Finite Length Scaling of Collapsing Directed Walks

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Abstract

We study the finite length scaling of self-interacting partially directed self-avoiding walks utilising enumeration data up to a total length of 6000 steps. This facilitates the evaluation of the numerical techniques available for calculating exponents at the $\theta$ point and in the collapsed phase of walk-type models. Another consequence is the conjecture of a new scaling theory for the collapsed region of the phase diagram and the suggestion that this should be applicable to the wider range of undirected problems including interacting SAW. We provide a phenomenological picture of the phase transition in terms of the condensation of droplets that allows us to understand the various length scales involved in the problem.

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1 Introduction

Substantial progress has been made on the elucidation of the properties of an isolated polymer chain [1] from various lattice models in statistical mechanics. Mostly, these have been based upon self–avoiding walks (SAW) which have been studied on a variety of lattices and in several dimensions. A canonical example is the interacting SAW (ISAW) model on a regular lattice where attractive nearest neighbour interactions introduce a thermal field. Two dimensional systems are often of interest from a directly physical point of view and coupled with the recent enthusiasm [2] concerning lattice models in two dimensions it comes as no surprise to find a wealth of work on the ISAW on two dimensional lattices [3]. Many results have been conjectured for this model though no exact solution exists.

A closely related model, that of partially directed walks with similar self–interactions (IPDSAW), has been proposed as a viable alternative to shed some light on the ISAW problem [4]. We have undertaken a thorough study of this model and several results have already been found including much exact information [5]. The scaling of the properties of walk systems with the length of the walk is the fundamental information requested from these models and while much can be inferred from analysis it is difficult to compute these properties directly. Moreover, it is interesting to compare the finite length estimates of quantities to the exact values known in the thermodynamic limit. Here, we shall describe a complete study of the scaling of the system with walk length in an attempt to draw some wider conclusions about interacting walk problems. In doing so we shall not only provide a phenomenological picture of the behaviour of the model but also expose generic features of these problems as yet unrecognised. This work has provided the impetus for two recent announcements [6, 7].

Partially directed walks are self-avoiding walks that have only steps in the positive $x$ (horizontal) direction while having steps in both positive and negative vertical directions. In figure 1 an allowed configuration is shown including a representation of which steps (representing monomers) interact. The basic problem is that of evaluating the canonical partition function, given by

$$Q_L(T) = \sum_{\text{configurations}} c_L(I) \omega(T)^I$$

(1)

where $\omega = \exp(J/k_B T)$; $J$ being some positive coupling constant. Here, $c_L(I)$ is the number of allowed configurations of length $L$ that have $I$ interacting sets of monomers. The
A common procedure is to consider instead the generalised canonical ensemble and introduce a fugacity $z$ for the walk length. The generalised partition function, or equivalently a generating function, is then found from summing over walk lengths as

$$G(z, \omega(T)) = \sum_{L=0}^{\infty} z^L Q_L(T).$$

It is then not too difficult to show that the closest singularity to the origin, $z_\infty$ say, of $G(z, \omega)$ (considering $z$ the variable and $\omega$ as a parameter) is related directly to the canonical free energy as

$$z_\infty = \exp(f_\infty(T)/k_B T).$$

It is however not guaranteed a priori that all averages of properties in one ensemble will tally with the other [8].

In the analytic work already presented [5] the discussion has centred on the generating function $G(z, \omega)$ and its derivatives (including extensions to $G(z, \omega)$). Thermodynamically, the free energy contains a lone singularity, or critical point at some finite temperature. The behaviour of the thermodynamic free energy $f_\infty(T)$, the internal energy $u_\infty(T)$ and the specific heat $c_\infty(T)$ as functions of temperature are given in figure 2. This has been viewed as analogous to a similar behaviour in the ISAW problem where the critical point is understood as a collapse transition. Aptly named, this transition signifies the abrupt change of finite length scaling of the average size of the walks and is believed to be associated with the $\theta$–point transition in polymer systems. Hence the study of this transition in the IPDSAW system is of some importance for the understanding of the ISAW model.

As pointed out by Nordholm [8], the relationship between the two ensembles is clear at high temperatures down to and including the critical point point in these systems. Therefore, analysis in the generalised ensemble can be confidently translated to the canonical. However, at low temperatures the situation is not well understood. Here the generating function converges at its radius of convergence and quantities such as the average length are finite. It is clear then that taking the limit of going to the radius of convergence is not always the same as the limit $L \to \infty$! This breakdown of the connection between the ensembles provides
the need for numerical techniques to be employed. However, knowing how to solve for the generating function allows much more to be achieved by series analysis than for a completely unsolved problem. We, of course, can also confirm that appropriate exponents are the same in both ensembles when required by theory. In addition, even for the generating function some effectively numerical work needs to be done to extract some exponents because of the nature of the solution as the functions involved are not well understood [5].

