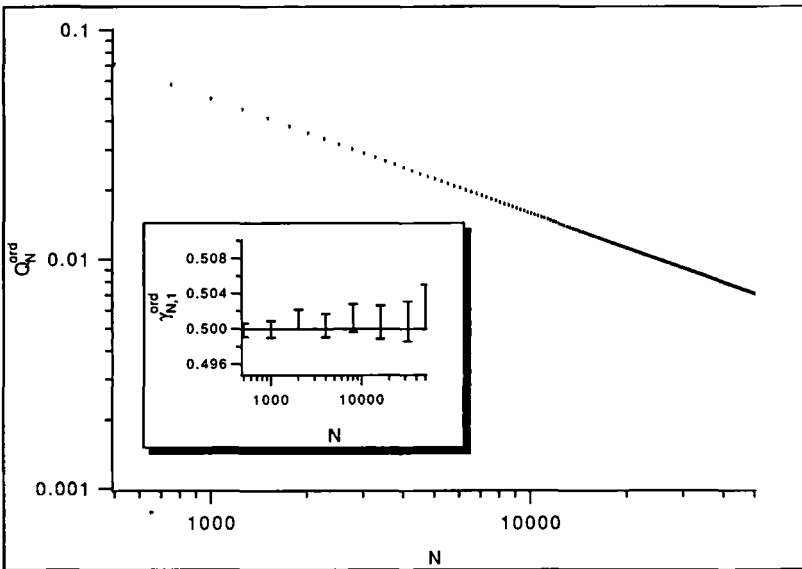
$$\gamma + \nu = 2\gamma_1 - \gamma_{11} \tag{21}$$

Fig. 7. The probability of open trails Q_N^{ord} in the presence of an absorbing boundary plotted versus the length N in a double-logarithmic plot, indicating a power-law decay. The inset shows local estimates $\gamma_{1,N}^{\text{ord}}$ of the closure exponent γ_1^{ord}. The horizontal line corresponds to the value $\gamma_1^{\text{ord}} = 1/2$.

with $\gamma = 1$ and $\nu = 1/2$, it follows that

$$\gamma_{11}^{ord} = -1/2 \qquad \text{and} \qquad \gamma_1^{ord} = 1/2 \tag{22}$$

To test this argument, we measure the probability Q_N^{ord} that trails are open at length N. Figure 7 shows a pure power-law decay, leading to a value of $\gamma_1^{ord} = 0.501(3)$, which confirms the above scaling argument.

With completely reflecting boundary conditions (which correspond to $w_s = 3$) we have by construction $Q_N = 1$, so that also $\gamma_1 = 1$. Therefore we are in a different scaling regime, which we thus identify with the special transition. Using Eq. (21) gives

$$\gamma_{11}^{sp} = 1/2 \qquad \text{and} \qquad \gamma_1^{sp} = 1 \tag{23}$$

To confirm that ($w = 3$, $w_s = 3$) is the surface adsorption point (at bulk collapse), we measured the number of surface contacts $M_{s,N}$ as a function of N. We reiterate from the introduction that below the adsorption transition, this quantity is expected to be bounded, and above it, it is expected to scale linearly with N, whereas at the special transition we expect a non-trivial power-law behavior

