Self-avoiding trails with nearest neighbour interactions on the square lattice

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Work in collaboration with A. L. Owczarek and T. Prellberg
Outline

1. Lattice polymers
2. Collapsing polymers
3. Nearest-Neighbour Interacting Self-Avoiding Trails
4. Conclusions
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1. Lattice polymers
2. Collapsing polymers
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Consider a walk on a some regular lattice

\[ \phi_n = \{x_0 \equiv 0, x_1, \ldots, x_n\} \]

where \( x_i \) and \( x_{i+1} \) are lattice neighbours.

- Require \( x_i \) to be all distinct (e.g. \( x_i \neq x_j \) if \( i \neq j \)).
Fundamental quantities

- We are interested in their number
  \[ Z_n \approx \mu^n n^{\gamma-1}, \]

- and in their size (ad. es. end-to-end distance)
  \[ R_n^2 = \langle |x_n|^2 \rangle \approx n^{2\nu} \]

- \( \gamma \) and \( \nu \) are universal exponent.

- These exponents can be understood as those of a magnetic system with \( O(N) \) symmetry in the limit \( N \to 0 \).

- Exact values can be obtained using Coulomb Gas arguments
  \[ \nu = 3/4 \text{ and } \gamma = 43/32 \]

- “Dilute polymers” phase
Self-Avoiding Trail (SAT)

- A model for polymers with loops or polymers in thin layers.

\[ \phi_n = \{ x_0 \equiv 0, x_1, \ldots, x_n \} \]

where we now require

\[ x_i x_{i+1} \neq x_j x_{j+1} \text{ if } i \neq j \] (bond avoidance)

CG predicts crossings to be an irrelevant perturbation of the dilute universality class.

Indeed, there is numerical evidence that the SAT exponents are the same as SAW.
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We introduce an attractive self interaction (contacts $m_c$).

and define the partition function:

$$Z_n(\omega) = \sum_{\phi \in SAW_n} \omega^{m_c(\phi)}$$

Energy: $u_n = \langle m_c \rangle / n$, Specific heat: $c_n = (\langle m_c^2 \rangle - \langle m_c \rangle^2) / n$
Collapse transition

- As the interaction increases we reach a critical point.
  
  \[ \theta\text{-point} \]
  
  dilute \[ \omega_c \] dense \[ \omega \]

- The collapse transition corresponds to a tri-critical point of the \( O(N \to 0) \) magnetic system.

- Finite-size quantities are expected to obey a scaling form

  \[ c_n(\omega) \sim n^{\alpha \phi} C((\omega - \omega_c)n^\phi) \]

  where \( C(x) \) is a scaling function and \( 0 < \phi \leq 1 \).

  - Exponents \( \alpha \) and \( \phi \) satisfy the tri-critical relation

    \[ 2 - \alpha = \frac{1}{\phi} \]
Exact $\theta$-point exponents

- The presence of vacancies induce short-range interactions on SAWs.
- $\theta$-point is obtained at the point where the vacancies percolate
- Full set of exponents can be obtained
  \[ \phi = \frac{3}{7}, \quad \alpha = -\frac{1}{3} \quad \text{and} \quad \nu = \frac{4}{7}. \]
- Specific heat does not diverge (exponent $\alpha\phi = -\frac{1}{7}$)
- Third derivative does diverge (exponent $(\alpha + 1)\phi = \frac{2}{7}$)
Interacting Self-Avoiding Trails (ISAT)

- Introduce a same-site interaction on trails

Let $m_t$ be the number of doubly visited sites, we define

$$Z_n^{ISAT}(\omega) = \sum_{\psi \in SAT_n} \omega^{m_t(\psi)}.$$ 

- Energy: $u_n = \langle m_t \rangle / n$, Specific heat: $c_n = (\langle m_t^2 \rangle - \langle m_t \rangle^2) / n$
ISAT Collapse

