# The expected number of inversions after *n* adjacent transpositions

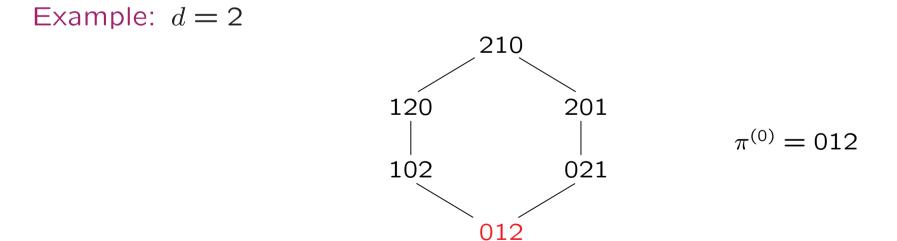
Mireille Bousquet-Mélou CNRS, LaBRI, Bordeaux, France

ArXiv 0909:0103

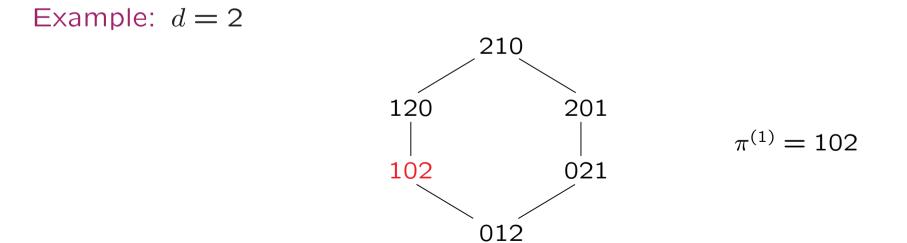
Aurora Borealis Combinatorics



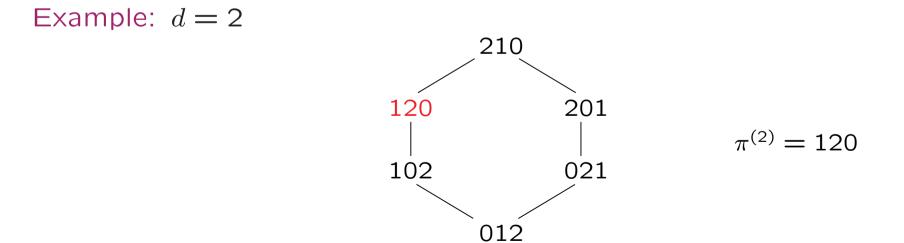
- Consider the symmetric group  $\mathfrak{S}_{d+1}$  on the elements  $\{0, 1, \ldots, d\}$ .
- Start from the identity permutation  $\pi^{(0)} = 012 \cdots d$ .
- Apply an adjacent transposition, taken uniformly at random (probability 1/d for each).
- Repeat.



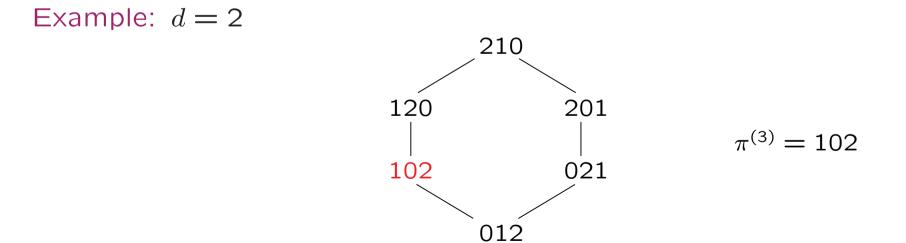
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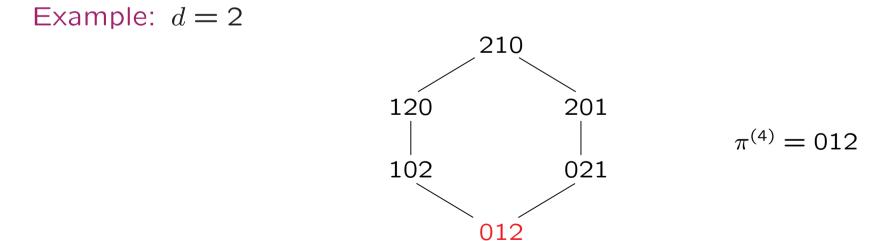
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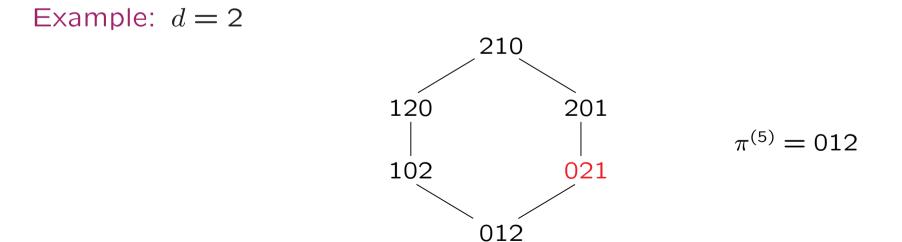
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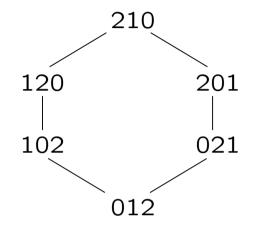


