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

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Inaugural ANZAMP Annual Meeting 2012, Lorne

arXiv:1210.7092

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

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Outline

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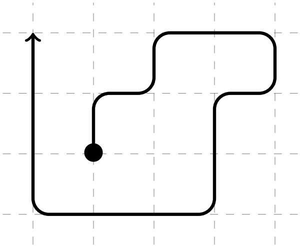
Self-Avoiding Walk (SAW)



- 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

$$Z_n \simeq \mu^n n^{\gamma-1},$$

- and in their size (ad. es. end-to-end distance)

$$R_n^2 = \langle |x_n|^2 \rangle \simeq n^{2\nu}$$

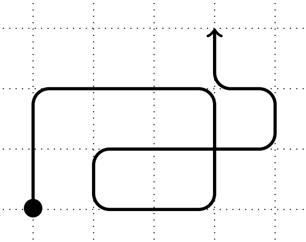
- γ and ν are universal exponent.
- These exponents can be understood as those of a magnetic system with $O(N)$ symmetry in the limit $N \to 0$.
- Exact values can be obtained using Coulomb Gas arguments

$$\nu = 3/4 \text{ and } \gamma = 43/32$$

- “Dilute polymers” phase

Self-Avoiding Trail (SAT)

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



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

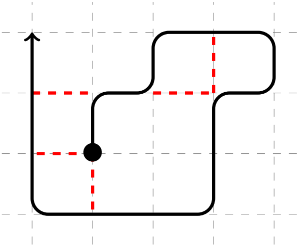
where we now require $\overline{x_i x_{i+1}} \neq \overline{x_j x_{j+1}}$ if $i \neq j$ (bond avoidance)

- 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

Outline

Interacting Self-Avoiding Walks (ISAW)

- We introduce an attractive self interaction (contacts m_c).



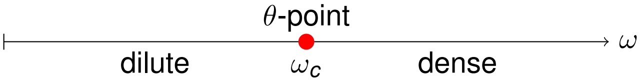
- and define the partition function:

$$Z_n(\omega) = \sum_{\phi \in \mathrm{SAW}_n} \omega^{m_c(\phi)}$$

- 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.



- 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

$$c_n(\omega) \sim n^{\alpha\phi}\, \mathcal{C}\big((\omega - \omega_c)n^{\phi}\big)$$

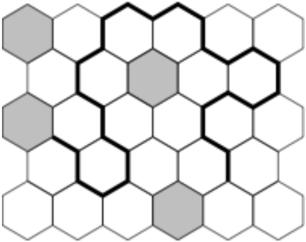
where $\mathcal{C}(x)$ is a scaling function and $0 < \phi \leq 1$.

- Exponents α and ϕ satisfy the tri-critical relation

$$2 - \alpha = \frac{1}{\phi}$$

Exact θ-point exponents

- The presence of vacancies induce short-range interactions on SAWs.
- θ-point is obtained at the point where the vacancies percolate



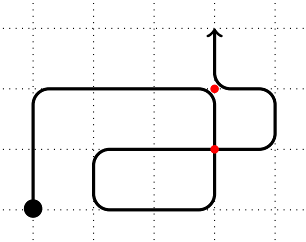
- Full set of exponents can be obtained

$$\phi = 3/7, \quad \alpha = -1/3 \quad \text{and} \quad \nu = 4/7.$$

- Specific heat does not diverge (exponent $\alpha\phi = -1/7$)
- Third derivative does diverge (exponent $(\alpha + 1)\phi = 2/7$)

Interacting Self-Avoiding Trails (ISAT)

- Introduce a same-site interaction on trails



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

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

- 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

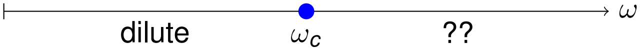
- As shown by Owczarek and Prellberg on the square lattice there is a collapse transition with estimated exponents

$$\phi_{\text{IT}} = 0.84(3) \quad \text{and} \quad \alpha_{\text{IT}} = 0.81(3)$$

- Additionally, the scaling of end-to-end distance was found to be consistent with

$$R_n^2 \simeq n\,(\log n)^2$$

- Clearly different from the θ-point
- No predictions for these exponents
- Phase diagram



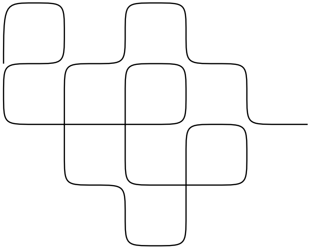
ISAT collapsed state

- 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

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



[1] AB, A.L. Owczarek, T. Prellberg, arXiv:1210.7196

We have seen two models of the polymer collapse.

