

# Statistical mechanics of forced and adsorbing directed polymers

Nicholas Beaton

School of Mathematics and Statistics  
University of Melbourne

Monash Workshop on Self-interacting Processes  
29-31 August, 2017



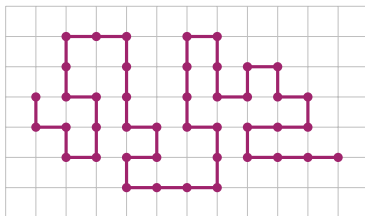
THE UNIVERSITY OF  
MELBOURNE



Australian Government  
Australian Research Council

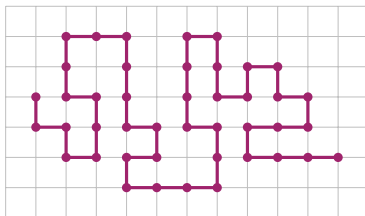
# Self-avoiding walks & polygons

A **self-avoiding walk** (SAW) on a lattice is a walk which never visits the same vertex twice.

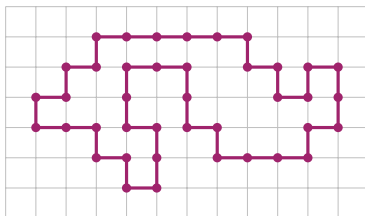


# Self-avoiding walks & polygons

A **self-avoiding walk** (SAW) on a lattice is a walk which never visits the same vertex twice.

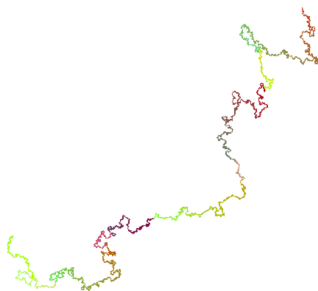
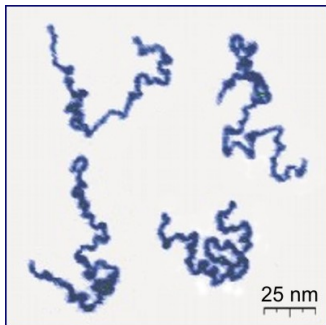


A **self-avoiding polygon** (SAP) is a simple closed loop on the lattice (ie. a SAW which returns to its starting position).



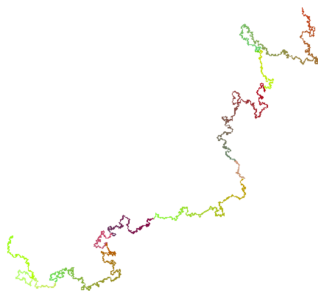
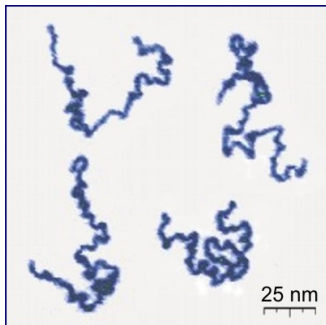
## Self-avoiding walks & polygons

SAWs and SAPs were originally conceived in the 1940s as a model of **long polymer chains** like polyethylene or DNA:



# Self-avoiding walks & polygons

SAWs and SAPs were originally conceived in the 1940s as a model of **long polymer chains** like polyethylene or DNA:



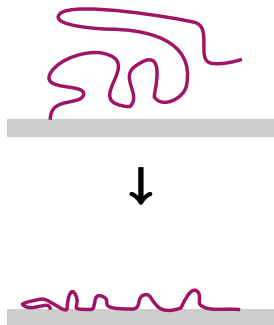
The self-avoidance constraint mimics the **excluded volume** of the monomers in the polymer. Geometric properties like the **radius of gyration** of long polymers in dilute solution closely match those of SAWs in 3D.

# Interacting polymers & phase transitions

Polymers experience various physical and chemical interactions with their environment, each other, and themselves, including

## Interacting polymers & phase transitions

Polymers experience various physical and chemical interactions with their environment, each other, and themselves, including **surface adsorption**,



## Interacting polymers & phase transitions

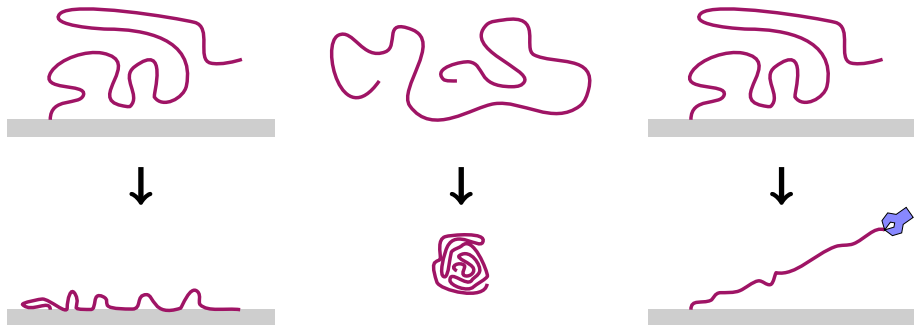
Polymers experience various physical and chemical interactions with their environment, each other, and themselves, including **surface adsorption**, **collapse**





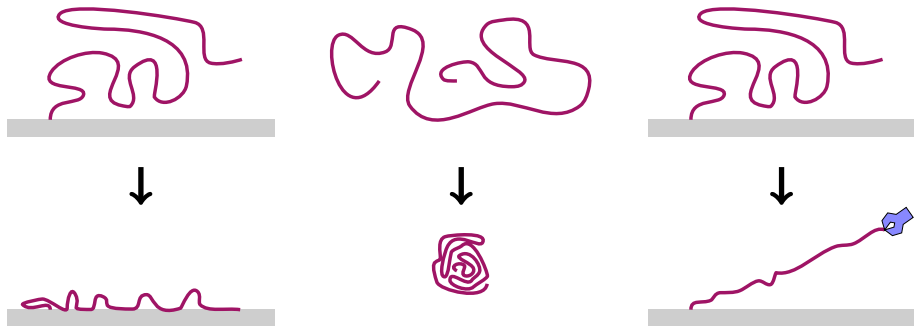
## Interacting polymers & phase transitions

Polymers experience various physical and chemical interactions with their environment, each other, and themselves, including **surface adsorption**, **collapse** and **force-induced stretching**.



## Interacting polymers & phase transitions

Polymers experience various physical and chemical interactions with their environment, each other, and themselves, including **surface adsorption**, **collapse** and **force-induced stretching**.



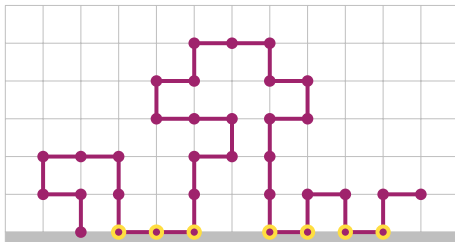
These interactions may lead to **phase transitions** at a **critical temperature** or **force**.

## Adsorbing walks

Interactions can be modelled with SAWs by including an **energy term**.

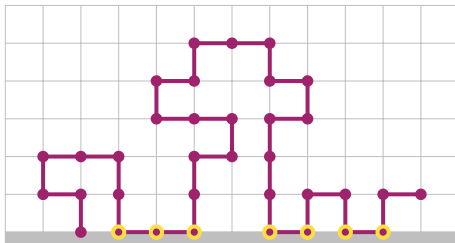
## Adsorbing walks

Interactions can be modelled with SAWs by including an **energy term**. e.g. For adsorption, put the SAWs in a half-space of the lattice and associate an energy with each **visit** to the boundary:



## Adsorbing walks

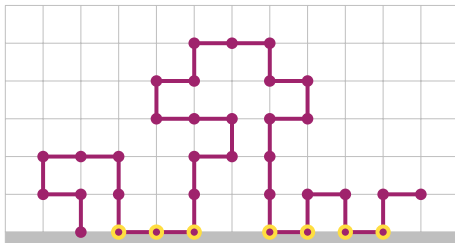
Interactions can be modelled with SAWs by including an **energy term**. e.g. For adsorption, put the SAWs in a half-space of the lattice and associate an energy with each **visit** to the boundary:



Let  $c_n(v)$  be the number of  $n$ -step SAWs which start on the boundary (counted up to translation) and have  $v$  visits to the boundary (excluding the first vertex). So the above walk is counted by  $c_{34}(7)$ .