So the first benefits of this study are simply the quantitative understanding of the low temperature phase of this system and the confirmation that the exact results do hold at higher temperatures. The first of these has led us in two directions.

Firstly, the collapsed phase has not been well understood for any walk problems. As a step towards a better understanding we will consolidate a scaling theory for the partition function for $T \leq T_c$ introduced by Owczarek et al [6] and subsequently expanded to a full scaling theory of the collapse transition [7]. This scaling theory is partly based on a connection with the droplet model of fluid condensation and can be viewed as a non–trivial example of a model displaying some of the behaviour of the fluid model while also having extra features.

The second benefit of looking more closely numerically at this problem and especially at the collapsed phase is the development of a phenomenological picture of the transition which we have inferred from a detailed study of the length scales involved. These length scales include the end–to–end distances in the two directions (as this is a directed problem). A physical “bubble” or droplet picture can be put forward as a heuristic explanation of the behaviour of the length scales. It is commonly assumed that it does not matter what one chooses to measure, the radius of gyration or the end–to–end distance, to find the length scale of global importance. We show how this assumption about length scales can fail at low temperatures, at least in directed problems.

Another reason for undertaking this numerical work is a comparison with other work on the ISAW problem. Again this provides us with an opportunity to give some insight into the procedures employed elsewhere. The analogous critical point in the ISAW problem has been understood to be a tricritical point in an extended “phase” diagram. This diagram is often taken as either the $(z, \omega)$ plane or the $(T, L)$ plane. It has recently been shown that it is reasonable to identify a tricritical-like point in the $(z, \omega)$ plane or singularity diagram. This diagram for the IPDSAW system is given in figure 3. We have verified [5] that in
the generalised ensemble of the IPDSAW system that the generating function does indeed have the crossover form and we have calculated the high-temperature and critical exponents. Now with the added understanding of the low temperature radius of convergence line as a line of condensation-like (first order) singularities we are certainly able to see the point as tricritical-like. Moreover, there exists unconfirmed conjectures [3] of the tricritical exponent values in the ISAW problem. In particular, the crossover exponent has been the subject of some dispute. We give a numerical reason why the estimates of that value may be far from their true values. This involves the exponent relation $2 - \alpha = \frac{1}{\phi}$, where $\alpha$ is the divergence index for the canonical specific heat and $\phi$ is the crossover exponent. We reveal that while this relationship does indeed hold in the thermodynamic limit it is very slowly asymptotically correct. Corrections-to-scaling strongly affect numerical estimates. Hence, the use of the relation can lead to erroneous results since it is often assumed to strictly be the case in finite length studies.

The paper is divided into three main sections. The first presents the model and the method used to generate the enumeration data. The second explains the results of studying the partition function. The warning concerning the crossover exponent is supported here with numerical evidence. The scaling at low temperatures leads to the Fisher droplet model extension and the new walk exponents. In the third section the length scales of the problem are examined and the phenomenological picture of the collapse transition is revealed.

2 The Method of Enumeration

Here, we describe the model and then present the method of generating the series enumeration data used in our analysis.

The configurations of this model are partially directed walks on a two-dimensional square lattice with nearest-neighbour interactions. For convenience, we demand that these walks end with a horizontal segment. Due to the directed nature of this problem, we can describe these configurations in a natural way through the length $r_i$ of vertical segments between two horizontal steps, measured in the positive $y$-direction. Thus, we associate to each configuration an $N$-tuple $(r_1, r_2, \ldots, r_N)$ corresponding to a configuration of total length $L = \sum_{i=1}^{N} |r_i| + N$. 

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The energy due to the nearest–neighbour interactions for each of these configurations is

\[ U(r_1, r_2, \ldots, r_N) = -J u(r_1, r_2, \ldots, r_N) \tag{5} \]

where

\[ u(r_1, r_2, \ldots, r_N) = \sum_{i=1}^{N-1} \min(|r_i|, |r_{i+1}|) \mathcal{H}(-r_i r_{i-1}) \tag{6} \]

with \( \mathcal{H}(x) \) being the Heaviside step function. We assign weights \( x \) for steps in the horizontal direction and \( y \) for steps in the vertical direction. The canonical partition function is

\[ Q_L(x, y, \omega) = \sum_{N=1}^{L} x^N \sum_{|r_1|+|r_2|+\ldots+|r_N|=L-N} y^{L-N} \omega^{u(r_1, r_2, \ldots, r_N)} \tag{7} \]

where we have set \( \omega = \exp(\beta J) \).

