Surface critical behaviour of the interacting self-avoiding trail on the square lattice

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Abstract
The surface critical behaviour of the interacting self-avoiding trail is examined using transfer matrix methods coupled with finite-size scaling. Particular attention is paid to the critical exponents at the ordinary and special points along the collapse transition line. The phase diagram is also presented.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Lattice self-avoiding walks have been used as models for real, linear polymers in solution for over 3 decades [1]. The quality of the solvent may be introduced by the inclusion of short-ranged interactions in the model; typically an attractive energy is included for non-consecutive nearest-neighbour occupied lattice sites. This model is the standard interacting self-avoiding walk (ISAW) model or the \( \Theta \)-point model [2, 3]. The model has been shown to accurately predict the critical behaviour of a wide range of real linear polymers in solution, not only in the high-temperature phase, but also at the collapse transition, which occurs as the temperature is lowered, at the \( \Theta \) temperature. The model is successful because it captures the strong entropic repulsion between different portions of the polymer chain (the self-avoidance), as well as the effect of the difference of affinity between monomer–monomer contacts and monomer–solvent contacts (attractive interaction).

Whilst the relevant physical dimension in polymer physics would usually be \( d = 3 \), the ISAW model has been much studied in two dimensions. This is partly motivated by the realization that \( d = 3 \) is the upper critical dimension of the collapse transition, and that the model in two dimensions provides an interesting playground. In this paper we shall concentrate on the two-dimensional square lattice.

One could ask whether the ISAW is a special model, or whether other models which include the same basic ingredients would have the same critical behaviour. Two related
models were introduced to examine this question: the O \((n = 0)\) model introduced by Nienhuis, which we will refer to in this paper as the vertex-interacting self-avoiding walk (VISAW) model \([4]\), and the interacting self-avoiding trail (ISAT) model \([5]\). In both of these models the self-avoidance constraint is relaxed in that lattice sites may be visited more than once, but the lattice bonds may only be visited once. In the VISAW model the walk is not allowed to cross, but in the ISAT model the walk is allowed to cross.

Whilst the VISAW and ISAT models have the same critical behaviour as the ISAW in the high-temperature phase \([4, 6]\), the situation is different at the collapse transition. For the VISAW model, a mapping to an integrable 19 vertex model allows the exact calculation of the correlation exponent \(\nu = 12/23\) and the exponent \(\gamma = 53/46\) \([7]\), as compared to \(\nu = 4/7\) and \(\gamma = 8/7\) for the ISAW at the collapse transition \([8]\). The situation for the ISAT model is far less clear. Early studies found a number of contradictory results \([9–12]\). Some authors claimed that the results were compatible with the ISAT model and the ISAW model being in the same universality class at the collapse transition \([10]\), whilst others found results which were incompatible \([11, 12]\). Recently this model was re-examined using transfer matrices \([13]\), and the conclusion arrived at was that the transition was similar to the collapse transition in the VISAW model (they have the same correlation length exponent \(\nu\) but different \(\gamma\) exponents). The collapse transition for both the VISAW and ISAT models is clearly not in the usual \(\Theta\)-point transition; the collapse transition in these models has an extra transition line leaving it separating two distinct dense phases.

In our previous study of the ISAT model \([13]\), we gave results for the bulk-critical exponents and showed that these results were different from the results of Owczarek and Prellberg \([11]\). We argued that this was due to a breakdown of the usual identification of the \(\nu\) exponent with the geometrical exponent derived from the radius of gyration. In the current paper, we extend our study by introducing attractive interactions with a surface, and examine the surface critical behaviour of the model. In their paper \([11]\), Owczarek and Prellberg also presented some results for the surface critical behaviour. Some of their results corresponded to explicit calculations using Monte Carlo, and others were derived by plausibility arguments. Our results concord with their explicit results, but disagree with the others. The surface critical exponents we find are consistent with the bulk results found in \([13]\).

2. Model and transfer matrix calculation

The ISAT model studied here is defined as follows: consider all random walks on the square lattice which do not visit any lattice bond more than once. Doubly visited sites may correspond to either crossings or ‘collisions’; both are assigned an attractive energy \(-\varepsilon\). The walk is allowed to touch, but not cross, a surface defined as a horizontal line on the lattice. Each step along the surface is assigned an attractive energy \(-\varepsilon_s\). For the transfer matrix calculation that follows it is convenient to consider a strip of width \(L\) with an attractive surface both sides of the strip. This is not expected to change the behaviour in the thermodynamic limit \(L \to \infty\); the bulk critical behaviour should not depend on the boundary conditions and when calculating the surface critical behaviour, a walk adsorbed to one surface needs an infinite excursion in order to ‘see’ the other surface. Additionally, the finite-size scaling results which link the eigenvalues of the transfer matrix to the scaling dimensions \(x^s_o\) and \(x^s\) (see \((15)\) and \((16)\)) rely on the conformal mapping of the half plane (one adsorbing surface) onto a strip with two adsorbing surfaces \([14]\). A typical configuration for the ISAT is shown in figure 1.