- that implement the same ideas
  (excluded volume + short range attraction)
- whose collapse transitions lie in different universality classes.

There is no clear understanding of why this is the case.

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Geometry

self-avoiding walks
vs
self-avoiding trails

Interaction

nearest-neighbours
vs
multiply visited sites

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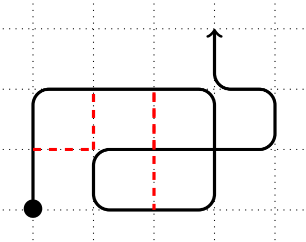
Definition



- 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

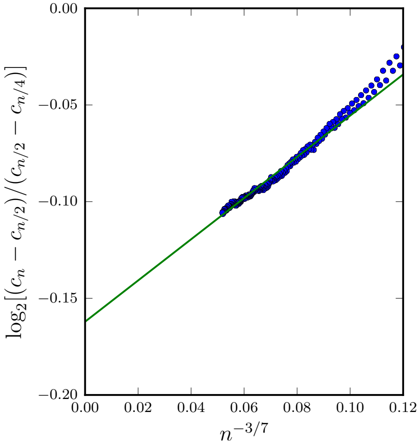
- Let c_n^p be specific-heat at peak at length n.
- We plotted the quantity

$$\log_2 \left[\frac{c_n^p - c_{n/2}^p}{c_{n/2}^p - c_{n/4}^p} \right] \xrightarrow{n \to \infty} \alpha\phi$$

- We find

$$\alpha_{\rm NT}\phi_{\rm NT} = -0.16(3),$$

vs a $-1/7 \approx -0.14$ (θ-point) and $\approx +0.68$ (ISAT).



Third-derivative behaviour

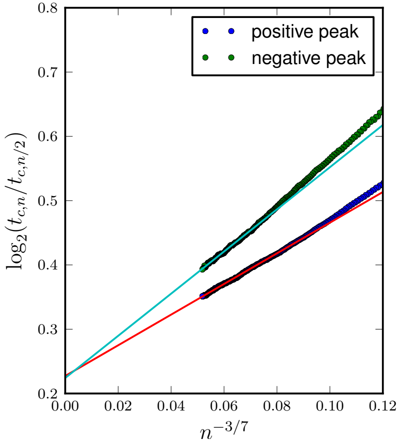
- Let t_n^p be the peak of the third derivative.
- The quantity

$$\log_2 \left[\frac{t_n^p}{t_{n/2}^p} \right] \xrightarrow{n\to\infty} (1+\alpha)\phi$$

- We find

$$(\alpha_{\mathrm{NT}} + 1)\phi_{\mathrm{NT}} = 0.23(5)$$

vs a θ-point value of $2/7 \approx 0.28$



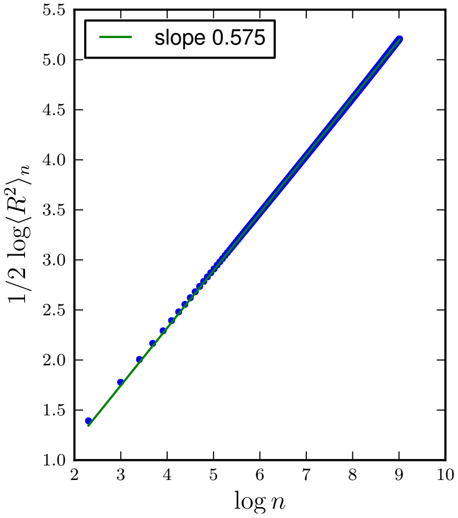
Radius scaling

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

$\nu \simeq 0.575(5)$

vs a θ-point value of

$\nu = 4/7 \simeq 0.571..$

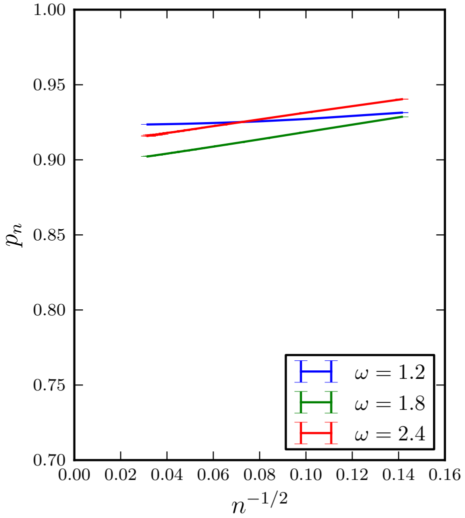


Characterisation of the low-temperature region

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



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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 θ-point.
- The θ-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.