In order to derive an efficient computational scheme for \( Q_L(x, y, \omega) \), it is convenient to consider the partition functions \( Z^r_L = Z^r_L(x, y, \omega) \) for walks of total length \( L+1 \) which start with a vertical segment of height \( r \), then

\[ Q_{L+1}(x, y, \omega) = \sum_{r=-L}^{L} Z^r_L. \tag{8} \]

(In the definition of \( Z^r_L \) we have chosen \( L+1 \) instead of \( L \), as it makes the indexing in the following equations more transparent.)

We can concatenate these walks to get a recursion relation for \( Z^r_L \) as follows:

\[ Z^r_L = xy^r \left\{ \delta_{r,L} + \sum_{s=-L+r+1}^{L-r-1} \omega^{u(r,s)} Z^{s}_{L-r-1} \right\} \tag{9} \]

for \( r = -L, \ldots, L \) and \( L = 0, 1, 2, \ldots \). It is this recursion relation which enables us to obtain very long series. Note that

\[ Z^{(0)}_L = xQ_L(x, y, \omega). \tag{10} \]

One can further use the symmetry \( Z^r_L = Z^{-(r)}_L \) and restrict to \( r \geq 0 \), then

\[ Z^r_L = xy^r \left\{ \delta_{r,L} + \sum_{s=0}^{L-r-1} Z^{s}_{L-r-1} + \sum_{s=1}^{L-r-1} \omega^{\min(r,s)} Z^{s}_{L-r-1} \right\}. \tag{11} \]

Considering \( Z^r_L \) as a matrix with indices \( L \) and \( r \) shows we have to recursively compute rows of a triangular matrix.
For the computation of the free energy \( f_L(\omega) \), internal energy \( u_L(\omega) \), and specific heat \( c_L(\omega) \), we need to compute first and second–order derivatives of \( Z_L^{(r)} \), further denoted by \( Z_{L,1}^{(r)} \) and \( Z_{L,2}^{(r)} \). Restricting \( x = y = 1 \) then yields the iteration scheme:

\[
Z_L^{(r)} = \sum_{s=0}^{L-r-1} Z_{L-r-1}^{(s)} + \sum_{s=1}^{L-r-1} \omega^{\min(r,s)} Z_{L-r-1}^{(s)} + \delta_r, \quad (12)
\]

\[
Z_{L,1}^{(r)} = \sum_{s=0}^{L-r-1} Z_{L-r-1,1}^{(s)} + \sum_{s=1}^{L-r-1} \omega^{\min(r,s)} (Z_{L-r-1,1}^{(s)} + \min(r,s) Z_{L-r-1}^{(s)}), \quad (13)
\]

\[
Z_{L,2}^{(r)} = \sum_{s=0}^{L-r-1} Z_{L-r-1,2}^{(s)} + \sum_{s=1}^{L-r-1} \omega^{\min(r,s)} (Z_{L-r-1,2}^{(s)} + 2 \min(r,s) Z_{L-r-1,1}^{(s)} + \min(r,s)^2 Z_{L-r-1}^{(s)}). \quad (14)
\]

Defining \( a_L(\omega) = \frac{1}{L} \log Z_L^{(0)} \) and recalling \( \omega = \exp(\beta J) \), we then have

\[
f_L(\omega) = -\frac{1}{\beta} a_L(\omega) = -\frac{1}{\beta L} \log Z_L^{(0)}, \quad (15)
\]

\[
u_L(\omega) = J \omega \frac{d}{d\omega} a_L(\omega) = J \frac{Z_L^{(0)}}{Z_L^{(0)}} Z_{L,1}^{(0)}, \quad (16)
\]

\[
c_L(\omega) = \beta J^2 \left( \omega \frac{d}{d\omega} \right)^2 a_L(\omega) = \beta J^2 \frac{Z_{L,2}^{(0)}}{Z_L^{(0)}} \left( \frac{Z_{L,1}^{(0)}}{Z_L^{(0)}} \right)^2. \quad (17)
\]

In the computation we rescale the matrix coefficients in the iteration scheme because they grow exponentially. As our computations concern the critical point and collapsed phase, this growth is given by \( \omega^{L-r} \), so that we actually store \( z_L^{(r)} = \omega^{r-L} Z_L^{(r)} \).