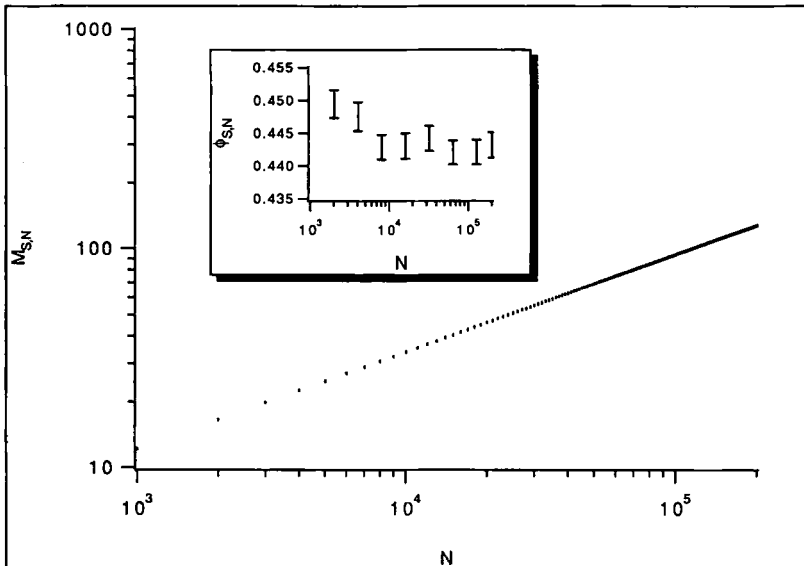$$M_{s,N} \sim MN^{\phi_s} \tag{24}$$

Fig. 8. The mean number of surface contacts $M_{s,N}$ in the presence of a reflecting boundary plotted versus the length N in a double-logarithmic plot, indicating a power-law dependence. The inset shows local estimates $\phi_{s,N}$ of the surface crossover exponent ϕ_s.

with some constant M. Figure 8 shows that our data are consistent with a well-defined surface crossover exponent $\phi_s \approx 0.44(1)$, which hence confirms that the point $w_s = 3$ is the special transition temperature (w_s^{ad}). This adsorption point has exponents different from those expected when the bulk is either at high or low temperatures. Hence, the very existence of a criticial adsorption point lends further credence to the argument that $w = w_{KGT}$ is the bulk collapse point.

3. CONCLUSION

We have studied the simulations of kinetic growth trails on the square lattice in the bulk and near a surface for long times (up to 10^6). Using the established (in the bulk and extended to surfaces) mapping to static self-avoiding trails interacting via contact attraction, we have argued that the temperature of this mapping, given by $w = 3$, lies precisely at the collapse point. This is the best hypothesis for the data accumulated and stems from (at least) five arguments culled from the data:

- The specific heat diverges and the crossover exponent is clearly greater than 0.8.
- We have tested the scaling relation $2 - \alpha = 1/\phi$, which should be valid only at the tricritical point, by calculating ϕ independently from the internal energy, and hence probed the consistency of the data.
- The internal density goes to zero logarithmically as a function of length, which violates physical ideas of the collapsed phase.
- The partition function scaling differs from that expected at low temperatures.[27]
- The surface simulations give a well-defined value of ϕ_s, which should not be possible at low temperatures, where surface adsorption is believed to be first order.

Table I. Best Estimates and Exact Conjectures for the Bulk Exponents for the Collapse Transaction of ISAT from Kinetic Growth Trail Simulations[a]

Exponent	ν	γ_t	α_t	ϕ	α
KGT	1/2(log)	1(log)	1(log)	$0.88^{+0.07}_{-0.05}$	$0.86^{+0.09}_{-0.07}$
DS walks	4/7	8/7	6/7	3/7	$-1/3$

[a] The annotation (log) indicates the presence of confluent logarithmic factors. These are to be compared to the values for the Duplantier and Saleur walk model.

Table II. Best Estimates and Exact Conjectures for the Surface Exponents for the Collapse Transition of ISAT from Kinetic Growth Trail Simulations[a]

Exponent	γ_1^{ord}	γ_{11}^{ord}	γ_1^{sp}	γ_{11}^{sp}	ϕ_s
KGT	1/2	−1/2	1	1/2	$0.440^{+0.005}_{-0.010}$
DS walks	4/7	−4/7	8/7	4/7	8/21

[a] The annotation (log) indicates the presence of confluent logarithmic factors. These are to be compared to the values for the Duplantier and Saleur walk model.

We believe these points taken together present a consistent view of the collapse transition in trails being at the temperature given by $w = w_{KGT} = 3$ (it is, however, still possible that some unseen pathology invalidates our conclusion). Our exact conjectures and numerical estimates of all the exponents are given in Tables I and II, and are seen to be quite different from those of the DS model.[14, 23, 24] On the other hand, while the collapse point has been identified, its tricritical nature has not been confirmed with great accuracy.

The results also shed light on the existence of a diffusion constant in the long-time limit of the related Lorentz lattice gas (Ruijgrok–Cohen mirror model). Our simulations show that the diffusion 'constant' diverges logarithmically and hence does not exist.