## Adsorbing walks

Interactions can be modelled with SAWs by including an **energy term**. e.g. For adsorption, put the SAWs in a half-space of the lattice and associate an energy with each **visit** to the boundary:



Let  $c_n(v)$  be the number of  $n$ -step SAWs which start on the boundary (counted up to translation) and have  $v$  visits to the boundary (excluding the first vertex). So the above walk is counted by  $c_{34}(7)$ .

The **partition function** for walks of length  $n$  is then

$$C_n(a) = \sum_v c_n(v) a^v$$

where  $a = e^{\epsilon/kT}$ ,  $\epsilon$  is the **energy of a single visit**,  $k$  is **Boltzmann's constant** and  $T$  is **absolute temperature**.

## Adsorbing walks

$C_n(a)$  is the normalisation for the **Boltzmann distribution**, where the probability of a walk with  $v$  visits is proportional to  $a^v$ :

$$\mathbb{P}(\omega) = \frac{a^{v(\omega)}}{C_n(a)}$$

If  $a$  is large, walks with lots of visits are favoured, while if  $a$  is small, walks with few visits are favoured. The expected number of visits is

$$\langle v \rangle_n = a \frac{\partial}{\partial a} \log C_n(a).$$

## Adsorbing walks

$C_n(a)$  is the normalisation for the **Boltzmann distribution**, where the probability of a walk with  $v$  visits is proportional to  $a^v$ :

$$\mathbb{P}(\omega) = \frac{a^{v(\omega)}}{C_n(a)}$$

If  $a$  is large, walks with lots of visits are favoured, while if  $a$  is small, walks with few visits are favoured. The expected number of visits is

$$\langle v \rangle_n = a \frac{\partial}{\partial a} \log C_n(a).$$

### Theorem (Hammersley, Torrie & Whittington 1982)

*The limit*

$$\kappa(a) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(a)$$

*exists for all  $a \geq 0$ . It is a non-decreasing log-convex function, and is thus continuous and almost-everywhere differentiable.*

This is the limiting **free energy** per step. The log-convexity implies that the limiting **density of visits** is

$$\delta(a) = \lim_{n \rightarrow \infty} \frac{1}{n} \langle v \rangle_n = a \frac{\partial}{\partial a} \kappa(a).$$



## Adsorbing walks

$C_n(1)$  just counts walks of length  $n$  in a half-space. So

$$\kappa(1) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1) = \kappa$$

is the **connective constant** of the lattice.

## Adsorbing walks

$C_n(1)$  just counts walks of length  $n$  in a half-space. So

$$\kappa(1) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1) = \kappa$$

is the **connective constant** of the lattice.

$C_n(0)$  counts walks with no visits to the surface. Those are half-space walks with an extra up-step at the start, so  $C_n(0) = C_{n-1}(1)$ , and hence

$$\kappa(0) = \kappa(1) = \kappa.$$

Since  $\kappa$  is non-decreasing, it must be constant for  $0 \leq a \leq 1$ .

## Adsorbing walks

$C_n(1)$  just counts walks of length  $n$  in a half-space. So

$$\kappa(1) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1) = \kappa$$

is the **connective constant** of the lattice.

$C_n(0)$  counts walks with no visits to the surface. Those are half-space walks with an extra up-step at the start, so  $C_n(0) = C_{n-1}(1)$ , and hence

$$\kappa(0) = \kappa(1) = \kappa.$$

Since  $\kappa$  is non-decreasing, it must be constant for  $0 \leq a \leq 1$ .

On the other hand, there is always a walk with  $n$  visits, so  $C_n(a) \geq a^n$ , and

$$\kappa(a) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(a) \geq \lim_{n \rightarrow \infty} \frac{1}{n} \log a^n = \log a.$$

## Adsorbing walks

$C_n(1)$  just counts walks of length  $n$  in a half-space. So

$$\kappa(1) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1) = \kappa$$

is the **connective constant** of the lattice.

$C_n(0)$  counts walks with no visits to the surface. Those are half-space walks with an extra up-step at the start, so  $C_n(0) = C_{n-1}(1)$ , and hence

$$\kappa(0) = \kappa(1) = \kappa.$$

Since  $\kappa$  is non-decreasing, it must be constant for  $0 \leq a \leq 1$ .

On the other hand, there is always a walk with  $n$  visits, so  $C_n(a) \geq a^n$ , and

$$\kappa(a) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(a) \geq \lim_{n \rightarrow \infty} \frac{1}{n} \log a^n = \log a.$$

So there must be a value  $1 \leq a_c \leq e^\kappa$  where  $\kappa(a)$  switches from constant to increasing, i.e. a point where it is **non-analytic**. This corresponds to the **critical temperature**, at which the **adsorption phase transition** occurs.

## Adsorbing walks

$C_n(1)$  just counts walks of length  $n$  in a half-space. So

$$\kappa(1) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1) = \kappa$$

is the **connective constant** of the lattice.

$C_n(0)$  counts walks with no visits to the surface. Those are half-space walks with an extra up-step at the start, so  $C_n(0) = C_{n-1}(1)$ , and hence

$$\kappa(0) = \kappa(1) = \kappa.$$

Since  $\kappa$  is non-decreasing, it must be constant for  $0 \leq a \leq 1$ .

On the other hand, there is always a walk with  $n$  visits, so  $C_n(a) \geq a^n$ , and

$$\kappa(a) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(a) \geq \lim_{n \rightarrow \infty} \frac{1}{n} \log a^n = \log a.$$

So there must be a value  $1 \leq a_c \leq e^\kappa$  where  $\kappa(a)$  switches from constant to increasing, i.e. a point where it is **non-analytic**. This corresponds to the **critical temperature**, at which the **adsorption phase transition** occurs.

When  $a < a_c$ , walks sampled from the Boltzmann distribution are **desorbed** and  $\delta(a) = 0$ . When  $a > a_c$ , walks sampled from the Boltzmann distribution are **adsorbed** and  $\delta(a) > 0$ .

## Adsorbing walks

$\kappa$  is not known exactly for any lattice except the 2D honeycomb lattice, where

$$\kappa = \log \sqrt{2 + \sqrt{2}} \quad [\text{Duminil-Copin \& Smirnov 2012}].$$

## Adsorbing walks

$\kappa$  is not known exactly for any lattice except the 2D honeycomb lattice, where

$$\kappa = \log \sqrt{2 + \sqrt{2}} \quad [\text{Duminil-Copin \& Smirnov 2012}].$$

Similarly  $a_c$  is not known exactly for any lattice except the 2D honeycomb lattice. Depending on which way the lattice is oriented, either

$$a_c = 1 + \sqrt{2} \quad [\text{NRB, Bousquet-Mélou, de Gier, Duminil-Copin \& Guttmann 2014}]$$

or

$$a_c = \sqrt{\frac{2 + \sqrt{2}}{1 + \sqrt{2} - \sqrt{2 + \sqrt{2}}}} \quad [\text{NRB 2014}].$$

## Pulled walks

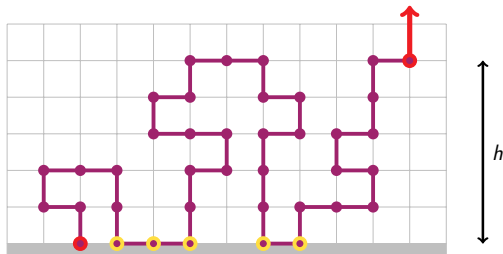
Can do something similar for pulled walks.





## Pulled walks

Can do something similar for pulled walks. Again take a polymer pinned to a surface at one end. To represent a force acting on the other end, in a direction perpendicular to the surface, let  $c_n(v, h)$  be the number of half-space walks with  $v$  visits and endpoint height  $h$ .