The partition function for the model is

\[
\mathcal{Z} = \sum_{\text{walks}} K^N \omega^N_s \tau^{N_t},
\]
Figure 1. A self-avoiding trail (SAT) model showing the vertex crossings and the vertex collisions, both weighted with a Boltzmann factor $\tau$. Surface contacts are weighted $\omega_s$ and a fugacity $K$ is introduced per walk step. The trail is shown on a strip of width $L = 5$.

where $K$ is the fugacity, $\omega_s = \exp(\beta \varepsilon S)$ and $\tau = \exp(\beta \varepsilon)$. $N$ is the length of the walk, $N_S$ is the number of steps on the surface and $N_I$ is the number of doubly visited sites.

The average length of the trail is controlled by the fugacity $K$ through

$$\langle N \rangle = K \frac{\partial \ln Z}{\partial K}. \quad (2)$$

As $K$ increases from zero, $\langle N \rangle$ increases, diverging at some value $K = K^*(\omega_s, \tau)$. To start we consider what happens in the absence of the adsorbing boundary. For $\tau$ small enough,

$$\langle N \rangle \sim (K^*(\omega_s, \tau) - K)^{-1}, \quad (3)$$

whilst for large enough $\tau$ the divergence is discontinuous. Whilst $\langle N \rangle$ is finite, the density of occupied bonds on an infinite lattice is zero, whilst once $\langle N \rangle$ has diverged the density is in general finite. For small enough $\tau$ the density becomes non-zero continuously at $K = K^*$ and for large enough $\tau$ the density jumps at $K = K^*$. $K^*$ may then be understood as the location of a phase transition, critical for $\tau < \tau_{\text{coll}}$ and first order for $\tau > \tau_{\text{coll}}$. The problem of infinite walks on the lattice is equivalent to setting $K = K^*$ and varying $\tau$; then it may be seen that for $\tau < \tau_{\text{coll}}$ the density is zero and is non-zero for $\tau > \tau_{\text{coll}}$. It then follows that $\tau_{\text{coll}}$ defines the collapse transition point.

Now let us consider the effect of the adsorbing boundary at constant $\tau$. For $\omega_s$ small, the entropic repulsion of the wall is strong enough for the walk to remain in the bulk. Once $\omega_s$ is large enough for the energy gain to overcome the entropic repulsion, the walk will visit the boundary a macroscopic number of times, and the walk adsorbs to the surface. These two behaviours are separated by $\omega_s = \omega^*_s$. For $\omega_s < \omega^*_s$ the behaviour of the walk is not influenced by the wall, and $K^*$ is independent of $\omega_s$. The transition $K = K^*$ if critical ($\tau \leq \tau_{\text{coll}}$) corresponds to ordinary critical behaviour. However, for $\omega_s > \omega^*_s$, $K^*$ is a function of $\omega_s$, and the transition is refered to as a surface transition. The point $K = K^*$, $\omega_s = \omega^*_s$ is referred to as the special critical point (again $\tau \leq \tau_{\text{coll}}$).

As the critical value $K^*$ is approached, and in the absence of a surface, the partition function (1) and the correlation length $\xi$ are expected to diverge, defining the standard exponents $\gamma$ and $\nu$:

$$\xi \sim |K - K^*|^{-\nu}, \quad (4)$$

$$Z \sim |K - K^*|^{-\gamma}. \quad (5)$$
The effect of the surface on the walk is to introduce an entropic repulsion, pushing the walk away from the surface. The number of allowed walks is reduced exponentially if the walk is constrained to remain near the surface, in particular if one or both ends of the walk are obliged to remain in contact with the surface. In this case the divergence of $Z$ is modified, and two new exponents are introduced, $\gamma_1$ and $\gamma_{11}$. Defining $Z_1$ and $Z_{11}$ as the partition functions for a walk with one end, and both ends, attached to the surface respectively, then