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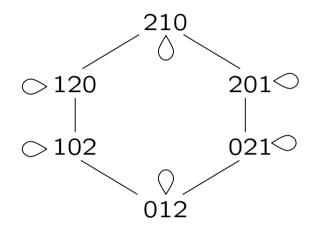
## Periodicity

This chain,  $\pi^{(0)}, \pi^{(1)}, \pi^{(2)}, \ldots$  is periodic of period 2: it takes an even number of steps to return to a point.



# **Aperiodic variants**

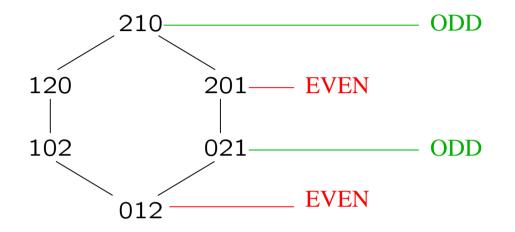
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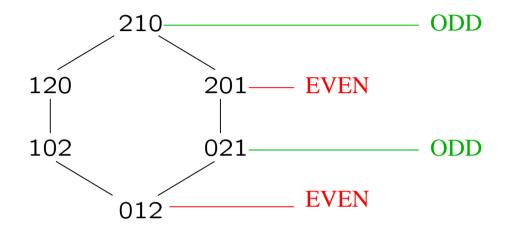
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- Or: consider the chains  $\left(\pi^{(2n)}\right)_n$  and  $\left(\pi^{(2n+1)}\right)_n$

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- Or: consider the chains  $\left(\pi^{(2n)}\right)_n$  and  $\left(\pi^{(2n+1)}\right)_n$

These three chains are aperiodic, irreducible and symmetric, and thus converge to the uniform distribution on their respective state spaces.

# **Motivations**

• 1980  $\rightarrow$  2010: Random walks in finite groups (Aldous, Diaconis, Letac, Saloff-Coste, Wilson...)

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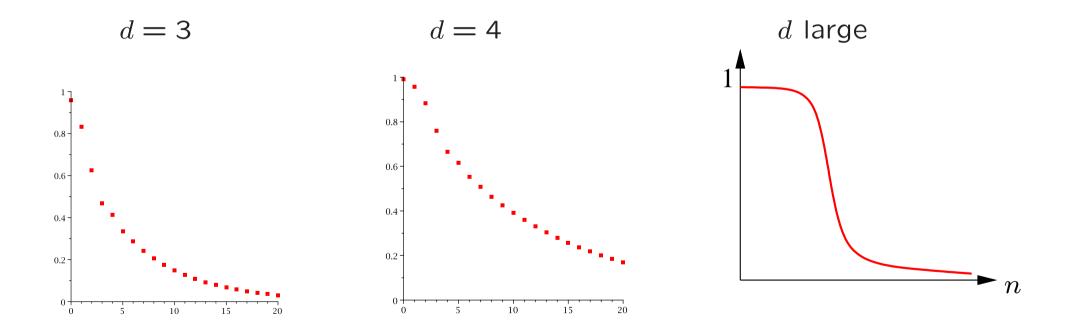
Tools: coupling techniques, representation theory...