So this walk is counted by  $c_{38}(5, 5)$ .

Now the two-variable partition function is

$$C_n(a, y) = \sum_{v, h} c_n(v, h) a^v y^h$$

where  $y = e^{f/kT}$ , and  $f$  is the force.

## Pulled walks

When  $a = 1$ , there are no interactions with the surface.

## Pulled walks

When  $a = 1$ , there are no interactions with the surface.

### Theorem (Janse van Rensburg et al 2009)

*The limit*

$$\lambda(y) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1, y)$$

*exists for all  $a \geq 0$ . It is a non-decreasing log-convex function, and is thus continuous and almost-everywhere differentiable.*

## Pulled walks

When  $a = 1$ , there are no interactions with the surface.

### Theorem (Janse van Rensburg et al 2009)

*The limit*

$$\lambda(y) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1, y)$$

*exists for all  $a \geq 0$ . It is a non-decreasing log-convex function, and is thus continuous and almost-everywhere differentiable.*

There is again a critical value  $1 \leq y_c \leq e^{\kappa}$  where  $\lambda(y)$  switches from constant  $\kappa$  to an increasing function of  $y$ . This time, however,

### Theorem (NRB 2015)

*The critical value*

$$y_c = 1$$

*for all lattices in all dimensions  $\geq 2$ .*

## Pulled walks

When  $a = 1$ , there are no interactions with the surface.

### Theorem (Janse van Rensburg et al 2009)

*The limit*

$$\lambda(y) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1, y)$$

*exists for all  $a \geq 0$ . It is a non-decreasing log-convex function, and is thus continuous and almost-everywhere differentiable.*

There is again a critical value  $1 \leq y_c \leq e^{\kappa}$  where  $\lambda(y)$  switches from constant  $\kappa$  to an increasing function of  $y$ . This time, however,

### Theorem (NRB 2015)

*The critical value*

$$y_c = 1$$

*for all lattices in all dimensions  $\geq 2$ .*

When  $y \leq 1$ , walks sampled from the Boltzmann distribution are **free**, and exhibit the same scaling behaviour (e.g. radius of gyration) as walks in the bulk. When  $y > 1$ , walks become **ballistic**, and move away from the surface at positive speed (i.e. height is  $O(n)$ ).

## Pulled walks

When  $a = 1$ , there are no interactions with the surface.

### Theorem (Janse van Rensburg et al 2009)

*The limit*

$$\lambda(y) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(1, y)$$

*exists for all  $a \geq 0$ . It is a non-decreasing log-convex function, and is thus continuous and almost-everywhere differentiable.*

There is again a critical value  $1 \leq y_c \leq e^{\kappa}$  where  $\lambda(y)$  switches from constant  $\kappa$  to an increasing function of  $y$ . This time, however,

### Theorem (NRB 2015)

*The critical value*

$$y_c = 1$$

*for all lattices in all dimensions  $\geq 2$ .*

When  $y \leq 1$ , walks sampled from the Boltzmann distribution are **free**, and exhibit the same scaling behaviour (e.g. radius of gyration) as walks in the bulk. When  $y > 1$ , walks become **ballistic**, and move away from the surface at positive speed (i.e. height is  $O(n)$ ).

Similar results when pulling at an angle to the surface.

## Adsorbing & pulled walks

The richer model is for **general  $a$  and  $y$** , so that walks can be **desorbed** by **pulling** hard enough from the surface.



## Adsorbing & pulled walks

The richer model is for **general  $a$  and  $y$** , so that walks can be **desorbed** by **pulling** hard enough from the surface.

### Theorem (Janse van Rensburg & Whittington 2013)

*The two-variable free energy*

$$\psi(a, y) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(a, y)$$

*exists for all  $a, y \geq 0$  and is equal to  $\max\{\kappa(a), \lambda(y)\}$ . It is a log-convex function, and is thus continuous and almost-everywhere differentiable.*

## Adsorbing & pulled walks

The richer model is for **general  $a$  and  $y$** , so that walks can be **desorbed** by **pulling** hard enough from the surface.

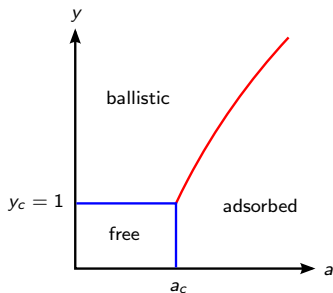
### Theorem (Janse van Rensburg & Whittington 2013)

The two-variable free energy

$$\psi(a, y) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(a, y)$$

exists for all  $a, y \geq 0$  and is equal to  $\max\{\kappa(a), \lambda(y)\}$ . It is a log-convex function, and is thus continuous and almost-everywhere differentiable.

This leads to the **phase diagram**



## Adsorbing & pulled walks

The richer model is for **general  $a$  and  $y$** , so that walks can be **desorbed** by **pulling** hard enough from the surface.

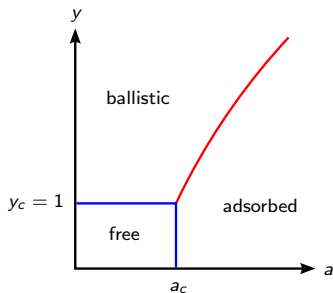
### Theorem (Janse van Rensburg & Whittington 2013)

The two-variable free energy

$$\psi(a, y) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(a, y)$$

exists for all  $a, y \geq 0$  and is equal to  $\max\{\kappa(a), \lambda(y)\}$ . It is a log-convex function, and is thus continuous and almost-everywhere differentiable.

This leads to the **phase diagram**



Adsorbed-ballistic phase boundary is curve defined by  $\kappa(a) = \lambda(y)$ .

## Adsorbing & pulled walks

The richer model is for **general  $a$  and  $y$** , so that walks can be **desorbed** by **pulling** hard enough from the surface.

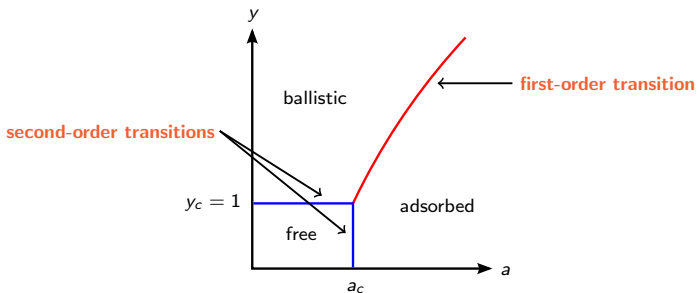
### Theorem (Janse van Rensburg & Whittington 2013)

The two-variable free energy

$$\psi(a, y) = \lim_{n \rightarrow \infty} \frac{1}{n} \log C_n(a, y)$$

exists for all  $a, y \geq 0$  and is equal to  $\max\{\kappa(a), \lambda(y)\}$ . It is a log-convex function, and is thus continuous and almost-everywhere differentiable.

This leads to the **phase diagram**



Adsorbed-ballistic phase boundary is curve defined by  $\kappa(a) = \lambda(y)$ .

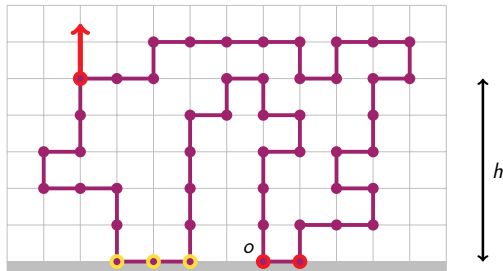
## Adsorbing & pulled polygons

Self-avoiding polygons are a model of **ring polymers**. Can do all the same physics with polygons, but not so obvious how to attach to the surface or apply force.

## Adsorbing & pulled polygons

Self-avoiding polygons are a model of **ring polymers**. Can do all the same physics with polygons, but not so obvious how to attach to the surface or apply force.

For simplicity we will fix one vertex  $o$  in the surface and apply the force at the **opposite vertex**.