$$Z_1 \sim |K - K^*|^{-\gamma_1} \quad (6)$$

$$Z_{11} \sim |K - K^*|^{-\gamma_{11}} \quad (7)$$

Whilst the bulk exponents, such as $\nu$ and $\gamma$, are the same at an ordinary critical point and at the special critical point, the surface exponents $\gamma_1$ and $\gamma_{11}$ differ. The exponents $\nu$, $\gamma$, $\gamma_1$ and $\gamma_{11}$ are related by the Barber relation [15]:

$$\nu + \gamma = 2\gamma_1 - \gamma_{11} \quad (8)$$

This partition function may be calculated exactly on a strip of length $L_x \to \infty$ and of finite width $L$ by defining a transfer matrix $T$. If periodic boundary conditions are assumed in the $x$-direction, the partition function for the strip is given by

$$Z_L = \lim_{L \to \infty} \text{Tr}(T^{L_x}). \quad (9)$$

The free energy per lattice site, the density, surface density and correlation length for the infinite strip may be calculated from the eigenvalues of the transfer matrix:

$$f(K, \omega_s, \tau) = \frac{1}{L} \ln (\lambda_0), \quad (10)$$

$$\rho(K, \omega_s, \tau) = \frac{K}{L\lambda_0} \frac{\partial \lambda_0}{\partial K}, \quad (11)$$

$$\rho_s(K, \omega_s, \tau) = \frac{\omega_s}{\lambda_0} \frac{\partial \lambda_0}{\partial \omega_s}, \quad (12)$$

$$\xi(K, \omega_s, \tau) = \left( \ln \frac{\lambda_0}{\lambda_1} \right)^{-1}, \quad (13)$$

where $\lambda_0$ and $\lambda_1$ are the largest and second largest (in modulus) eigenvalues.

Our first task is to find estimates of $K^*(\omega_s, \tau)$. For this, two distinct methods are used, which we now describe.

(i) For $K < K^*$ the largest eigenvalue of the transfer matrix $T$ corresponds to the empty lattice; the length of the walk is finite, but the lattice strip is infinitely long, and so the probability of finding a non-empty column is zero. The largest eigenvalue is then $\lambda_0 = 1$. The divergence of the walk length is identified with the value $K = K^*_L$ for which $\xi \to \infty$. This occurs when $\lambda_1 = \lambda_0 = 1$ [16].

(ii) An estimate for the critical point where the length of the walk diverges may be found using a phenomenological renormalization group for a pair of lattice widths [17], $L$ and $L'$. The estimated value of $K^*$ is given by the solution of the equation

$$\frac{\xi_L}{L} = \frac{\xi_{L'}}{L'}. \quad (14)$$
Both these methods give finite-size estimates $K^*_L(ω_s, τ)$ which should converge to the same value in the limit $L → ∞$.

The critical dimensions of the surface magnetic and energy fields may be calculated from the first few eigenvalues of the transfer matrix:

$$x^s_σ = \frac{L \ln |λ_0|}{π},$$

$$x^s_ε = \frac{L \ln |λ_2|}{π},$$

with $λ_2$ the eigenvalue with the third largest absolute value.

The surface scaling dimensions $x^s_σ$ and $x^s_ε$ may be related to the surface correlation length exponent $ν_s$ and the exponent $η_∥$, controlling the decay of the correlation function along the surface, through standard relations

$$ν_s = \frac{1}{1 - x^s_ε},$$

$$η_∥ = 2x^s_σ.$$  

The entropic exponent $γ_{11}$ is related to $η_∥$ through

$$γ_{11} = ν(1 - η_∥).$$

For a more detailed discussion of the transfer matrix method, and in particular how to decompose the matrix, the reader is referred to the article of Blöte and Nienhuis [4].

3. Results

For clarity, we will present separately the results found setting $λ_1 = 1$ and those found using the phenomenological renormalization group equation (14).

The finite-size results obtained are, where possible, extrapolated on the one hand using the Burlisch and Stoer (BST) extrapolation procedure [18] and on the other hand fitting to a three-point extrapolation scheme, fitting the following expression for the quantity $X_L$:

$$X_L = X_∞ + aL^{-b}.$$  

Calculating $X_∞$, $a$ and $b$ require three lattice widths. The extrapolated values $X_∞$ clearly will still depend weakly on $L$, and the procedure may be repeated; however, weak parity effects can be seen in their values, impeding further reasonable extrapolation by this method.