For the computation of the length–scale exponents, we take partial derivatives of (11) with respect to \( x \) and \( y \) and set up a corresponding iteration scheme. For the computation of the vertical end–to–end distance it is further necessary to distinguish between steps in the positive and negative directions; a straightforward but rather tedious generalisation of (9) similar to (A.1) of [5] is required to accomplish this task.

All the computations have been done using floating–point numbers with 17 digit precision, some up to \( L = 6000 \). Therefore it is necessary to discuss the accuracy of these enumerations as opposed to “exact” enumerations with symbolic manipulation programs. One observes that the terms in the sums are positive and decrease exponentially fast in \( \omega \) for \( \omega \geq \omega_c \). This implies that each of these sums is dominated by only a few terms, and the number of terms

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contributing to within the floating-point accuracy is in any case less than 50. Therefore
roundoff errors are negligible and the scheme is numerically stable within the given floating-
point accuracy. A comparison with results from exact enumeration data (computed up to
$L = 160$) [9] and computations with 34-digit accuracy (computed up to $L = 1000$) support
this conclusion.

The evaluation of the data involves two different methods. We compute effective exponent
estimates, that is, assuming that a quantity grows as\footnote{Note, in this paper we take $f(x) \sim g(x)$ to mean $\lim_{x \to x_0} f/g = \text{constant} \neq 0$ (rather than one). This avoids the frequent introduction of constants.}

\[ f(L) \sim L^\lambda \]  

we define an effective exponent as

\[ \lambda(L) = \frac{\log f(L) - \log f(L - 1)}{\log L - \log(L - 1)} \]  

and treat the resulting series with various series extrapolation methods. It turns out that
we can determine the order of the corrections–to–scaling quite accurately and can in turn
use this information in the extrapolations. This method is quite successful and gives rather
accurate error estimates.

The second method used in the numerical analysis is the method of differential approxi-
mants [10]. This method confirms our extrapolation results but in this case it turns out to
be less accurate as corrections–to–scaling are not accounted for. A well–known problem here
is also the quite subjective determination of error bounds from the various approximants.
However, for shorter series this method gives results closer to the exact values.

3 Results for the Partition Function

The canonical partition function is expected to have the following length scaling form at high
temperatures:

\[ Q_L \sim \mu^L L^{\gamma - 1} \]  

where $f_\infty(T) = -k_B T \log \mu(T)$ and $\gamma = \gamma_+$ for $T > T_c$ and $\gamma = \gamma_-$ for $T = T_c$. As previously
mentioned the exponent $\gamma$ can be extracted from the generating function provided the form
(20) holds. We will be interested in this section in two questions. What can we say about the ease of calculating exponents when the critical point crossover occurs. Secondly, we will discuss the form of the finite length scaling for the partition function at low temperatures where (20) does not hold.

3.1 Critical Point

Around the critical point the partition function should have the crossover scaling form [7]

$$Q_L(\omega) \sim [\mu_a(\omega)]^L L^{\gamma_t-1} \Theta(\delta \omega L^\phi)$$ (21)

where $\delta \omega = \omega_c - \omega$, $\mu_a(\omega)$ is the analytic part of $\mu$ and

$$\Theta(x) \sim \begin{cases} 
\mu_+^{1/\phi} x^{(\gamma_t-\gamma_t)/\phi} & x \to \infty \\
1 & x \to 0 \end{cases}$$ (22)

where $\mu_+$ is related to the singular part of the free energy.

The canonical specific heat $C_L(\omega)$ should also have a crossover scaling form

$$c_L(\omega) \sim L^{\alpha \phi} \Omega(\delta \omega L^\phi)$$ (23)

where

$$\Omega(x) \sim \begin{cases} 
x^{-\alpha} & x \to \infty \\
1 & x \to 0 \end{cases}$$ (24)

It has been shown [7] that under some general assumptions that the exponent relation

$$2 - \alpha = 1/\phi$$ (25)

should hold. Even though there exists an exact solution in the generalised ensemble we have used series analysis to find estimates of the values of the two exponents $\alpha$ and $\phi$ from canonical finite length data in an attempt to evaluate the numerical precision of the series analysis. As an aside we have verified that the canonical exponent $\gamma_t$ has indeed the same value as the exact generalised canonical answer.

