Multiple interacting directed walks

ANZAMP Annual Meeting

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Introduction

- (Multiple) directed walks can be considered as idealised models of polymers in a solution
- At the inaugural ANZAMP meeting, we featured a model of two interacting walks near an attractive surface
- Review the results, including some new ones
- Insights gained for solving models of $n > 2$ interacting walks

What's new

- Publication (JPhysA): *An exact solution of two friendly interacting directed walks near a sticky wall* - to appear soon
- Exact solution
- Polished phase diagram

Allowed walks

Consider two directed walks along the square lattice.
Let Ω be the class of allowed configurations.

- both walks begin at $(0,0)$, end on the x-axis.
- directed: can only take steps in the $(\pm 1, 0)$ directions.
- friendly: walks can share sites, but cannot cross

Interaction terms

- surface visit step: weight a
- shared site contact: weight c
- trivial walk consisting of zero steps has weight 1.

An example

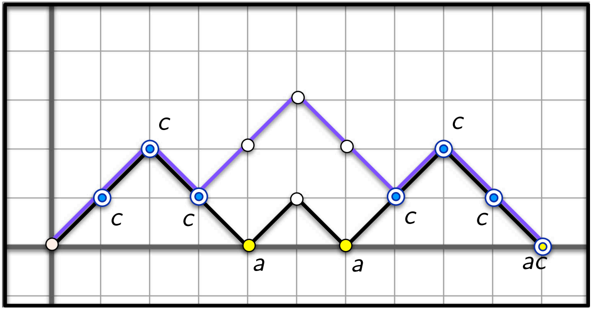


Figure: An allowed configuration of length 10. The overall weight is a^3c^7.

Generating function

We encode all the counting information of every configuration in the generating function:

$$G(a,c) \equiv G(a,c;z) = \sum_{\varphi \in \Omega} w(\varphi) z^{|\varphi|}$$

- $w(\varphi)$ is the weight associated with a given config.
- $|\varphi|$ is the number of paired steps.
- e.g. prev. slide, $w(\varphi) = a^3 c^7$ and $|\varphi| = 10$.

Reduced free energy

With the generating function, we can also determine the reduced free energy $\psi(a, c)$ of the system.

$$\psi(a, c) = -\log z_s(a, c)$$

where $z_s(a, c)$ is smallest real and positive singularity of $G(a, c)$ w.r.t z

Order parameters

Define suitable order parameters to identify phases of the system.
The limiting average surface contacts

$$\mathcal{A}(a, c) \equiv \lim_{L \to \infty} \frac{\langle m_a \rangle}{L} = a \frac{\partial \psi}{\partial a}$$

and the limiting average number of shared sites

$$\mathcal{C}(a, c) \equiv \lim_{L \to \infty} \frac{\langle m_c \rangle}{L} = c \frac{\partial \psi}{\partial c}$$

where m_a and m_c are the number of surface visits and shared contacts for a given config. resp.

Phases

- free: $\mathcal{A} = \mathcal{C} = 0$
- adsorbed: (a-rich) $\mathcal{A} > 0, \mathcal{C} = 0$
- zipped: (c-rich) $\mathcal{A} = 0, \mathcal{C} > 0$
- adsorbed-zipped: (ac-rich) $\mathcal{A} > 0, \mathcal{C} > 0$

Solution of $G(a,1)$

For the case where we ignore shared-contact effects, it was found in *Owczarek, Rechnitzer & Wong* ('12) that

$$G(a,1) = 1 + \sum_{i=1}^{\infty} z^{2i} \sum_{m=1}^{i} a^m \frac{m(m+1)(m+2)}{(i+1)^2(i+2)(2i-m)} \binom{2i}{i} \binom{2i-k}{i}. \tag{1}$$

Solution of $G(1, c)$

For the case where we ignore surface-visit effects, we were able to find the exact-solution to the generating function

$$G(1, c; z) = 1 + c^2 z^2 + c^3 (1 + 2z) z^4 + \left\{ \sum_{i=3}^{\infty} z^{2i} \sum_{m=3}^{2i} c^m \sum_{k=3}^{m} (-1)^{k+1} \frac{k(k-1)(k-2)(2i-k+1)(i-k+2)}{i^2(i-1)^2(i+1)(i-2)} \binom{m}{k} \times \binom{2i-k}{i-2} \binom{2i-k-1}{i-3} \right\}. \tag{2}$$

Solution of $G(a, c)$

Finally, we were able to express $G(a,c)$ in terms of $G(a,1)$ and $G(1,c)$

$$G(a,c;z) = \frac{1}{(a-1)(c-1)}\left[1 + \frac{p_0}{p_1 G\left(a,1;z\right) + p_2 G\left(1,c;z\right) + p_3}\right] \quad (3)$$

where p_i are polynomials in a, c and z. In particular ...