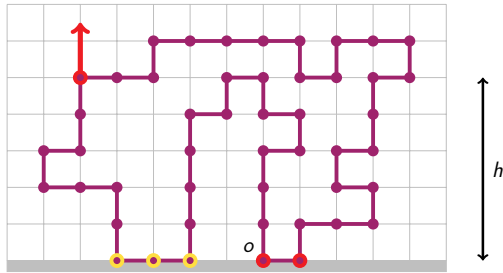


Let  $p_{2n}(v, h)$  be the number of half-space polygons of length  $2n$  with one marked vertex  $o$  in the surface,  $v + 2$  total vertices in the surface, and the vertex opposite  $o$  of height  $h$ . e.g. The above polygon is counted by  $p_{48}(4, 5)$ .

## Adsorbing & pulled polygons

Self-avoiding polygons are a model of **ring polymers**. Can do all the same physics with polygons, but not so obvious how to attach to the surface or apply force.

For simplicity we will fix one vertex  $o$  in the surface and apply the force at the **opposite vertex**.



Let  $p_{2n}(v, h)$  be the number of half-space polygons of length  $2n$  with one marked vertex  $o$  in the surface,  $v + 2$  total vertices in the surface, and the vertex opposite  $o$  of height  $h$ . e.g. The above polygon is counted by  $p_{48}(4, 5)$ .

The partition function is

$$P_{2n}(a, y) = \sum_{v, h} p_{2n}(v, h) a^v y^h.$$

## Adsorbing & pulled polygons

Things now depend on the **dimension**: in 2D, **at most half** of the vertices can be in the surface, but in  $\geq 3$  dimensions **all of the vertices** can be in the surface. In all dimensions the height is **at most half** of the length.



## Adsorbing & pulled polygons

Things now depend on the **dimension**: in 2D, **at most half** of the vertices can be in the surface, but in  $\geq 3$  dimensions **all of the vertices** can be in the surface. In all dimensions the height is **at most half** of the length.

### Theorem (Soteros 1992)

*The limiting free energy*

$$\kappa^P(a) = \lim_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, 1)$$

*exists for all  $a \geq 0$ . It is a non-decreasing and log-convex function of  $a$ , and is thus continuous and almost-everywhere differentiable. In  $\geq 3$  dimensions,  $\kappa^P(a) = \kappa(a)$ . In 2 dimensions,  $\kappa^P(a) \leq \kappa(a)$ .*

As with walks there is an **adsorption phase transition** at  $a = a_c^P$ . In  $\geq 3$  dimensions,  $a_c^P = a_c$ , while in 2 dimensions  $a_c^P \geq a_c$ . (Unknown if they are really the same.)

## Adsorbing & pulled polygons

Things now depend on the **dimension**: in 2D, **at most half** of the vertices can be in the surface, but in  $\geq 3$  dimensions **all of the vertices** can be in the surface. In all dimensions the height is **at most half** of the length.

### Theorem (Soteros 1992)

*The limiting free energy*

$$\kappa^P(a) = \lim_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, 1)$$

*exists for all  $a \geq 0$ . It is a non-decreasing and log-convex function of  $a$ , and is thus continuous and almost-everywhere differentiable. In  $\geq 3$  dimensions,  $\kappa^P(a) = \kappa(a)$ . In 2 dimensions,  $\kappa^P(a) \leq \kappa(a)$ .*

As with walks there is an **adsorption phase transition** at  $a = a_c^P$ . In  $\geq 3$  dimensions,  $a_c^P = a_c$ , while in 2 dimensions  $a_c^P \geq a_c$ . (Unknown if they are really the same.)

### Theorem (Guttmann, Janse van Rensburg, Jensen & Whittington 2017)

*The limiting free energy*

$$\lambda^P(y) = \lim_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(1, y)$$

*exists for all  $y > 0$ . In all dimensions,  $\lambda^P(y) = \lambda(\sqrt{y})$ .*

So polygons also become **ballistic** at  $y = y_c^P = y_c = 1$ .

## Adsorbing & pulled polygons

In  $\geq 3$  dimensions polygons work the same way as walks:

**Theorem (Guttmann, Janse van Rensburg, Jensen & Whittington 2017)**

*In  $\geq 3$  dimensions, the limiting free energy*

$$\psi^P(a, y) = \lim_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y)$$

*exists for all  $a \geq 0$  and  $y > 0$ . Moreover, it is equal to  $\max\{\kappa^P(a), \lambda^P(y)\}$ .*

Corresponding phase diagram.

## Adsorbing & pulled polygons

In  $\geq 3$  dimensions polygons work the same way as walks:

**Theorem (Guttmann, Janse van Rensburg, Jensen & Whittington 2017)**

*In  $\geq 3$  dimensions, the limiting free energy*

$$\psi^P(a, y) = \lim_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y)$$

*exists for all  $a \geq 0$  and  $y > 0$ . Moreover, it is equal to  $\max\{\kappa^P(a), \lambda^P(y)\}$ .*

Corresponding phase diagram.

In 2 dimensions, much less is known.

**Theorem (Guttmann, Janse van Rensburg, Jensen & Whittington 2017)**

*In 2 dimensions, when  $0 \leq a \leq 1$  or  $0 < y \leq 1$ , the limiting free energy*

$$\psi^P(a, y) = \lim_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y)$$

*exists, and is equal to  $\kappa^P(a)$  or  $\lambda^P(y)$  respectively.*

## Adsorbing & pulled polygons

For  $a, y > 1$ , there are only bounds:

$$\liminf_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y) \geq \max\{\kappa^P(a), \lambda^P(y)\}$$

and

$$\limsup_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y) \leq \max\{\kappa(a), \lambda^P(y)\}.$$

## Adsorbing & pulled polygons

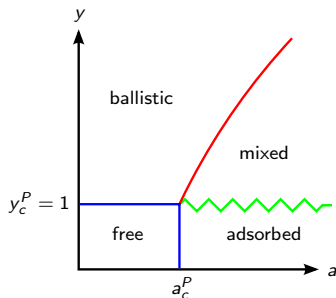
For  $a, y > 1$ , there are only bounds:

$$\liminf_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y) \geq \max\{\kappa^P(a), \lambda^P(y)\}$$

and

$$\limsup_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y) \leq \max\{\kappa(a), \lambda^P(y)\}.$$

**Numerical evidence** (series analysis) suggests that the phase diagram is more complicated, with possibly (at least) **4 phases**:



## Adsorbing & pulled polygons

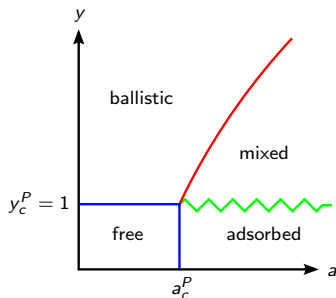
For  $a, y > 1$ , there are only bounds:

$$\liminf_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y) \geq \max\{\kappa^P(a), \lambda^P(y)\}$$

and

$$\limsup_{n \rightarrow \infty} \frac{1}{2n} \log P_{2n}(a, y) \leq \max\{\kappa(a), \lambda^P(y)\}.$$

**Numerical evidence** (series analysis) suggests that the phase diagram is more complicated, with possibly (at least) **4 phases**:



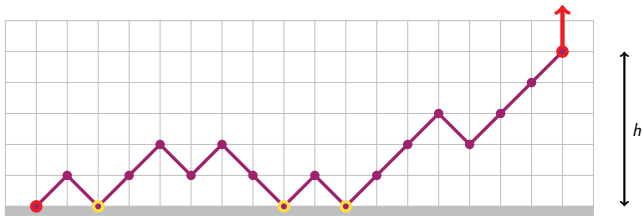
But the series are not very long so this is only speculation...





## Solvable models

**Solvable models** often exhibit similar physics as the more general cases, but allow for exactly analysis. The simplest solvable models use **directed paths**:



Let  $d_n(v, h)$  be the number of directed paths starting at  $(0, 0)$  and ending at  $(n, h)$ , staying in the upper half-plane and with  $v + 1$  vertices in the surface.