Our computation of these exponents is greatly aided by the fact that we know the critical temperature and the free energy at the critical point exactly. Therefore, we can compute the
exponents from

\[ Q_L(\omega_c) \omega_c^{-L} \sim L^{71-1}, \quad (26) \]
\[ 1 - u_L(\omega_c)/J \sim L^{(1-\alpha)\phi}, \quad (27) \]
\[ c_L(\omega_c) \sim L^{\alpha \phi}. \quad (28) \]

In figures 4 and 5 we plot the effective exponents for \( \alpha, \phi \) and \( \alpha + 1/\phi \). One can immediately see that the “true” values of these quantities, being 1/2, 2/3 and 2, are only slowly reached. This presents a warning [7] in the wider field of walk problems at a collapse transition when extrapolating finite length data.

We further analyse these data using two techniques. Firstly, second order inhomogeneous differential approximants (for the 2000-term series, only every 20th term is used). Secondly, from the figures we see that the correction terms are of order \( L^{-1/3} \); therefore we also extrapolate towards \( L = \infty \) by fitting to an expansion in powers of \( L^{-1/3} \) and get good results. We summarise these in the table ???.

The estimation of \( \gamma_t \) from the short series is quite accurate, whereas strong corrections to scaling make the estimations of \( \alpha \) and \( \phi \) quite problematic. Only with an a priori guess of the right correction terms (which by virtue of the consistent result proves itself correct a posteriori) can the correct value be extrapolated to a satisfactory accuracy. We caution that such a guess from shorter series is highly dangerous and it can result in a “self-fulfilling prophecy”.

The most important feature in this table is perhaps that the differential approximant method, even if applied to a rather “long” series of 100 terms when compared to its usual applications, gives \textit{wrong} results in the sense that even within quite a conservative error estimation the true value is outside that range. This is almost certainly because of the strong corrections-to-scaling not accounted for in the differential approximant analysis.

Furthermore, if we did not know the exact location of the critical point along with the free energy and internal energy we would have to resort to the usual procedure of determining the exponents from the scaling of the peak of the specific heat. The results [9] using 100 term series are \( \alpha = 1.30(5) \) and \( \phi = 0.45(3) \), with rather subjective error bounds. Since the exact values are 1/2 and 2/3 respectively, clearly this method is unsatisfactory! The problems with this last approach are due to the strong asymmetry of the collapse transition.
We have calculated the scaling functions $\Theta(x)$ and $\Omega(x)$ (see figures 6 and 7). These support the crossover scaling theory in the canonical ensemble. One can see also both the asymmetry of the scaling function and the size of the region of validity of the scaling function from these diagrams. The high temperature side convergences very slowly and this reinforce the remarks above and elsewhere [7] concerning the care that must be taken in analysing finite length data at collapse transitions.

### 3.2 Collapsed Phase

The scaling form (20) is the expected scaling form for the partition function in a wide range of walk/polygon models and hence polymer systems. This form induces a divergence in the generating function (see above) as one approaches the radius of convergence from below. From the exact solution it is clear that the generating function converges at its radius of convergence indicating an essential singularity of some type.

Previous work by Fisher [11] on the condensation of a fluid system can be adapted to our problem in the following way. We have conjectured that the scaling form

$$Q_L \sim [\mu_0(\omega)]^L [\mu_1(\omega)]^{L^\sigma} L^{\gamma - 1}$$

where $\sigma \approx 1/2$, is the appropriate asymptotic scaling in the collapsed region for general SAW type problems [6]. Here we shall present evidence to support this claim. We shall also consider the consequences for the critical point crossover scaling. This will introduce a further critical exponent $\chi$, thereby extending Fisher’s discussion.

From the exact solution we know already that $\mu_0(\omega) = \omega$. For the estimation of $\sigma$, we first compute an effective exponent $\sigma(L)$ from

$$\log(Q_L(\omega)^{-L}) \sim L^\sigma$$

at $\omega - \omega_c = 1, 2, \ldots, 64$ for $L \leq 6000$ in the collapsed phase. A plot against $L^{-1/2}$ (figure 8) suggests that in fact asymptotically $\sigma = 1/2$ in the collapsed regime. Using differential approximants on $\log(Q_L(\omega)^{-L})$, we confirm that $\sigma = 0.495(6)$.

Assuming $\sigma = 1/2$, we now proceed with an estimation of $\gamma - 1$. We compute estimates from a two–parameter fit to

$$\log(Q_L(\omega)^{-L}) \sim \log\mu_1 L^{1/2} + (\gamma - 1) \log L.$$
The result is shown in figure 9 and again we see convergence to a value of about 0.75 over a wide range of temperatures in the collapsed region. We remark that due to pathological behaviour of the zero temperature state these computations need to be done with series whose lengths are well above 100 in order to overcome these pathologies.