ACKNOWLEDGMENTS

REFERENCES

1. A. Malakis, *Physica* **84**:256 (1976).
2. Y. Shapir and Y. Oono, *J. Phys. A* **17**:L39 (1984).
3. H. A. Lim, A. Guha, and Y. Shapir, *J. Phys. A* **21**:773 (1988).
4. I. S. Chang, A. Guha, H. A. Lim, and Y. Shapir, *J. Phys. A* **21**:L559 (1988).
5. A. J. Guttmann, *J. Phys. A* **18**:567 (1985).
6. A. J. Guttmann, *J. Phys. A* **18**:575 (1985).
7. P.-G. de Gennes, *Phys. Lett.* **38A**:339 (1972).
8. J. des Cloizeaux, *J. Phys. (Paris)* **36**:281 (1975).
9. P. D. Gujrati, *Phys. Rev.* **24**:2096 (1981).
10. D. Napper, *Polymeric Stabilisation of Colloidal Dispersions* (Academic Press, London, 1983).

11. J. des Cloizeaux and G. Jannink, *Polymers in Solution* (Clarendon Press, Oxford, 1990).
12. P. Flory, *Principles of Polymer Chemistry* (Cornell University Press, Ithaca, New York, 1953).
13. P. G. de Gennes, *J. Phys. Lett. (Paris)* **36**:L55 (1975).
14. B. Duplantier and H. Saleur, *Phys. Rev. Lett.* **59**:539 (1987).
15. H. Meirovitch and H. A. Lim, *Phys. Rev. Lett.* **62**:2640 (1989).
16. I. S. Chang and H. Meirovitch, *Phys. Rev. Lett.* **69**:2232 (1992).
17. T. Prellberg and A. L. Owczarek, *J. Phys. A* **27**:1811 (1994).
18. M. T. Batchelor, A. L. Owczarek, K. Seaton, and C. M. Yung, Surface critical behaviour of an $O(n)$ loop model related to two Manhatten lattice walk problems, *J. Phys A.* (1994), to appear.
19. H. Meirovitch, I. S. Chang, and Y. Shapir, *Phys. Rev. A* **40**:2879 (1989).
20. I. S. Chang, H. Meirovitch, and Y. Shapir, *Phys. Rev. A* **41**:1808 (1990).
21. H. A. Lim, *Int. J. Mod. Phys.* **3**:385 (1992).
22. J. Lyklema, *J. Phys. A* **18**:L617 (1985).
23. C. Vanderzande, A. L. Stella, and F. Seno, *Phys. Rev. Lett.* **67**:2757 (1991).
24. A. Stella, F. Seno, and C. Vanderzande, *J. Stat. Phys.* **73**:21 (1993).
25. D. Bennett-Wood, A. L. Owczarek, and T. Prellberg, *Physica A* **206**:283 (1994).
26. B. Nienhuis, *Phys. Rev. Lett.* **49**:1062 (1982).
27. A. L. Owczarek, T. Prellberg, and R. Brak, *Phys. Rev. Lett.* **70**:951 (1993).
28. A. Coniglio, N. Jan, I. Majid, and H. E. Stanley, *Phys. Rev. B* **35**:3617 (1987).
29. H. Saleur, *J. Phys. A* **20**:455 (1987).
30. H. Meirovitch and H. A. Lim, *Phys. Rev. A* **39**:4186 (1989).
31. R. Brak, A. L. Owczarek, and T. Prellberg, *J. Phys. A.* **26**:4565 (1993).
32. R. M. Bradley, *Phys. Rev. A* **41**:914 (1990).
33. H. Meirovitch and H. A. Lim, *Phys. Rev. A* **38**:1670 (1988).
34. P. M. Binder, *Complex Systems* **1**:559 (1987).
35. M. H. Ernst and P. M. Binder, *J. Stat. Phys.* **51**:981 (1988).
36. T. M. Ruijgrok and E. G. D. Cohen, *Phys. Lett.* **133**:415 (1988).
37. X. P. Kong and E. G. D. Cohen, *Phys. Rev. B* **40**:4838 (1989).
38. R. M. Ziff, X. P. Kong, and E. G. D. Cohen, *Phys. Rev. A* **44**:2410 (1991).
39. D. Knuth, *The Art of Computer Programming, Vol. 3: Sorting and Searching* (Addison-Wesley, Reading, Massachusetts, 1969).
40. P. Coddington, Syracuse University Preprint SSC5 526 (1993).
41. P. L. L'Ecuyer and S. Cote, *ACM Trans. Math. Soft.* **17**:98 (1991).
42. X. P. Kong and E. G. D. Cohen, *Physica D* **47**:9 (1991).