Define the **partition function**

$$D_n(a, y) = \sum_{v, h} d_n(v, h) a^v y^h$$

and **generating function**

$$D(t; a, y) = \sum_{n \geq 0} D_n(a, y) t^n.$$

## Adsorbing & pulled directed paths

Then  $D(t; a, y)$  satisfies a simple **functional equation**:

$$D(t; a, y) = 1 + t(y + \bar{y})D(t; a, y) + t(a - 1)[y^1]D(t; a, y) - t\bar{y}D(t; a, 0)$$

where  $\bar{y} = y^{-1}$ .

## Adsorbing & pulled directed paths

Then  $D(t; a, y)$  satisfies a simple **functional equation**:

$$D(t; a, y) = 1 + t(y + \bar{y})D(t; a, y) + t(a - 1)[y^1]D(t; a, y) - t\bar{y}D(t; a, 0)$$

where  $\bar{y} = y^{-1}$ . This can be solved with the **kernel method**, giving

$$D(t; a, y) = \frac{2(1 - 2t^2 + \sqrt{1 - 4t^2})}{(1 - 2t^2a + \sqrt{1 - 4t^2})(1 - 2ty + \sqrt{1 - 4t^2})}.$$

## Adsorbing & pulled directed paths

Then  $D(t; a, y)$  satisfies a simple **functional equation**:

$$D(t; a, y) = 1 + t(y + \bar{y})D(t; a, y) + t(a - 1)[y^1]D(t; a, y) - t\bar{y}D(t; a, 0)$$

where  $\bar{y} = y^{-1}$ . This can be solved with the **kernel method**, giving

$$D(t; a, y) = \frac{2(1 - 2t^2 + \sqrt{1 - 4t^2})}{(1 - 2t^2a + \sqrt{1 - 4t^2})(1 - 2ty + \sqrt{1 - 4t^2})}.$$

The **dominant singularity** (i.e. the one closest to the origin) of  $D(t; a, y)$  (viewed as a function of  $t$ ) determines the asymptotic behaviour of  $D_n(a, y)$ , which in turn determines the free energy.

When  $y = 1$ ,

$$\kappa^D(a) = \begin{cases} \log 2 & \text{if } a \leq 2 \\ \log a - \frac{1}{2} \log(a - 1) & \text{if } a > 2, \end{cases}$$

while if  $a = 1$  then

$$\lambda^D(y) = \begin{cases} \log 2 & \text{if } y \leq 1 \\ \log(y^2 + 1) - \log y & \text{if } y > 1. \end{cases}$$

## Absorbing & pulled directed paths

Then  $D(t; a, y)$  satisfies a simple **functional equation**:

$$D(t; a, y) = 1 + t(y + \bar{y})D(t; a, y) + t(a - 1)[y^1]D(t; a, y) - t\bar{y}D(t; a, 0)$$

where  $\bar{y} = y^{-1}$ . This can be solved with the **kernel method**, giving

$$D(t; a, y) = \frac{2(1 - 2t^2 + \sqrt{1 - 4t^2})}{(1 - 2t^2a + \sqrt{1 - 4t^2})(1 - 2ty + \sqrt{1 - 4t^2})}.$$

The **dominant singularity** (i.e. the one closest to the origin) of  $D(t; a, y)$  (viewed as a function of  $t$ ) determines the asymptotic behaviour of  $D_n(a, y)$ , which in turn determines the free energy.

When  $y = 1$ ,

$$\kappa^D(a) = \begin{cases} \log 2 & \text{if } a \leq 2 \\ \log a - \frac{1}{2} \log(a - 1) & \text{if } a > 2, \end{cases}$$

while if  $a = 1$  then

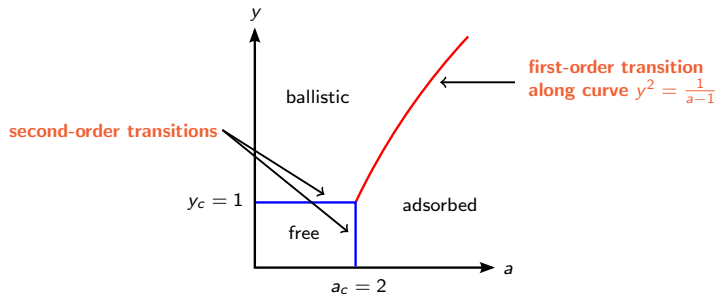
$$\lambda^D(y) = \begin{cases} \log 2 & \text{if } y \leq 1 \\ \log(y^2 + 1) - \log y & \text{if } y > 1. \end{cases}$$

Then

$$\psi^D(a, y) = \max\{\kappa^D(a), \lambda^D(y)\}.$$

## Adsorbing & pulled directed paths

The phase diagram matches that of SAWs, but here we can exactly locate the phase boundaries:



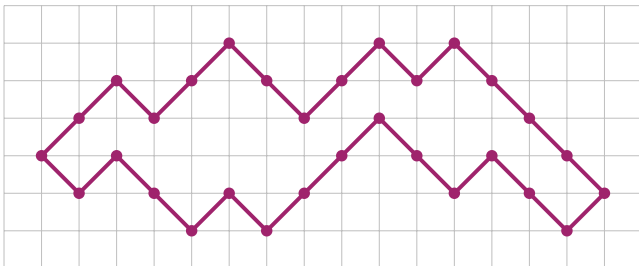
## Directed polygons

That worked well, so what about polygons?

# Directed polygons

That worked well, so what about polygons?

The simplest model is **staircase polygons**:



Two directed paths, starting and ending at the same vertices but otherwise avoiding each other.

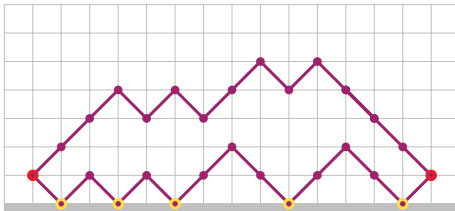


# Adsorbing & pulled staircase polygons

Focus on two cases:

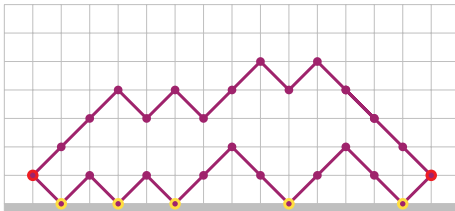
## Adsorbing & pulled staircase polygons

Focus on two cases: the **two ends** fixed at the surface (**grafted** staircase polygons)

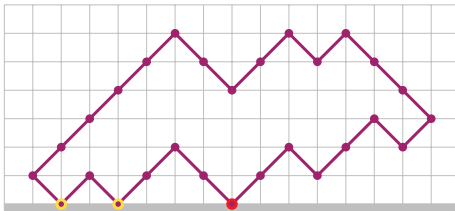


## Adsorbing & pulled staircase polygons

Focus on two cases: the **two ends** fixed at the surface (**grafted** staircase polygons)

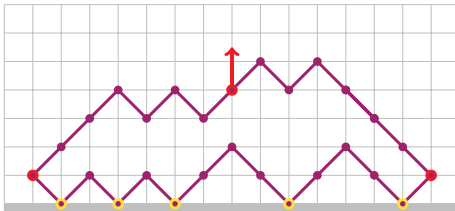


or the **middle vertex** on the bottom fixed at the surface (**centred** staircase polygons)

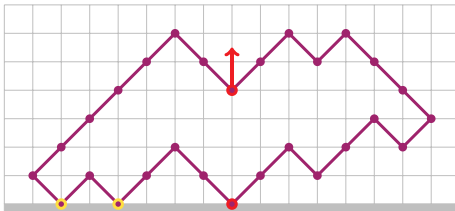


## Adsorbing & pulled staircase polygons

Focus on two cases: the **two ends** fixed at the surface (**grafted** staircase polygons)



or the **middle vertex** on the bottom fixed at the surface (**centred** staircase polygons)



In both cases, count vertices in the surface as visits and apply the force at the **middle vertex** on the top.