Extrapolation of $\gamma_-$ by fitting successively to

$$\log(Q_L(\omega)\omega^{-L}) \sim \log \mu_1 L^{1/2} + (\gamma_- - 1) \log L + \sum_{i=0}^{n} a_n L^{-n/2}$$

results in a very accurate determination of $\mu_1(\omega)$ and a value of $\gamma_- = 0.250000(5)$, which by its accuracy is an indirect confirmation of $\sigma = 1/2$. The direct estimation of $\sigma$ is less accurate because the differential approximants cannot account for either $\mu L^\sigma$ asymptotics or, upon taking the logarithm, for the logarithmic correction term.

Of further interest is the crossover that occurs as $\omega \to \omega_c$. A crossover scaling form for the collapsed region is again given by

$$Q_L(\omega) \sim [\mu_\omega(\omega)]^L L^{\gamma t - 1} \Theta(\delta\omega L^\phi)$$

whereas comparison with (29) implies that

$$\Theta(x) \sim \begin{cases} \mu_\omega^{1/\phi} |x|^\sigma/\phi & \text{for } x \to -\infty \\ \mu_\omega^{(\gamma_- - \gamma_t)/\phi} |x|^{(\gamma_- - \gamma_t)/\phi} & \text{for } x \to 0. \end{cases}$$

(34)

This, together with (21) describes the complete crossover scaling form as outlined in [7]. (In our model, we have an even slightly simpler scaling form due to $\mu_\omega(\omega) = \omega$ and $\mu_- = 1$ in the collapsed phase.)

To test this scaling form, we note that as a consequence we have asymptotically

$$\mu_1(\omega) \sim \mu_\omega^{[\delta\omega]^\chi} \quad \text{with} \quad \chi = \frac{\sigma}{\phi} = \frac{3}{4},$$

so that the independent computation of the exponent $\chi$ can serve as a verification. In order to check its predicted value, we compute $\mu_1(\omega)$ for $\omega \to \omega_c$. We fit again using (31), but now with $\gamma_-$ specified. Naturally this extrapolation gets worse when we approach $\omega_c$, as we have to extrapolate into the crossover regime itself. The results are shown in figure 10, and one can see that the error increases as the critical point is approached. Clearly the numerical results are compatible with a slope of $\chi = \frac{3}{4}$.

We conclude this section with summarising the exponent values in the collapsed phase in table ??.
4 Results for the Length Scales

The examination of the “size” of the objects is a central task of the analysis of walk models. We present results on the end–to–end displacements of the walks as functions of length and temperature and in the following subsection provide a simple phenomenological picture and scaling theory to explain the results.

The quantities of initial interest are the average horizontal $\langle R_x \rangle$ and vertical $\langle R_y \rangle$ end–to–end displacements:

$$\langle R_{x,y} \rangle = \sum_{\text{configurations}} R_{x,y} c_L(I) \omega^I / Q_L. \quad (36)$$

This supplies us with some measure of the global size of the walks. Note that $R_x$ is simply equal to the number of horizontal steps $L_x$ while this correspondence does not hold for $R_y$. One can compute the corresponding generalised canonical averages by introducing three fugacities into the generating function associated with the horizontal steps and with the vertical steps from folds that move in the positive and negative (a different fugacity) $y$ directions (as one moves along the walk in the positive $x$ direction) [5]. However, as stressed before, the low temperature results are not useful since the generalised canonical averages converge at the radius of convergence of the generating function.

Also of interest is the average length of each vertical fold. This will give a measure of the local size and is defined as

$$\langle h \rangle = \sum_{\text{configurations}} \left( \sum_i h_i / L_x \right) c_L(I) \omega^I / Q_L, \quad (37)$$

where $i$ labels the folds of an individual walk and $h_i = |r_i|$.

As $L \rightarrow \infty$ the size of the walks become large and the end–to–end displacements are expected to scale as

$$\langle R_{x,y} \rangle \sim L^{\nu_{x,y}}. \quad (38)$$

We define also $\nu_h$ by

$$\langle h \rangle \sim L^{\nu_h}. \quad (39)$$

Utilising the recurrence relations, we have calculated effective exponents for $\langle R_{x,y} \rangle$ and $\langle h \rangle$ as functions of $L$ from series up to $L = 600$. The reason for this much shorter series is
that the amount of computer memory needed to keep track of the geometric information is naturally much larger than for the computation of the generating function alone. The results are shown in Figures 11, 12 and 13.