• More recently: Computational biology (N. Beresticky, Durrett, Eriksen, Hultman, H. Eriksson, K. Eriksson, Sjöstrand...)

A transposition: a gene mutation

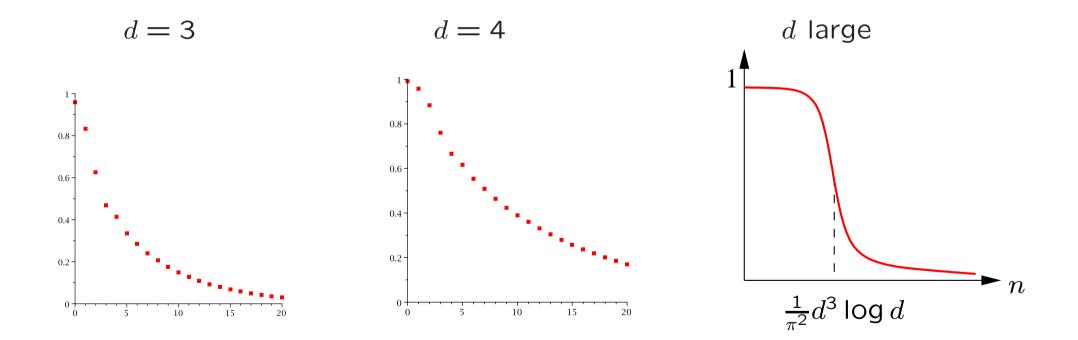
• Mixing time: How much time does it take to "reach" the uniform distribution?

The total variation distance between the distribution at time n and the uniform distribution on  $\mathfrak{S}_{d+1}$ :



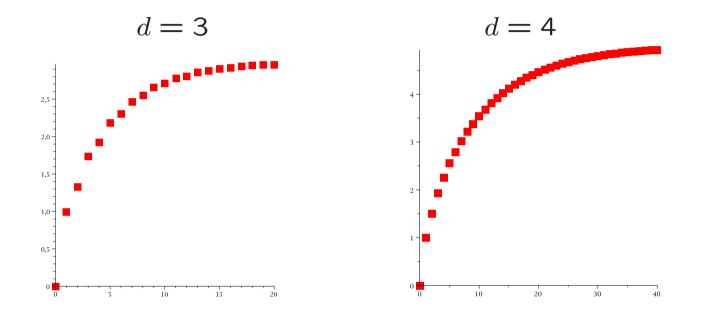
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[Aldous 83, Diaconis & Saloff-Coste 93, Wilson 04]

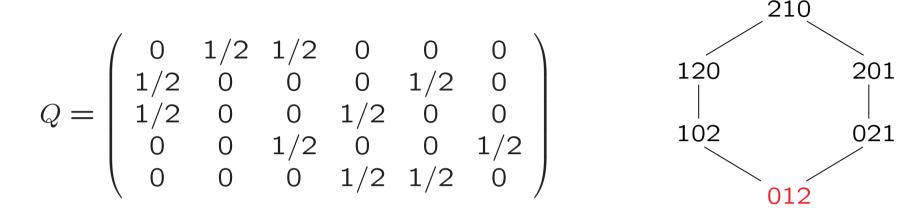
• Focus on observables, for instance the inversion number  $\mathcal{I}_{d,n} = inv(\pi^{(n)})$ . The expected value of the inversion number,  $I_{d,n} := \mathbb{E}(\mathcal{I}_{d,n})$ :



 $\implies$  Estimate the number of transpositions (mutations) that have occurred, and hence the evolutionary distance between species.

Of particular interest: what happens before mixing.

Let  $Q = (Q_{\sigma,\tau})$  be the transition matrix of the chain:



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$$Q = \begin{pmatrix} 0 & 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 \\ 1/2 & 0 & 0 & 1/2 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 & 1/2 \\ 0 & 0 & 0 & 1/2 & 1/2 & 0 \end{pmatrix}$$

$$Q = \begin{pmatrix} 210 \\ 120 \\ 0 \\ 120 \\ 102 \\ 021 \\ 102 \\ 012 \\$$

• For all 
$$\sigma \in \mathfrak{S}_{d+1}$$
, let

$$G_{\sigma}(t) := \sum_{n \ge 0} \mathbb{P}\left(\pi^{(n)} = \sigma\right) t^n$$

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is a rational series in t.