## Adsorbing & pulled staircase polygons

Let  $s_{4n}^G(v, h)$  (resp.  $s_{4n}^C(v, h)$ ) be the number of grafted (resp. centred) staircase polygons of total length  $4n$ , with  $v$  vertices in the surface and middle vertex of height  $h$ .

Define **partition functions** in the usual way:

$$S_{4n}^G(a, y) \quad \& \quad S_{4n}^C(a, y).$$

(Everything can be adapted to total length  $4n + 2$  as well.)

## Adsorbing & pulled staircase polygons

Let  $s_{4n}^G(v, h)$  (resp.  $s_{4n}^C(v, h)$ ) be the number of grafted (resp. centred) staircase polygons of total length  $4n$ , with  $v$  vertices in the surface and middle vertex of height  $h$ .

Define **partition functions** in the usual way:

$$S_{4n}^G(a, y) \quad \& \quad S_{4n}^C(a, y).$$

(Everything can be adapted to total length  $4n + 2$  as well.)

Can once again write down **functional equations** for the **generating functions**, but this time they are too complicated to solve explicitly.

## Adsorbing & pulled staircase polygons

Let  $s_{4n}^G(v, h)$  (resp.  $s_{4n}^C(v, h)$ ) be the number of grafted (resp. centred) staircase polygons of total length  $4n$ , with  $v$  vertices in the surface and middle vertex of height  $h$ .

Define **partition functions** in the usual way:

$$S_{4n}^G(a, y) \quad \& \quad S_{4n}^C(a, y).$$

(Everything can be adapted to total length  $4n + 2$  as well.)

Can once again write down **functional equations** for the **generating functions**, but this time they are too complicated to solve explicitly.

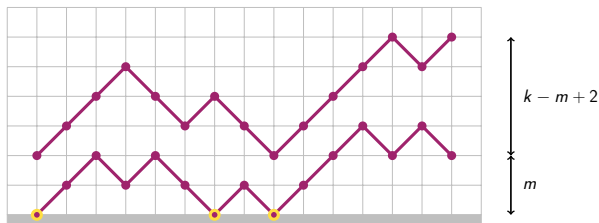
Fortunately, we have another way: can count **pairs of nonintersecting paths** directly.



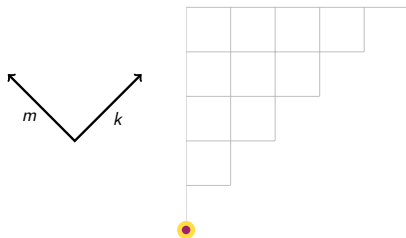


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

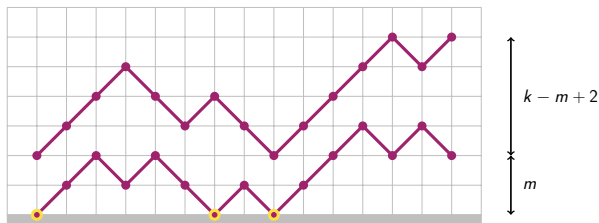


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

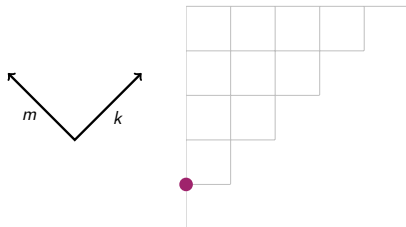


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

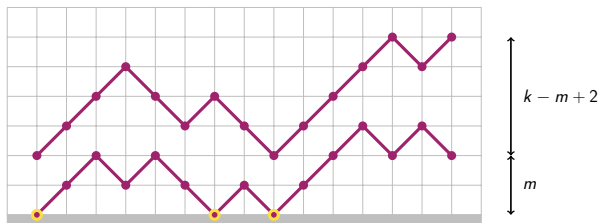


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

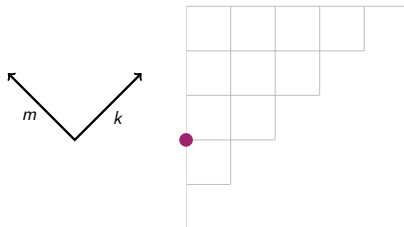


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

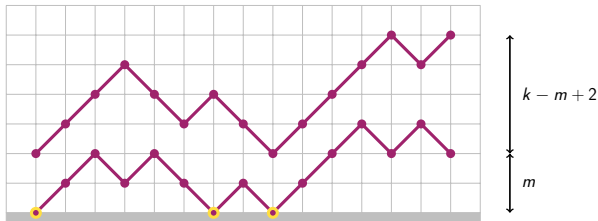


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

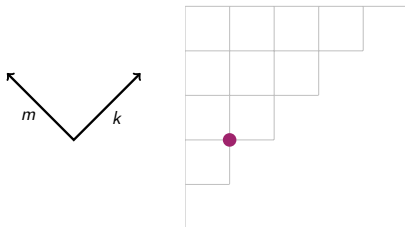


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

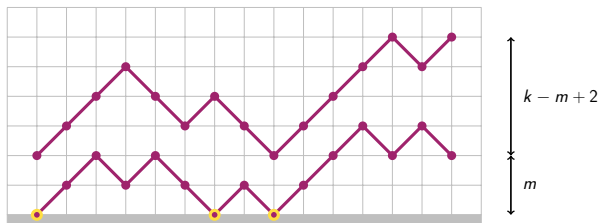


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

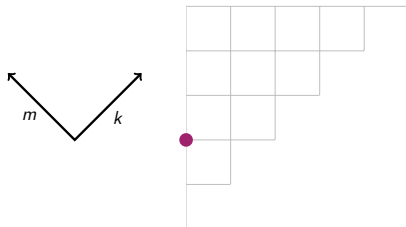


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

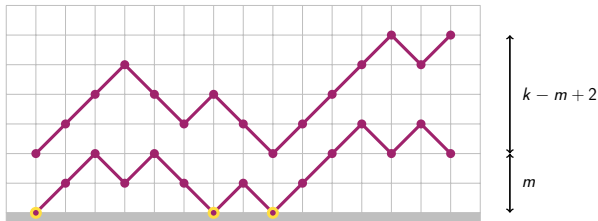


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

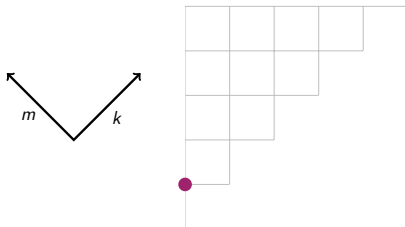


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

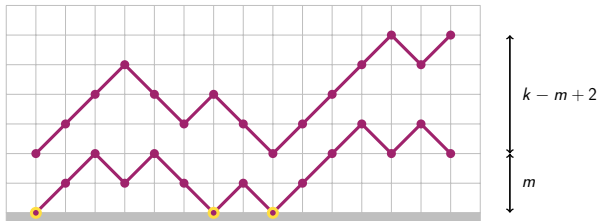


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

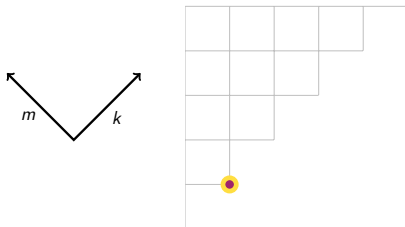


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

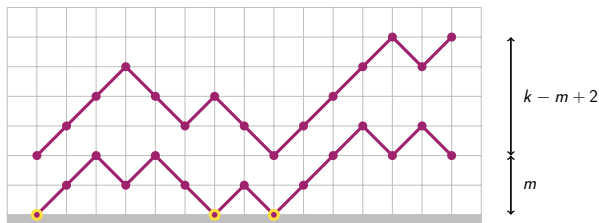


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

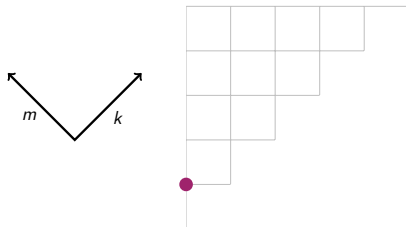


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights on the surface:



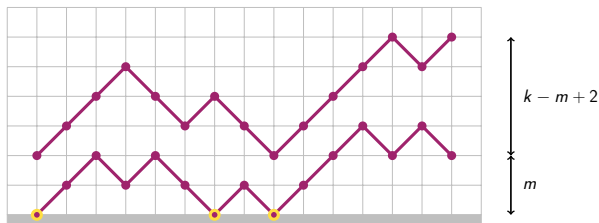
These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :



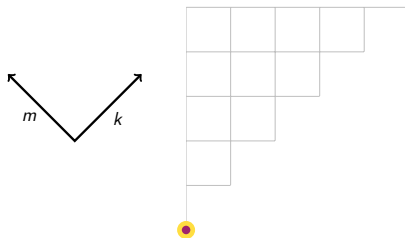


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

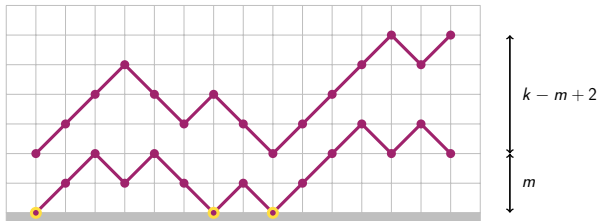


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

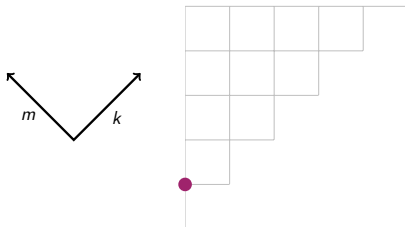


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

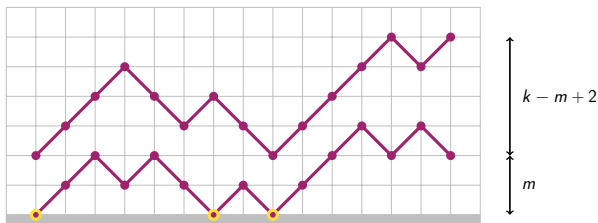


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

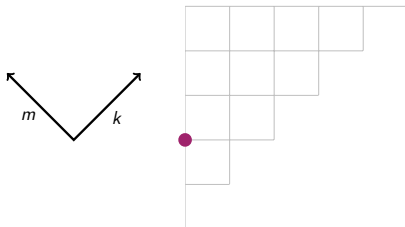


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

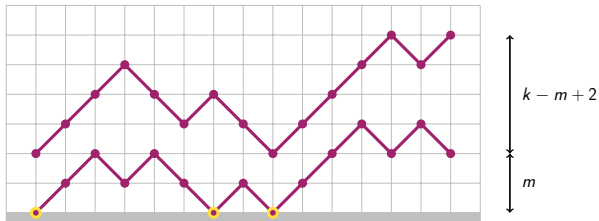


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

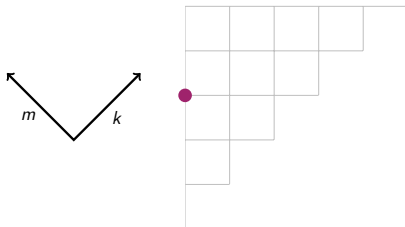


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights on the surface:

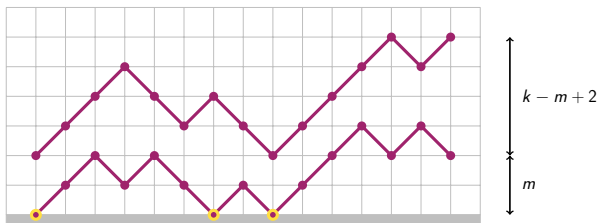


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

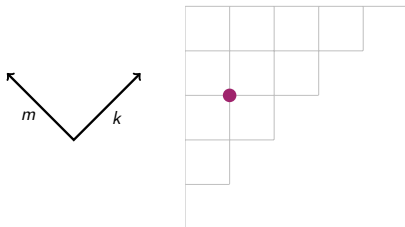


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:

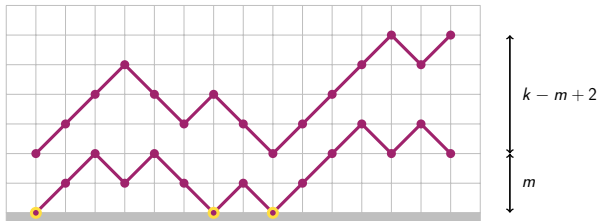


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

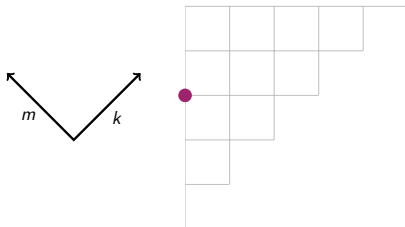


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights on the surface:

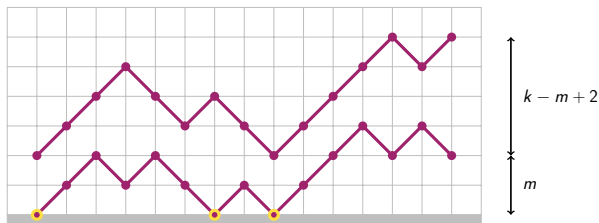


These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :

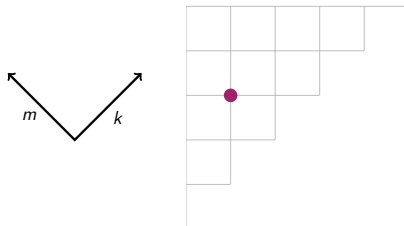


## Grafted polygons via pairs of paths

Let  $r_{n,k,m}(a)$  be the total weight of all non-intersecting pairs of paths which start at  $(0,0)$  (resp.  $(0,2)$ ) and end at  $(n,m)$  (resp.  $(n,k+2)$ ), with the bottom path accumulating a weights  $a$  on the surface:



These are in bijection a single path in an **octant of  $\mathbb{Z}^2$** :



## Grafted polygons via pairs of paths

The  $r_{n,k,m}(a)$  satisfy a recurrence, which can be solved with a **Bethe ansatz**. When  $a = 1$ ,

$$r_{n,k,m}(1) = \frac{(k+3)(m+1)(k-m+2)(k+m+4)}{4(n+1)(n+2)(n+3)^2} \binom{n+3}{\frac{1}{2}(n+k+6)} \binom{n+3}{\frac{1}{2}(n+m+4)}.$$



## Grafted polygons via pairs of paths

The  $r_{n,k,m}(a)$  satisfy a recurrence, which can be solved with a **Bethe ansatz**. When  $a = 1$ ,

$$r_{n,k,m}(1) = \frac{(k+3)(m+1)(k-m+2)(k+m+4)}{4(n+1)(n+2)(n+3)^2} \binom{n+3}{\frac{1}{2}(n+k+6)} \binom{n+3}{\frac{1}{2}(n+m+4)}.$$

Then for general  $a$ ,

$$r_{n,k,m}(a) = a \sum_{w=0}^n (a-1)^w \sum_{p=0}^w s_{n,k+2p,m+2w-2p}(1).$$

## Grafted polygons via pairs of paths

Grafted polygons can then be formed by gluing together two pairs of paths with the same  $m$  and  $k$ , multiplying by  $y^{k+2}$ , and summing over  $m, k$ :

$$S_{4n}^G(a, y) = \frac{1}{a} \sum_{k=0}^{n-1} r_{n-1, k, 0}(1)^2 y^{k+2} + \sum_{k=0}^{n-1} \sum_{m=1}^k r_{n-1, k, m}(a)^2 y^{k+2}.$$

## Grafted polygons via pairs of paths

Grafted polygons can then be formed by gluing together two pairs of paths with the same  $m$  and  $k$ , multiplying by  $y^{k+2}$ , and summing over  $m, k$ :

$$S_{4n}^G(a, y) = \frac{1}{a} \sum_{k=0}^{n-1} r_{n-1,k,0}(1)^2 y^{k+2} + \sum_{k=0}^{n-1} \sum_{m=1}^k r_{n-1,k,m}(a)^2 y^{k+2}.$$