3.1. Results setting $λ_1 = 1$

In figure 2 we present the curves of $K^*_L(ω_s, τ)$ as a function of $ω_s$ for $τ = 0$. The case where $τ = 0$ corresponds to the pure self-avoiding walk in the presence of an attractive surface is already studied using transfer matrices [19, 20]. The ISAT maps onto the kinetic SAT model when $τ = 3$. It was conjectured that the kinetic SAT corresponded to the collapsing SAT, leading to the identification $τ_{coll} = 3$ [11]. This identification seems to be verified by the results presented in [11] and [13]. The curves of $K^*_L(ω_s, τ)$ for $τ = 3$ are shown in figure 3. The values calculated from the intersections of successive curves are shown in table 1 which places the special surface transition for $τ = 3$ at $K^* = 0.3333 ± 0.0001$, $ω^*_s = 2.427 ± 0.002$. We calculated the finite-size estimates for the density $ρ_L(K^*, ω^*_s)$. These
estimates can be seen to have a finite limit of $\rho_\infty = 0.35 \pm 0.02$. In table 1 we also give this reciprocal fractal dimension calculated at the special transition for $\tau = 3$. Whilst the question of the density at the special point in the infinite lattice limit remains open, given the lattice widths used in our calculation, we can clearly see that we recover a geometrical exponent compatible with the results of Owczarek and Prellberg [11]. This indicates that the thermal exponent $\nu$ and the geometrical exponent $1/d_f$ are likely to be different for this model at the collapse transition.

For both $\tau = 0$ and $\tau = 3$ the curves may clearly be seen to cross at a point, which defines the adsorption transition $\omega_s^*(\tau)$. By varying $\tau$ we may map out the adsorption line, and hence find the phase diagram in the $K = K^*(\omega_s, \tau)$ plane. This is shown in figure 4. The vertical line, corresponding to the collapse transition, has been added by hand at $\tau_{\text{coll}} = 3$; the boundary is not expected to influence the location of the collapse transition until the walk adsorbs to the boundary; the surface interaction below $\omega_s^*$ will have a finite perpendicular correlation length $\xi_{\perp}$ associated with it. In the thermodynamic limit, the bulk of the lattice
Table 1. Location of the special point calculated by setting $\lambda = 1$ and solving $K_L^*(\varpi^*_s, \tau) = K_{L+1}^*(\varpi^*_s, \tau)$ for $\tau = 3$. The results have then been extrapolated using the BST extrapolation scheme. The reciprocal fractal dimension $1/d_f$ is given, calculated from the densities $\rho_L$ and $\rho_{L+1}$.

| $L$ | $\varpi^*_s$ | $K^*$ | $\rho_{L+1}$ | $1/d_f$ |
|-----|---------------|-------|---------------|---------|
| 3   | 2.220 342     | 0.340 394 | 0.501 949     | 0.565 358 |
| 4   | 2.267 276     | 0.337 428 | 0.474 241     | 0.545 825 |
| 5   | 2.296 043     | 0.336 003 | 0.455 622     | 0.534 034 |
| 6   | 2.315 608     | 0.335 210 | 0.442 176     | 0.526 218 |
| 7   | 2.329 838     | 0.334 723 | 0.431 958     | 0.520 713 |
| 8   | 2.340 687     | 0.334 403 | 0.423 892     | 0.516 664 |
| 9   | 2.349 254     | 0.334 182 | 0.417 336     | 0.513 588 |
| 10  | 2.356 203     | 0.334 022 | 0.411 881     | 0.511 191 |
| 11  | 2.361 962     | 0.333 904 | 0.407 254     | 0.509 286 |
| BST $\infty$ | 2.4267 | 0.3333 | 0.3539 | 0.498 |

Three-point extrapolated results

| $L$ | $\varpi^*_s$ | $K^*$ | $\rho_{L+1}$ | $1/d_f$ |
|-----|---------------|-------|---------------|---------|
| 3   |               |       |               |         |
| 4   | 2.4227        | –     | –             | –       |
| 5   | 2.4250        | 0.333 267 | 0.327 394 | 0.488 281 |
| 6   | 2.4262        | 0.333 291 | 0.332 348 | 0.490 432 |
| 7   | 2.4271        | 0.333 304 | 0.334 328 | 0.491 926 |
| 8   | 2.4277        | 0.333 312 | 0.334 880 | 0.493 045 |
| 9   | 2.4281        | 0.333 317 | 0.334 636 | 0.493 983 |

Figure 4. Phase diagram in the $K = K_L^*(\varpi, \tau)$ plane found setting $\lambda = 1$ and identifying the adsorption transition with the solutions of $K_L^*(\varpi_s, \tau) = K_{L+1}^*(\varpi_s, \tau)$.

will not be an influenced surface, and bulk collapse should be unaffected. It is only at $\varpi^*_s$, were $\xi^*_s \to \infty$, that the bulk will be influenced by the surface, and the walk will adsorb to the surface. This picture has been proven for the case of the adsorption of collapsing self-avoiding polygons in three dimensions [21].