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• The GF of the expected inversion number

$$\sum_{n\geq 0} \mathsf{I}_{d,n} t^n = \sum_{n\geq 0} \left( \sum_{\sigma\in\mathfrak{S}_{d+1}} \mathsf{inv}(\sigma) \mathbb{P}\left(\pi^{(n)} = \sigma\right) \right) t^n = \sum_{\sigma\in\mathfrak{S}_{d+1}} \mathsf{inv}(\sigma) G_{\sigma}(t)$$

is rational as well.

#### A formula for the expected inversion number

Theorem: The expected number of inversions after n adjacent transpositions in  $\mathfrak{S}_{d+1}$  is

$$\mathsf{I}_{d,n} = \frac{d(d+1)}{4} - \frac{1}{8(d+1)^2} \sum_{k,j=0}^{d} \frac{(c_j + c_k)^2}{s_j^2 s_k^2} x_{jk}^n,$$

where

$$c_k = \cos \alpha_k, \quad s_k = \sin \alpha_k, \quad \alpha_k = \frac{(2k+1)\pi}{2d+2},$$

and

$$x_{jk} = 1 - \frac{4}{d}(1 - c_j c_k).$$

#### Remarks

- The series  $\sum_{n} I_{d,n} t^{n}$  is rational.
- For d large enough  $(d \ge 8)$ ,  $I_{d,n}$  increases, as n grows, to  $\frac{d(d+1)}{4}$ , which is the average inversion number of a random permutation in  $\mathfrak{S}_{d+1}$ .

#### Another formula for the expected inversion number [Eriksen 05]

$$\mathsf{I}_{d,n} = \sum_{r=1}^{n} \frac{1}{d^r} \binom{n}{r} \sum_{s=1}^{r} \binom{r-1}{s-1} (-4)^{r-s} g_{s,d} h_{s,d},$$

with

$$g_{s,d} = \sum_{\ell=0}^{d} \sum_{k \ge 0} (-1)^k (p - 2\ell) {\binom{2\lceil s/2 \rceil - 1}{\lceil s/2 \rceil + \ell + k(d+1)}}$$

and

$$h_{s,d} = \sum_{j \in \mathbb{Z}} (-1)^j \binom{2\lfloor s/2 \rfloor}{\lfloor s/2 \rfloor + j(d+1)}.$$

Based on [Eriksson & Eriksson & Sjöstrand 00]

Beresticky & Durrett 08: "it is far from obvious how to extract useful asymptotic from this formula".

Combinatorialists could not throw in the sponge!

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## The expected inversion number: asymptotics

Three regimes, as d and n tend to  $\infty$ 

• When n is "small", each step of the chain increases the inversion number with high probability. For example,

$$\operatorname{inv}(\pi^{(1)}) = 1, \qquad \mathbb{P}\left(\operatorname{inv}(\pi^{(2)}) = 2\right) = 1 - \frac{1}{d}, \qquad \mathbb{P}\left(\operatorname{inv}(\pi^{(n)}) = n\right) = 1 - O\left(\frac{1}{d}\right)$$

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• An intermediate regime?

# Small times: linear and before

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• Linear regime. If  $n \sim \kappa d$ ,

$$\frac{\mathsf{d}_{d,n}}{n} = f(\kappa) + O(1/d)$$

where

$$f(\kappa) = \frac{1}{2\pi\kappa} \int_0^\infty \frac{1 - \exp(-8\kappa t^2/(1+t^2))}{t^2(1+t^2)} dt$$
$$= \sum_{j\geq 0} (-1)^j \frac{(2j)!}{j!(j+1)!^2} (2\kappa)^j.$$

The function  $f(\kappa)$  decreases from f(0) = 1 to  $f(\infty) = 0$ .