The asymptotics can be computed by using Stirling's approximation and replacing the sums with integrals. The free energy turns out to be

$$\psi^G(a, y) = \frac{1}{2} \kappa^D(a) + \frac{1}{2} \lambda^D(\sqrt{y}).$$

## Grafted polygons via pairs of paths

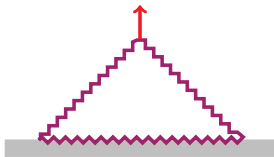
Grafted polygons can then be formed by gluing together two pairs of paths with the same  $m$  and  $k$ , multiplying by  $y^{k+2}$ , and summing over  $m, k$ :

$$S_{4n}^G(a, y) = \frac{1}{a} \sum_{k=0}^{n-1} r_{n-1,k,0}(1)^2 y^{k+2} + \sum_{k=0}^{n-1} \sum_{m=1}^k r_{n-1,k,m}(a)^2 y^{k+2}.$$

The asymptotics can be computed by using Stirling's approximation and replacing the sums with integrals. The free energy turns out to be

$$\psi^G(a, y) = \frac{1}{2} \kappa^D(a) + \frac{1}{2} \lambda^D(\sqrt{y}).$$

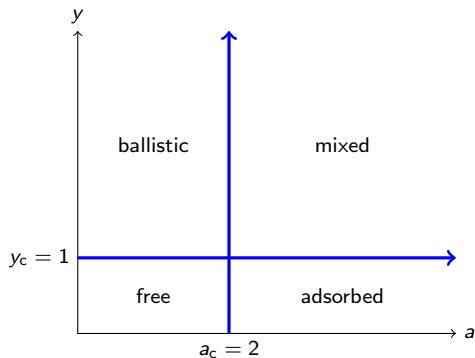
i.e. The bottom path acts as an adsorbing directed path, and the top path acts like a pulled directed path with half the force:



Impossible to desorb by pulling.

## Grafted polygons via pairs of paths

The phase diagram is simple:



All phase transitions are second-order.

## Centred polygons via pairs of paths

A similar approach can be used for centred staircase polygons.

## Centred polygons via pairs of paths

A similar approach can be used for centred staircase polygons.

This time

$$\psi^C(a, y) = \frac{1}{2}\lambda^D(\sqrt{y}) + \frac{1}{2}\max\{\lambda^D(\sqrt{y}), \kappa^D(a)\}.$$

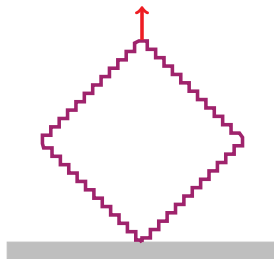
## Centred polygons via pairs of paths

A similar approach can be used for centred staircase polygons.

This time

$$\psi^C(a, y) = \frac{1}{2} \lambda^D(\sqrt{y}) + \frac{1}{2} \max\{\lambda^D(\sqrt{y}), \kappa^D(a)\}.$$

Now pulling hard enough does induce desorption:





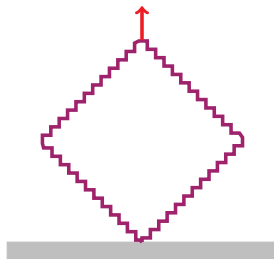
## Centred polygons via pairs of paths

A similar approach can be used for centred staircase polygons.

This time

$$\psi^C(a, y) = \frac{1}{2} \lambda^D(\sqrt{y}) + \frac{1}{2} \max\{\lambda^D(\sqrt{y}), \kappa^D(a)\}.$$

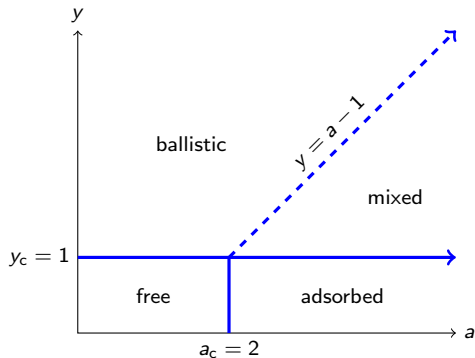
Now pulling hard enough does induce desorption:



But the converse (adsorb strongly enough to overcome force) is still impossible.

## Centred polygons via pairs of paths

The phase diagram now resembles what the numerics suggest for SAPs:



Ballistic-mixed transition is first-order, all others are second-order.

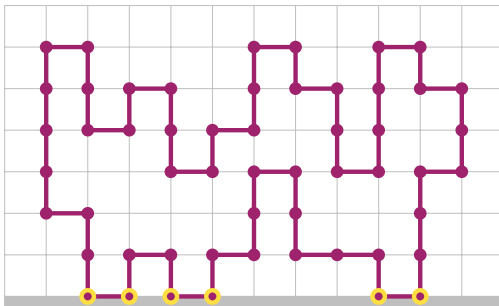
## Generalisations

A more general model for staircase polygons requires only that there is **at least one vertex** in the surface somewhere. In that case the free energy turns out to be the **same as centred polygons**.

## Generalisations

A more general model for staircase polygons requires only that there is **at least one vertex** in the surface somewhere. In that case the free energy turns out to be the **same as centred polygons**.

A model which more closely resembles that of SAPs might be **column-convex polygons**:

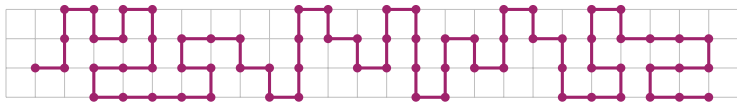


But this may not be amenable to generating-function or Bethe ansatz methods.



## Restricting the lattice instead

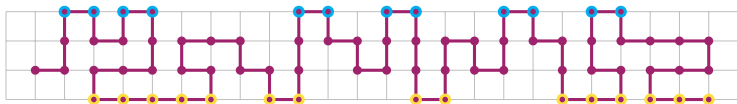
Can instead induce directedness by restricting the walks/polygons to a **narrow strip** (2D) or **tube** (3D):



The physics here is quite different though – there are **no phase transitions** in such geometry.

## Restricting the lattice instead

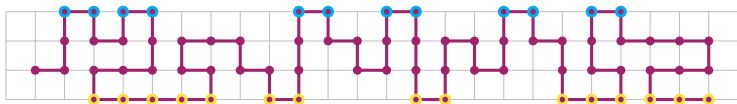
Can instead induce directedness by restricting the walks/polygons to a **narrow strip** (2D) or **tube** (3D):



The physics here is quite different though – there are **no phase transitions** in such geometry. But we can do other things, e.g. measure the **force** that the walk/polygon exerts on the boundaries of the strip, and how this changes if we add adsorption weights to the top and bottom.

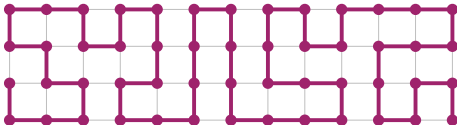
## Restricting the lattice instead

Can instead induce directedness by restricting the walks/polygons to a **narrow strip** (2D) or **tube** (3D):



The physics here is quite different though – there are **no phase transitions** in such geometry. But we can do other things, e.g. measure the **force** that the walk/polygon exerts on the boundaries of the strip, and how this changes if we add adsorption weights to the top and bottom.

Can also apply forces in the horizontal direction, causing the walks/polygons to become **space-filling** (Hamiltonian):





## References

NRB, *Adsorbing staircase polygons subject to a force*, arXiv:1706.07653, submitted.

NRB, J. W. Eng & C. E. Soteris, *Polygons in restricted geometries subjected to infinite forces*, J. Phys. A: Math. Theor. **49** (2016), 424002.

## References

NRB, *Adsorbing staircase polygons subject to a force*, arXiv:1706.07653, submitted.

NRB, J. W. Eng & C. E. Soteris, *Polygons in restricted geometries subjected to infinite forces*, J. Phys. A: Math. Theor. **49** (2016), 424002.

Thank you!