Having set $\tau = 3$ using the conjecture from the kinetic SAT model, there are different methods for estimating the location of the special surface transition, where collapse and
adsorption occur simultaneously. The simplest is to use the crossings of $K^*$ to estimate the adsorption point $\omega_s^*$, results for which are shown in table 1. However, we may also use the scaling behaviour of the order parameter to set up a phenomenological renormalization scheme. An order parameter for the adsorption transition may be defined as

$$O(K, \omega_s, \tau) = \frac{\langle N_s^c \rangle}{\langle N \rangle}.$$  \hfill (21)

For a continuous adsorption transition, the order parameter $O$ vanishes for $\omega_s < \omega_s^*$ whilst for $\omega_s > \omega_s^*$ $O$ is finite. At the transition point the order parameter is expected to scale as

$$O_L(\omega_s) \approx L^{-(1 - \phi_s)/\nu} O[L^\nu(\omega_s - \omega_s^*)].$$  \hfill (22)

Defining $Y_{L,L'}$ by

$$Y_{L,L'}(\omega_s) = -\frac{\ln[O_L(\omega_s)/O_{L'}(\omega_s)]}{\ln[L/L']}$$  \hfill (23)

we may set up a phenomenological RG scheme for estimating the adsorption transition, as well as the exponent $\phi_s$. These are given by the solutions of the equation

$$Y_{L,L+1}(\omega_s^*) = Y_{L+1,L+2}(\omega_s^*) = Y_L,$$  \hfill (24)

where $Y_L$ is the finite size estimate of the exponent $Y_\infty = (1 - \phi_s)/\nu$.

Plots of the order parameter are shown in figure 5 and results for $Y_L$ are shown in table 2. The values $Y_L$ are far from their asymptotic values, and the extrapolation using BST is not very conclusive. The best estimate from BST is $Y_\infty = 1.08$. Plotting this value along with the data points shows it to be a low estimate. A reasonable extrapolation of the points seems to be $Y_\infty = 1.12 \pm 0.05$, although these values should be taken with care.

3.2. Results from phenomenological RG

In the previous section we calculated our estimate $K^*(\omega_s, \tau)$ by setting $\lambda_1 = 1$. This gives an overestimate of $K^*$. Calculating $K^*$ using equation (14) gives more asymptotic results, but at the cost of needing two lattice widths, reducing the number of available data points for extrapolation. Additionally, the phenomenological RG method used identifies both the ordinary and the special surface transitions. The phase diagram in the $(K, \omega_s)$ plane is shown

| $L$ | $\omega_s^*$ | $K^*$ | $Y_L = (1 - \phi_s)/\nu$ |
|-----|-------------|------|-------------------------|
| 3   | 2.644 273   | 0.306 760 | 0.635 164           |
| 4   | 2.612 544   | 0.315 671 | 0.675 046           |
| 5   | 2.587 753   | 0.320 837 | 0.714 237           |
| 6   | 2.568 090   | 0.324 099 | 0.751 030           |
| 7   | 2.552 274   | 0.326 280 | 0.784 704           |
| 8   | 2.539 271   | 0.327 805 | 0.815 357           |
| 9   | 2.528 203   | 0.328 916 | 0.843 678           |
| 10  | 2.519 807   | 0.329 713 | 0.866 822           |

BST $\infty$ 2.431 0.3339 see the text and caption

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in figure 6 for $\tau = 3$. It may be seen that there are two points on the phase diagram where the lines seem to cross at (or close to) a point. These two points are the fixed points corresponding to the ordinary and the special surface transitions. The location of these points may be estimated using a three width phenomenological RG scheme. From equations (13)–(15) and (18) it may be seen that we may identify the fixed points with crossings of $\eta_0$, and find corresponding estimates for $\eta_0$. The plots of $\eta_0$ as a function of $\omega_s$ for $\tau = 3$ are shown in figure 7, whilst the phase diagram in the $\tau, \omega_s$ plane with $K = K^*$ is shown in figure 8. The estimates for the location of the fixed points for the ordinary and special transitions, along with the corresponding exponent estimates, are shown in tables 3 and 4.

The results presented in tables 3 and 4 are calculated setting $\tau = 3$. The identification $\tau_{\text{coll}}$ may be checked by looking for the special transition fixed point in the full phase diagram at the cost of using an extra (fourth) lattice width. Unconstrained results are shown in table 5. Extrapolated values of $\tau$ give $\tau_{\text{coll}} = 3.000 \pm 0.001$, which is consistent with the identification used elsewhere.