As above, we can extract estimates of the exponents at high, critical and low temperatures, shown in table ???. The estimation of the numerical values again involved differential approximants on the one hand and an extrapolation procedure with an assumed corrections–to–scaling form on the other. The assumed corrections–to–scaling were integer powers of $L^{-1}$ in the extended phase, $L^{-1/3}$ at the critical point, and $L^{-1/2}$ in the collapsed phase. The high and critical temperature exponents agree, as expected, with the exact calculation [5].

The results for $T > T_c$ converge quite fast to the exact results of $\nu_x = 1$, $\nu_y = 1/2$, and $\nu_h = 0$, with the anticipated correction to scaling of $L^{-1}$. This allows us to visualise the dominant walk configurations in the extended phase as elongated and such walks are effectively free partially directed random walks with a finite local fold length. For later comparison we mention that here the vertical radius of gyration scales in the same way as the vertical end–to–end distance.

At $T_c$ the estimates converge at a greatly reduced rate to the exact values of $2/3, 1/3, 1/3$ while the theoretic correction term $L^{-1/3}$ has a much stronger effect. The predominant walks are now those in which the local length is as large as the overall size. So the radius of gyration, the end–to–end distance and the local size all scale together.

Most curious, at first, are the low temperature results which are precisely the ones that have not been found exactly. Conventional wisdom would say that the walks collapse to compact objects and so any radius of gyration would scale as the length to the exponent $1/d$, where $d$ is the lattice dimension. This wisdom also dictates that it does not matter which length scale one chooses to measure (the actual radius of gyration or the end–to–end distance) as the same exponent should appear. We have found strong evidence that the vertical end–to–end displacement exponent is in fact not $1/2$ but $1/4$! However, with some simple arguments one can show that the global size of the object in the vertical direction must scale with an exponent of at least $1/2$. The average local size (that is, the fold length) certainly seems to scale with the exponent $1/2$, and the global size must be as large as the local one! In the next section we explain these intriguing results.
4.1 Scaling Theory

The key to understanding these results is to understand that the dominant configurations at low temperatures are droplet or bubble–like. In fact one can view the the collapse transition as a fluid condensation transition by placing “particles” on the dual lattice wherever there exists monomer–monomer interactions. Then at high temperatures we have an infinite string of finite droplets (see figure 14) while at low temperatures a single infinite drop exists (see figure 15).

As the results stand, one feature that is immediately clear is that the relationship

\[ \nu_x = 2\nu_y \] (40)

always holds. This leads us to the idea that the centre–of–mass of the configurations at any temperature acts like a free partially directed walk. The other ingredient needed to make sense of the 1/4 value for \( \nu_y \) is the following. Let \( h_i \) be the height of the \( i \)-th fold in a configuration and \( \langle h_i \rangle \) be the average height over walks of length \( L \). If we let \( i \) and \( L - i \) simultaneously be proportional to \( L \) then we can safely assume that \( \langle h_i \rangle \sim L^{1/2} \). However, if \( \nu_y = 1/4 \) then we should have \( \nu_1 \leq 1/4 \) where \( \langle h_L \rangle = \langle h_1 \rangle \sim L^{\nu_1} \). We have estimated the value of \( \nu_1 \) (Figure 16) and found that it is in fact close to 0. We conjecture that it is in fact zero (although we do not comment on whether \( \langle h_1 \rangle \) is finite in the thermodynamic limit). We then see that the dominant configurations are bubble–like, rather than say square as one might also expect.

We may introduce a shape scaling form for the bubble as

\[ \langle h_i \rangle \sim L^{\nu_h} H(iL^{-\nu_h}) \] (41)

where

\[ H(x) \sim x^{1-\nu_1/\nu_h} \] (42)

for \( x \to 0 \) and \( x \to 1 \). The exponent \( \rho = \nu_h(1 - \nu_1/\nu_h) \) is a shape exponent describing the shape of the ends of the bubble. In this case \( \nu_1 = 0 \) so \( \rho = 1/2 \) giving a locally spherical shape.

To summarise: since the number of “centre–of–mass” steps, which is of the order of \( L^{1/2} \), perform a partially directed walk this “centre–of–mass” walk has an average vertical
displacement of the order of $L^{1/4}$. Given that the length of the first and last segments scale with powers less than a quarter then the total vertical end–to–end displacement scales as $L^{1/4}$. Hence this does not contradict the fact that the global vertical size of the walks scale with the power 1/2, as the walks form bubble shaped objects on average.

Acknowledgements

The authors thank Keith Briggs for carefully reading the manuscript and are grateful to the Australian Research Council for financial support. They also thank Keith Briggs for his willingness to continually extend his differential approximant program [?] to suit our growing needs.

