Swelling-collapse transition of self-attracting walks

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We study the structural properties of self-attracting walks in d dimensions using scaling arguments and Monte Carlo simulations. We find evidence of a transition analogous to the Θ transition of polymers. Above a critical attractive interaction \( u_c \), the walk collapses and the exponents \( \nu \) and \( k \), characterizing the scaling with time \( t \) of the mean square end-to-end distance \( \langle R^2(t) \rangle \) and the average number of visited sites \( \langle S \rangle \), are universal and given by \( \nu = 1/\left(d+1 \right) \) and \( k = d/(d+1) \). Below \( u_c \), the walk swells and the exponents as with no interaction, i.e., \( \nu = 1/2 \) for all \( d \), \( k = 1/2 \) for \( d = 1 \) and \( k = 1 \) for \( d > 2 \). At \( u_c \), the exponents are found to be in a different universality class.

In this Rapid Communication we present scaling arguments and extensive numerical simulations for \( \langle R^2(t) \rangle \) and \( \langle S \rangle \) that strongly suggest the existence of a critical attraction \( u_c \) in \( d \geq 2 \), with three different universality classes for \( u > u_c \), \( u < u_c \), and \( u = u_c \). Below \( u_c \), the SATW is in the universality class of random walks, with \( \nu = 1/2 \) and \( k = 1/2 \). Above \( u_c \), the SATW collapses and the exponents change to \( \nu = 1/(d+1) \) and \( k = d/(d+1) \). At the critical point, the exponents are \( \nu_c = 0.40 \pm 0.01 \) and \( k_c = 0.80 \pm 0.01 \) in \( d = 2 \) and \( \nu_c = 0.32 \pm 0.01 \) and \( k_c = 0.91 \pm 0.03 \) in \( d = 3 \) [11]. The existence of \( u_c \) is in striking similarity to the Θ point phenomenon of linear polymers [4,5] where three different universality classes for \( T > \Theta \), \( T = \Theta \), and \( T < \Theta \) exist.

We used Monte Carlo simulations to study \( \langle R^2(t) \rangle \) and \( \langle S \rangle \). Figure 1 shows representative results of \( \langle R^2(t) \rangle \) for several values of \( u \) in \( d = 3 \). For large values of \( u \) the curves bend down toward the slope of \( 2 \nu \equiv 0.5 \) while for small values of \( u \) the curves bend up toward the slope of \( 2 \nu \equiv 1 \). At some intermediate critical value \( u_c \approx 1.9 \), the slope is approximately \( 2 \nu_c \approx 0.64 \). The mean number of visited sites \( \langle S \rangle \) shows a similar behavior, with \( k \approx 1 \) below \( u_c \), \( k_c \)

FIG. 1. The mean square end-to-end distance \( \langle R^2(t) \rangle \) vs \( t \) up to \( t = 10^8 \) time steps averaged over 1000 configurations for each attraction \( u = 0, 1.5, 1.9, 2.25, \) and \( 4 \) in \( d = 3 \). Note that for large values of \( u \) the curves bend down toward the slope of \( 2 \nu = 1/2 \), while for small values of \( u \) the curves bend up toward the slope of \( 2 \nu = 1 \).
The number of visited sites scales with the rms displacement $R_{\text{rms}}$ as

$$ R_{\text{rms}} \sim t^{\alpha}, $$

where $\alpha$ is the exponent that characterizes the long-time behavior of the mean square displacement. For values related to the $\Theta$ transition, we find the best collapse for $\alpha = 5.0$; for $d = 2$ for $u_c = 0.40$, $k_c = 0.80$, and $u_c = 0.88$, we find the best collapse for $\alpha = 7$. The straight lines represent the exponents given in Table 1.

$$ k = vd, \quad u \gg u_c. \quad (3) $$

For sufficiently strong attraction it takes a very long time for the walker to jump to an unvisited site. Before doing this, the walker diffuses around on the visited sites, which are located with equal probability on any of the cluster sites. Hence the mean cluster growth rate is proportional to the ratio between the number of boundary sites and the total number of the cluster sites $[3, 12]$:

$$ \frac{d\langle S \rangle}{dt} \sim \left( \frac{\langle R \rangle^{d-1}}{\langle R \rangle^d} \right)^{\alpha - 1} \sim t^{-\nu}. \quad (4) $$

Thus $\langle S \rangle \sim t^{-\nu + 1}$. Combining this result with Eqs. (1b) and (3), we obtain

$$ \nu = 1/2, \quad \alpha = 5.0; \quad u_c = 1.92 \pm 0.03. $$

### Table I

Comparison of the exponents $\nu$ and $k$ as well as the estimated values for the transition points $u_c$ for random walks (RW) and $\Theta$ for SAW's on hypercubic lattices. For values related to the $\Theta$ transition, see Ref. [5] and references therein.