In the results presented above we have used (14), or equivalently (15), to identify the fixed points. However, the correlation length defined using the largest and third largest eigenvalues also diverges in the thermodynamic limit, and so we may use a phenomenological RG based
Figure 6. $K^*_L(\omega_s, \tau)$ calculated using phenomenological RG for $\tau = 3$.

Figure 7. Exponent $\eta\|\perp\|$ from crossings of $\xi/L$ for $\tau = 3$ and $L' = L + 1$.

on $x$, using (16). This leads to estimates for $\nu_s$, the correlation exponent along the surface as well as alternative estimates for the location of the fixed points. The results are shown in table 6.

In table 2 we calculated estimates, $Y_L$, of $Y_\infty = (1 - \phi_s)/\nu$ from (23) and (24), calculating $K^*(\omega_s, \tau)$ by setting $\lambda_0 = 1$. In table 7 we present the analogous calculation but with $K^*$ calculated using phenomenological RG.

3.3. Summary of results

The transfer matrix calculation gives the exponent $\eta\|$ directly. At the ordinary transition we find a value $\eta^{\text{ord}}_\| = 1.9213 \pm 0.0001$. Using the results conjectured in [13], $\nu = 12/23$ and $\gamma = 22/23$ with (8) and (19), we find $\gamma^{\text{ord}}_\| = 0.499$ and $\gamma^{\text{ord}}_{11} = -0.481$. These values agree with the value $\gamma^{\text{ord}}_\|$ calculated with Monte Carlo in [11], but not with the value of $\gamma^{\text{ord}}_{11}$. It should be noted that the values were obtained using $\nu = 12/23$. At the special transition we find $\eta^{\text{sp}}_\| = -0.085 \pm 0.003$, leading to $\gamma^{\text{sp}}_\| = 1.022$ and $\gamma^{\text{sp}}_{11} = 0.566$. Again, $\gamma^{\text{sp}}_\|$ is consistent with the value given in [11], but not $\gamma^{\text{sp}}_{11}$, and again we used the value $\nu = 12/23$. In both
cases in [11] the values of $\gamma_{11}$ are calculated using the assumed values of $\nu = 1$ and $\nu = 1/2$, which we believe not to be the correct values.

We calculated $\phi_s$ in three ways.

(i) From the result $v_s = 1.275 \pm 0.002$ and using $v = 12/23$ leads to $\phi_s = v/v_s = 0.414$.
(ii) Using $\gamma_{11} = (1 - \phi_s)/\nu = 1.12 \pm 0.05$ from table 2, giving $\phi_s = 0.405$.
(iii) Using $\gamma_{11} = (1 - \phi_s)/\nu = 1.19 \pm 0.05$ from table 7, giving $\phi_s = 0.379$.

In all three cases the result is close but a little lower than the value $\phi_s = 0.440 \pm 0.010$ given in [11], but the determination of this exponent is the least accurate of the results presented here.
### Table 4. Special point location for $\tau = 3$ and estimates for $\eta_{sp}^\parallel$. The three-point extrapolations are shown in the second half of the table.

| $L$ | $\omega^*$ | $K^*$ | $\eta_{sp}^\parallel$ |
|-----|------------|-------|-----------------------|
|     |            |       |                       |
| 3   | 2.462 062  | 0.332 813 | $-0.110 939$         |
| 4   | 2.451 809  | 0.333 074 | $-0.105 536$         |
| 5   | 2.446 565  | 0.333 181 | $-0.102 198$         |
| 6   | 2.443 407  | 0.333 234 | $-0.099 858$         |
| 7   | 2.441 324  | 0.333 264 | $-0.098 106$         |
| 8   | 2.439 855  | 0.333 283 | $-0.096 728$         |
| 9   | 2.438 768  | 0.333 294 | $-0.095 606$         |
| 10  | 2.437 932  | 0.333 302 | $-0.094 666$         |
| BST $\infty$ | 2.432 45 | 0.333 31 | $-0.084 49$ |
|     |            |       |                       |

Three-point extrapolated results

| $L$ | $\omega^*$ | $K^*$ | $\eta_{sp}^\parallel$ |
|-----|------------|-------|-----------------------|
| 3   | 2.434 491  | 0.333 327 | $-0.086 941$         |
| 4   | 2.433 346  | 0.333 328 | $-0.083 971$         |
| 5   | 2.433 139  | 0.333 332 | $-0.083 208$         |
| 6   | 2.432 852  | 0.333 340 | $-0.082 012$         |
| 7   | 2.432 683  | 0.333 317 | $-0.081 190$         |
| 8   | 2.432 473  | 0.333 339 | $-0.079 932$         |