References

A Figures

1. A typical partially directed walk with interactions represented by grey bonds between nearest neighbour steps.

2. Plots of the thermodynamic limit free energy $f_\infty(T)$, internal energy $u_\infty(T)$ and specific heat $c_\infty(T)$ against the temperature variable $\omega$ calculated from a continued fraction expansion [5]. The specific heat is zero for $\omega > \omega_c$.

3. The singularity diagram for the discrete IPDSAW model. Important points, including free walks at $\omega = 1$ and the tricritical collapse point are shown.

4. Estimates for the exponents $\alpha$ and $\phi$ at the collapse transition are plotted against a corrections–to–scaling term of $L^{-1/3}$ for $L$ up to 2000. The exact values are $1/2$ and $2/3$ respectively. This plot shows that the series are only slowly convergent.

5. To demonstrate the slow asymptotic truth of the relation $2 - \alpha = 1/\phi$ a plot of $\alpha + 1/\phi$ is shown. The leftmost point corresponds to $L = 2000$.

6. Estimates for the scaling function $\Theta(x)$ of the partition function (up to a constant) are shown for lengths $L = 250, 500, 1000, 2000, 4000$.

7. Estimates for the scaling function $\Omega(x)$ of the specific heat (up to a constant) are shown for lengths $L = 250, 500, 1000, 2000, 4000$.

8. Estimates for the exponent $\sigma$ plotted against a corrections–to–scaling term, for a range of temperatures, for $L$ up to 6000. The “temperatures” are, from top to bottom, $\omega = \omega_c + 64.0, 32.0, 16.0, 8.0, 4.0, 2.0, 1.0$.

9. Estimates for the exponent $\gamma - 1$, computed by fitting the calculated partition function to the full form (29) for $L$ up to 6000. Again these cover the same range of temperatures as in Figure 8. from top to bottom (on the left hand side). Fitting these curves with 3rd and 4th order polynomials in $L^{-1/2}$ produces remarkably stable results.

10. To provide an estimate for the new exponent $\chi$ a log–log plot of $\mu_1$ is given against the “temperature” difference to the critical point $(\omega - \omega_c)$. A 6000 term series was used to calculate $\mu_1$. The straight line has slope $3/4$. 

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11. The high temperature ($\omega = 1.0$) length scale exponents can be estimated from this plot of $\nu_{\parallel}, \nu_{\perp}$ and $\nu_h$. The corrections should be of the order $1/L$ (from the exact solution) and so we use this as the variable against which we plot. A 600 term series was used here because of the greater complexity of the series needed to calculate length scale exponents.

12. The critical temperature ($\omega = 3.382975...$) length scale exponents can be estimated from this plot of $\nu_{\parallel}, \nu_{\perp}$ and $\nu_h$. Here the corrections to scaling should be of the order $(L^{-1/3})$. A 600 term series was used.

13. The low temperature ($\omega = 6.0$) length scale exponents can be estimated from this plot of $\nu_{\parallel}, \nu_{\perp}$ and $\nu_h$. Here the corrections to scaling should be of the order $(L^{-1/2})$. A 600 term series was used.

14. A picture showing the dominant type of configurations at low temperature; these being described as bubble–like.

15. A picture showing the dominant type of configurations at high temperatures for comparison. Finite size droplets form up to the size of the thermal correlation length $\xi_x$.

16. The growth exponent for the length of the first segment $h_1$ denoted by $\nu_T = 1$ is plotted here against $L^{-1/2}$. It clearly converges to a value less than $1/4$ and probably converges to zero.
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<th>exact results</th>
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<td>$\gamma_t$</td>
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<td>0.3334(2)</td>
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<tr>
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<td>0.62(2)</td>
<td>0.51(1)</td>
<td>0.5000(1)</td>
<td>1/2</td>
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<td>0.69(1)</td>
<td>0.6667(1)</td>
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<td>$\alpha + 1/\phi$</td>
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<td>1.96(2)</td>
<td>2.0000(2)</td>
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Table 1: Numerical estimations for $\gamma_t$, $\alpha$, and $\phi$. 
Table 2: Conjectured values for $\sigma$, $\gamma_-$, and $\chi$.

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<td>$\sigma$</td>
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<tr>
<td>$\gamma_-$</td>
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<td>$\chi$</td>
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Table 3: End–to-end displacement and average fold length exponents.

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<td>$2/3$</td>
<td>0.3338(5)</td>
</tr>
<tr>
<td>$T &lt; T_c$</td>
<td>0.501(1)</td>
<td>0.251(1)</td>
<td>0.502(2)</td>
</tr>
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