Solution of $G(a, c)$ cont'd

$$
\begin{aligned}
p_0(a, c; z) &= (a-1)(c-1)^2(a-c)(ac-c-a) \\
&\quad - (c-1)\left(2a - a^2 + 3c - 3ac + a^2c - 2\right) a^2c^2z^2 - (a-1)a^2c^4z^4, \\
p_1(a, c; z) &= (a-1)a^2c^3(1-a-c+ac)z^4, \\
p_2(a, c; z) &= (a-1)a(c-1)^3c^2z^2, \\
p_3(a, c; z) &= (a-1)(c-1)^2(a-c) \\
&\quad - a^2(c-1)c^2\left[1 + c(a-2)\right]z^2 + (a-1)a^2c^4z^4.
\end{aligned}
$$

Key point: With solutions to $G(a, 1)$ and $G(1, c)$ we additionally have solved for $G(a, c)$. More on the relation later.

Phase diagram

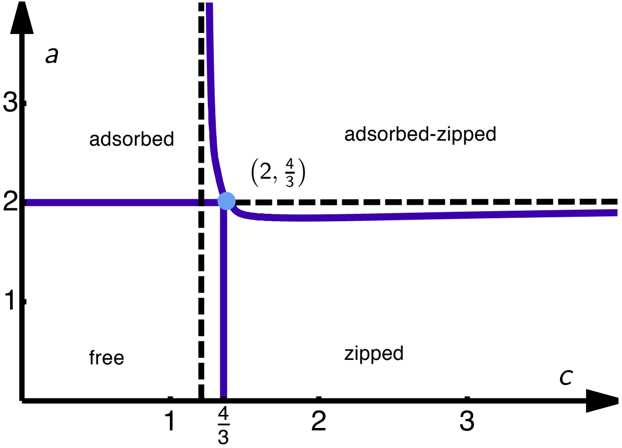


Figure: All transitions are second-order while the critical point where all boundaries meet (filled circle) occurs when $a = 2$ and $c = 4/3$

n interacting walks

Recall

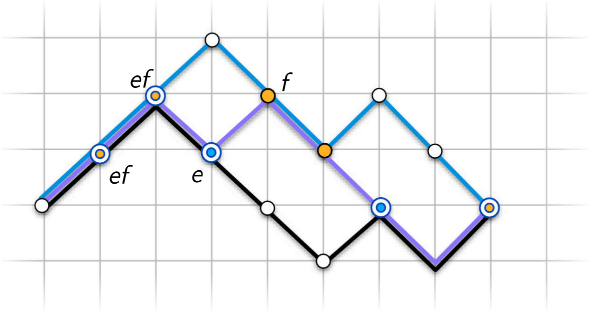
$$G(a,c;z) = \frac{1}{(a-1)(c-1)}\left[1 + \frac{p_0}{p_1 G\left(a,1;z\right) + p_2 G\left(1,c;z\right) + p_3}\right]$$

- Able to isolate interaction effects
- To our knowledge, such a decomposition previously unseen in the literature
- Should we expect this kind of decomposition for similar models ($n > 2$ interacting walks) ?

n interacting walks cont'd

- Relation for $G(a, c)$ obtained analytically, but not very illuminating for understanding general case
- Ideally, we would like a combinatorial proof
- But as a start, consider the case where $n = 3$ to see if we can repeat the process used for $G(a, c)$

Three walks in bulk



Let Δ be comb. class of three directed friendly walks in bulk

$$H(e,f) \equiv H(e,f;z) = \sum_{\varphi \in \Delta} w(\varphi) z^{|\varphi|}$$

Some notation - coefficient extraction

Treating $H(e, f)$ as a power series in e, we have

$$H(e, f) = \sum_{i \geq 0} A_i(f, z) e^i, \quad A_i(f, z) \in \mathbb{Z}[f, z]$$

and we denote the coefficient $A_i(f, z)$ as

$$[e^i] H(e, f) \equiv A_i(f, z)$$

Three walks in bulk cont'd

Solving for general $H(e, f)$ by the exact same process as $G(a, c)$ has not been possible. But we do know

- Combinatorial relation:

$$H(1, f) = \frac{-2fz + [e^1]H(e, f)}{f^2 z^2} \tag{4}$$

- We can find $[e^1]H(e, f)$ using same techniques as for $G(a, c)$
- By symmetry, we can also solve for $H(e, 1)$

Three walks in bulk cont'd

Most importantly, for the equal interaction case (i.e.$f = e$) we have found that

$$H(e,e) = \frac{1}{(e-1)^2}\left[1 + \frac{q_0}{q_1 H\left(e,1;z\right) + q_3}\right]$$

where q_i are polynomials in e and z.

- Closely resembles decomposition for $G(a,c)$
- Suggests that we can also relate $H(e,f)$ in terms of $H(1,f)$ and $H(e,1)$!

To do

- Explicitly solve $H(1, f)$ and $H(e, 1)$
- Find relation for $H(e, f)$ in terms of $H(1, f)$ and $H(e, 1)$ (?)

Distant future

- Can we generalize for arbitrary n interacting directed walks?
- i.e. relate $H(e_1, e_2, \ldots, e_{n-1})$ to $H(e_1, 1, 1, \ldots, 1)$, $H(1, e_2, 1, \ldots, 1)$, $\ldots H(1, 1, \ldots, e_{n-1})$

Thanks!