### Table 5. Special point location with $\tau$ unconstrained, using four lattice widths. Estimates for $\eta_{sp}^\parallel$ are also shown. The three-point extrapolations are shown in the second half of the table.

| $L$ | $\omega^*$ | $K^*$ | $\eta_{sp}^\parallel$ |
|-----|------------|-------|-----------------------|
|     |            |       |                       |
| 3   | 3.132 743  | 2.514 601 | 0.329 697 | $-0.123 477$ |
| 4   | 3.074 773  | 2.486 484 | 0.331 186 | $-0.115 417$ |
| 5   | 3.048 363  | 2.472 046 | 0.331 897 | $-0.110 607$ |
| 6   | 3.033 676  | 2.463 154 | 0.332 307 | $-0.107 244$ |
| 7   | 3.024 799  | 2.457 278 | 0.332 562 | $-0.104 764$ |
| 8   | 3.019 029  | 2.453 143 | 0.332 731 | $-0.102 840$ |
| 9   | 3.015 082  | 2.450 106 | 0.332 848 | $-0.101 298$ |
| BST $\infty$ | 2.99 967 | 2.440 | 0.333 291 | $-0.0874$ |
|     |            |       |                       |

Three-point extrapolated results

| $L$ | $\omega^*$ | $K^*$ | $\eta_{sp}^\parallel$ |
|-----|------------|-------|-----------------------|
| 3   | 3.003 123  | 2.438 430 | 0.333 265 | $-0.091 790$ |
| 4   | 2.997 885  | 2.432 266 | 0.333 423 | $-0.084 854$ |
| 5   | 3.000 002  | 2.433 993 | 0.333 345 | $-0.086 107$ |
| 6   | 3.000 077  | 2.433 675 | 0.333 338 | $-0.085 025$ |
| 7   | 3.000 388  | 2.433 813 | 0.333 325 | $-0.084 784$ |

### 4. Discussion

In this paper we have investigated the surface critical behaviour of the ISAT. The results confirm the identification of the collapse transition as occurring at $K_{coll} = 1/3$ and $\tau_{coll} = 3$ and locates the adsorption transition for $\tau_{coll} = 3$ at $\omega_s = 2.45 \pm 0.05$. For the standard ISAW model an additional line has been observed in the collapsed phase, separating a region where
Table 6. Special point location with $\tau = 3$ by applying the phenomenological RG method using $x_s^\epsilon$, leading to estimates for $\nu_s = 1/(1 - x_s^\epsilon)$. The three-point extrapolations are shown in the second half of the table.

| $L$ | $\omega_s^*$ | $K^*$ | $\nu_s$ |
|-----|--------------|------|--------|
| 3   | 2.380 861    | 0.334 825 | 1.352 725 |
| 4   | 2.423 360    | 0.333 648 | 1.309 484 |
| 5   | 2.439 110    | 0.333 307 | 1.291 723 |
| 6   | 2.445 939    | 0.333 198 | 1.283 136 |
| 7   | 2.449 061    | 0.333 167 | 1.278 793 |
| 8   | 2.450 430    | 0.333 166 | 1.276 705 |
| 9   | 2.450 901    | 0.333 175 | 1.275 924 |
| 10  | 2.450 890    | 0.333 188 | 1.275 943 |
| BST $\infty$ | 2.451 2   | 0.333 2 | 1.275  |

Three-point extrapolated results

| $L$ | $\omega_s^*$ | $K^*$ | $\nu_s$ |
|-----|--------------|------|--------|
| 3   | 2.456 846    | –    | 1.267 398 |
| 4   | 2.454 952    | –    | 1.268 746 |
| 5   | 2.453 232    | –    | 1.271 502 |
| 6   | 2.451 999    | –    | 1.273 811 |
| 7   | 2.451 239    | –    | 1.275 283 |
| 8   | –            | –    | 1.276 304 |

Table 7. Location of the special point calculated by fixing $K^*$ by phenomenological RG and solving $Y_L(\omega_s^*, \tau) = Y_{L+1}(\omega_s^*, \tau)$ for $\tau = 3$. The results are have then been extrapolated using the BST extrapolation scheme.