<table>
<thead>
<tr>
<th>RW</th>
<th>SAW</th>
</tr>
</thead>
<tbody>
<tr>
<td>$d = 2$</td>
<td>$d = 3$</td>
</tr>
<tr>
<td>$u &lt; u_c$</td>
<td>$u = u_c$</td>
</tr>
<tr>
<td>$v$</td>
<td>1/2</td>
</tr>
<tr>
<td>$k$</td>
<td>1</td>
</tr>
<tr>
<td>$u_c = 0.88 ± 0.05$</td>
<td>$\theta_0 = 0.65 ± 0.03$</td>
</tr>
<tr>
<td>$d = 3$</td>
<td>$d = 3$</td>
</tr>
<tr>
<td>$v$</td>
<td>1/2</td>
</tr>
<tr>
<td>$k$</td>
<td>1</td>
</tr>
<tr>
<td>$u_c = 1.92 ± 0.03$</td>
<td>$\theta_0 = 0.5 ± 0.03$</td>
</tr>
</tbody>
</table>
Because of universality we assume that these results, which are in agreement with the exact values \( \nu = 1/2 \) and \( k = 1/2 \) in \( d = 1 \) [10], and are supported by our extensive Monte Carlo simulations in \( d = 2 \) and 3, are valid for all \( u > u_c \). Indeed, Fig. 2 suggests that the predictions for \( u > u_c \) [Eq. (5)] are approached asymptotically. We note that in \( d = 2 \) the relation \( k = \nu d \) also holds for \( u \leq u_c \), while in \( d = 3 \) the numerical results yield \( k > \nu d \) for \( u < u_c \). Since the mass of the generated clusters scales like \( M \sim S \sim R^{k/d} \), \( k/\nu \) corresponds to the fractal dimension \( d_f \) of the cluster. In \( d = 2 \) the clusters are compact for all \( u \) as \( k/\nu = d_f = d \). In \( d = 3 \) they are compact for \( u > u_c \), while for \( u < u_c \) the fractal dimension of clusters generated by simple random walks \( d_f = 2 < d \) is obtained. At the criticality, we find \( d_f = 2.84 \pm 0.25 \), but we cannot rule out the possibility that \( d_f = d \).

To understand the behavior in the critical regime we suggest the following scaling approach. Guided by Fig. 1, we assume that there exists a crossover time \( t_\xi \) below which the exponent \( n \) is close to \( n_c \). Above which \( n \) approaches \( 1/2 \) for \( u < u_c \) and \( 1/(d+1) \) for \( u > u_c \). This suggests the scaling relations

\[
R(t) \sim t^{n_c} g_\pm (t/t_\xi),
\]

and

\[
S(t) \sim t^{k_c} g_\pm (t/t_\xi),
\]

where

\[
t_\xi = |u - u_c|^{-\alpha}.
\]

The plus sign refers to \( u > u_c \), the minus sign to \( u < u_c \), and the exponent \( \alpha \) has to be determined numerically. As \( t_\xi \) is assumed to be the only relevant time scale, the scaling functions bridge the short time and the long time regime. To match both regimes, we require that \( f_\pm (x) = \text{const} \) for \( x < 1 \) \( (t < t_\xi) \), and \( f_+ (x) \sim x^{(d+1)/2 - n_c} \), \( f_- (x) \sim x^{1/2 - n_c} \) for \( x > 1 \). Analogous results are expected for \( g_\pm (x) \), with \( g_\pm (x) = \text{const} \) for \( x < 1 \), and \( g_+ (x) \sim x^{d/(d+1) - k_c} \), \( g_- (x) \sim x^{1 - k_c} \) for \( x > 1 \).

To test the scaling theory and to determine the exponent \( \alpha \), we plotted \( \langle R^2 (t) \rangle/t^2 \) and \( \langle S(t) \rangle/t_\xi^2 \) as functions of \( t/t_\xi \) for several values of \( \alpha \) in \( d = 2 \) and 3. We obtained the best data collapse for \( \alpha = 5.0 \pm 0.5 \) in \( d = 3 \) and \( \alpha = 7 \pm 1 \) in \( d = 2 \), which are shown in Fig. 3(a) and 3(b), respectively. The excellent data collapse strongly supports the above scaling assumptions.

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[6] Note that, in the original definition by Sapozhnikov, \( p \sim \exp x(-nu) \), with \( u < 0 \) [3]; for convenience we use \( p \sim \exp (+nu) \), with \( u > 0 \).

[7] The SAW corresponds to the case \( \alpha \to -1 \) and \( g < 0 \) of the generalized true self-avoiding walk model of Oettinger [2], where the probability \( p_i \) for moving to the neighboring site \( i \) depends on the number of previous visits \( n_i \) of site \( i \) through \( p_i \sim \exp(-gn_i^{\alpha+1}) \).


[11] These results could be found only because of the large number of time steps \( t \) taken in our simulations, revealing the asymptotic behavior of the exponents.