- As shown by Owczarek and Prellberg on the square lattice there is a collapse transition with estimated exponents
  \[ \phi_{IT} = 0.84(3) \quad \text{and} \quad \alpha_{IT} = 0.81(3) \]

- Additionally, the scaling of end-to-end distance was found to be consistent with
  \[ R_n^2 \sim n (\log n)^2 \]

Clearly different from the \( \theta \)-point

- No predictions for these exponents
- Phase diagram
ISAT collapsed state

If we consider that proportion $p_n$ of sites which are not doubly occupied

$$p_n = \frac{n - 2\langle m_t \rangle}{n}.$$ 

it is found\(^1\) that in the low temperature region

$$p_n \sim n^{-1/2} \rightarrow 0 \quad \text{as} \quad n \rightarrow \infty.$$ 

\(^{1}\)AB, A.L. Owczarek, T. Prellberg, arXiv:1210.7196
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- that implement the same ideas
  (excluded volume + short range attraction)
- whose collapse transitions lie in different universality classes.

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<thead>
<tr>
<th>Geometry</th>
<th>Interaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>self-avoiding walks</td>
<td>nearest-neighbours</td>
</tr>
<tr>
<td>vs</td>
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</tr>
<tr>
<td>self-avoiding trails</td>
<td>multiply visited sites</td>
</tr>
</tbody>
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**Geometry**

- self-avoiding walks vs self-avoiding trails

**Interaction**

- nearest-neighbours vs multiply visited sites
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Definition

Let $m_c(\psi_n)$ be the number of contacts, we define

$$Z_n^{\text{NT}}(\omega) = \sum_{\psi_n \in \text{SAT}_n} \omega^{m_c(\psi_n)}.$$ 

Energy: $u_n = \langle m_c \rangle / n$, Specific heat: $c_n = (\langle m_c^2 \rangle - \langle m_c \rangle^2) / n$
Specific-heat behaviour

- Let $c_n^p$ be specific-heat at peak at length $n$.
- We plotted the quantity
  \[
  \log_2 \left[ \frac{c_n^p - c_{n/2}^p}{c_{n/2}^p - c_{n/4}^p} \right] \xrightarrow{n \to \infty} \alpha \phi
  \]
- We find
  \[
  \alpha_{NT} \phi_{NT} = -0.16(3),
  \]
  vs a $-1/7 \approx -0.14$ ($\theta$-point) and $\approx +0.68$ (ISAT).
Third-derivative behaviour

- Let $t_n^p$ be the peak of the third derivative.
- The quantity
  \[
  \log_2 \left\{ \frac{t_n^p}{t_n^{p/2}} \right\} \overset{n \to \infty}{\longrightarrow} (1 + \alpha) \phi
  \]
- We find
  \[
  (\alpha_{NT} + 1) \phi_{NT} = 0.23(5)
  \]
  vs a $\theta$-point value of $2/7 \approx 0.28$
Radius scaling

Assuming ISAW crossover exponent $\phi = \frac{3}{7}$, we can determine precisely the critical point go to greater lengths.

$$\nu \simeq 0.575(5)$$

vs a $\theta$-point value of

$$\nu = \frac{4}{7} \simeq 0.571..$$
Characterisation of the low-temperature region

Plot of the proportion of steps visiting the same site once, at different temperatures above and below the critical point.

The scale $n^{-1/2}$ chosen is the natural low temperature scale.

In all cases: $\lim_{n \to \infty} p_n > 0$. 

In the graph, the proportion $p_n$ is plotted against $n^{-1/2}$ for different values of $\omega$. The graph shows that $p_n$ increases as $n^{-1/2}$ decreases, indicating a higher proportion of steps visiting the same site at lower temperatures.
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Summary

- We simulated a model of self-avoiding trails with nearest-neighbour interaction.
- We presented evidence that its collapse transition is in the same universality class as the $\theta$-point.
- The $\theta$-point seems to be robust when allowing crossings.
- While crossings are expected to be relevant in the dense phase, the dense phase seems also unaffected.
- CG predictions might not hold in presence of crossings.
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Thanks.