| $L$ | $K^*$ | $\omega_s^*$ | $Y_L$ |
|-----|------|--------------|------|
| 3   | 0.326 892 | 2.675 620   | 0.715 973 |
| 4   | 0.329 234 | 2.622 565   | 0.767 296 |
| 5   | 0.330 545 | 2.587 417   | 0.809 961 |
| 6   | 0.331 343 | 2.562 356   | 0.845 875 |
| 7   | 0.331 858 | 2.543 648   | 0.876 360 |
| 8   | 0.332 207 | 2.529 207   | 0.902 462 |
| 9   | 0.332 451 | 2.517 800   | 0.924 981 |
| 10  | 0.332 634 | 2.507 957   | 0.945 751 |
| BST $\infty$ (3-8) | 0.333 377 | 2.427 | 1.19 |

Three point extrapolated results

| $L$ | $\omega_s^*$ | $K^*$ | $\nu_s$ |
|-----|--------------|------|--------|
| 3   | 0.330 183    | 2.348 631 | — |
| 4   | 0.331 123    | 2.369 608 | — |
| 5   | 0.333 704    | 2.388 620 | — |
| 6   | 0.333 557    | 2.401 071 | — |
| 7   | 0.333 463    | 2.413 110 | — |
| 8   | 0.333 647    | 2.222 366 | — |

the collapsed walk is adsorbed to the surface from a region where the walk is desorbed from the surface [22]. This transition corresponds to a wetting of the surface by the perimeter of the collapsed globule, and so does not correspond to a singularity in the bulk-free energy. Whilst
the method used in this paper does not naturally throw up this transition line, an a posteriori reexamination of the order parameter defined in (21) for the standard ISAW model does show a signature of this transition (see the curves in [20]). Such a signature seems to be absent in this model, see figure 5 for plots with $\tau = 4 > \tau_{\text{coll}}$. Whilst this should not be taken as a strong indication, it would be of interest to examine whether such a line does exist in this model, or whether the particular type of collapse suppresses this transition.

In conclusion, in the paper we use finite-size scaling and transfer matrix methods to investigate the surface critical behaviour of the ISAT model. Using the conjectured results for $\nu$ and $\gamma$ from [13] ($\nu = 12/23$ and $\gamma = 22/23$) we find values of $\gamma_{\text{ord}}^1$ and $\gamma_{\text{sp}}^1$ in agreement with the numerical results of Owczarek and Prellberg [11]. We do not, however, find agreement with the conjectured values of $\gamma_{\text{ord}}^{11}$ or $\gamma_{\text{sp}}^{11}$. The values of $\nu$ and $\gamma$ needed for this agreement are different from the values $\nu = 1/2$ and $\gamma = 1$ proposed in [11].

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References

[1] Vanderzande C 1998 Lattice Models of Polymers (Cambridge: Cambridge University Press)
[2] Flory P 1971 Principles of Polymer Chemistry (Ithaca: Cornell University Press)
[3] de Gennes P G 1975 J. Phys. Lett. 36 L55
[4] Blöte H W J and Nienhuis B 1989 J. Phys. A: Math. Gen. 22 1415
[5] Massih A R and Moore M A 1975 J. Phys. A: Math. Gen. 8 237
[6] Guim I, Blöte H W J and Burkhardt T W 1997 J. Phys. A: Math. Gen. 30 413
[7] Warnaar S O, Batchelor M T and Nienhuis B 1992 J. Phys. A: Math. Gen. 25 3077
[8] Duplantier B and Saleur H 1987 Phys. Rev. Lett. 59 539
[9] Lyklema J 1985 J. Phys. A: Math. Gen. 18 L617
[10] Meirovitch H and Lim H A 1988 Phys. Rev. A 38 R1670
[11] Owczarek A L and Prellberg T 1995 J. Stat. Phys. 79 951
[12] Owczarek A L and Prellberg T 2007 Physica A 373 433
[13] Foster D P 2009 J. Phys. A: Math. Theor. 42 372002
[14] Cardy J 1986 Phase Transitions and Critical Phenomena ed Domb and Lebowitz vol XI (New York: Academic)
[15] Barber M N 1973 Phys. Rev. B 8 407
[16] Derrida B and Herrmann H G 1983 J. Physique 44 1365
[17] Nightingale M P 1976 Physica A 83 561
[18] Bulirsch R and Stoer J 1964 Numer. Math. 6 413
[19] Henkel M and Schütz G 1988 J. Phys. A: Math. Gen. 21 2617
[20] Veal A R, Yeomans J M and Jug G 1991 J. Phys. A: Math. Gen. 24 827
[21] Vrbová T and Whittington S G 1996 J. Phys. A: Math. Gen. 29 6253
[22] Singh Y, Giri D and Kumar S 2001 J. Phys A 34 L67