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• Cubic regime. If  $n \sim \kappa d^3$ ,

$$rac{\mathbf{I}_{d,n}}{d^2} \sim g(\kappa)$$

where

$$g(\kappa) = \frac{1}{4} - \frac{16}{\pi^4} \left( \sum_{j \ge 0} \frac{e^{-\kappa \pi^2 (2j+1)^2/2}}{(2j+1)^2} \right)^2.$$

The function  $g(\kappa)$  increases from g(0) = 0 to  $g(\infty) = 1/4$ .

## Around the mixing time (super-cubic regime)

Assume  $n \sim \kappa d^3 \log d$ .

• If  $\kappa < 1/\pi^2$ , there exists  $\gamma > 0$  such that

$$\mathsf{I}_{d,n} \leq \frac{d(d+1)}{4} - \Theta(d^{1+\gamma}),$$

• If  $\kappa > 1/\pi^2$ , there exists  $\gamma > 0$  such that

$$I_{d,n} = \frac{d(d+1)}{4} - O(d^{1-\gamma}).$$

• For the critical value  $\kappa = 1/\pi^2$ , the following refined estimate holds: if  $n \sim 1/\pi^2 d^3 \log d + \alpha d^3 + o(d^3)$ , then

$$\mathsf{I}_{d,n} = \frac{d(d+1)}{4} - \frac{16d}{\pi^4} e^{-\alpha \pi^2} (1 + o(1))$$

# The intermediate regime

• If  $d \ll n \ll d^3$ ,

$$\frac{\mathsf{I}_{d,n}}{\sqrt{dn}} \to \sqrt{\frac{2}{\pi}}.$$

Remark. For a related continuous time chain, the normalized inversion number  $\mathcal{I}_{d,n}/\sqrt{dn}$  converges in probability to  $\sqrt{2/\pi}$  [Beresticky & Durrett 08]

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# Where are the inversions? [Eriksson et al. 00]

For  $i \leq j$ , let  $p_{i,j}^{(n)}$  be the probability that there is an inversion at time n in the positions i and j + 1:

$$p_{i,j}^{(n)} = \mathbb{P}(\pi_i^{(n)} > \pi_{j+1}^{(n)}).$$

 $\bullet$  The expected number of inversions at time n is

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• The numbers  $p_{i,j}^{(n)}$  can be described recursively by examining where were the values  $\pi_i^{(n)}$  and  $\pi_{j+1}^{(n)}$  at time n-1. For instance:

-i = j and the *n*th transposition has switched the *i*th and i + 1st values:

$$\left(1-p_{i,j}^{(n-1)}\right)rac{1}{d}$$

 $- 0 \neq i = j \neq d$  and the *n*th transposition has not changed the values at positions *i* and *i* + 1,

$$p_{i,j}^{(n-1)}\left(1-\frac{3}{d}\right).$$

– etc.

#### A recursion for the inversion probabilities

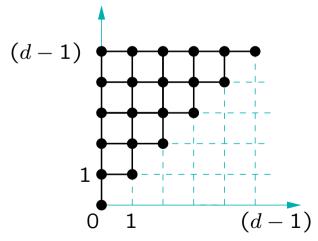
Lemma. The inversion probabilities  $p_{i,j}^{(n)}$  are characterized by:

$$p_{i,j}^{(0)} = 0 \quad \text{for} \quad 0 \le i \le j < d,$$

and for  $n \geq 0$ ,

$$p_{i,j}^{(n+1)} = p_{i,j}^{(n)} + \frac{1}{d} \sum_{(k,\ell)\leftrightarrow(i,j)} \left( p_{k,\ell}^{(n)} - p_{i,j}^{(n)} \right) + \frac{\delta_{i,j}}{d} \left( 1 - 2p_{i,j}^{(n)} \right),$$

where  $\delta_{i,j} = 1$  if i = j and 0 otherwise, and the neighbour relations  $\leftrightarrow$  are those of the following graph:



 $\rightsquigarrow$  A (weighted) walk in a triangle.

### A functional equation for the GF of the inversion probabilities

Let P(t; u, v) be the generating function of the numbers  $p_{i,j}^{(n)}$ :

$$P(t; u, v) \equiv P(u, v) := \sum_{n \ge 0} t^n \sum_{0 \le i \le j < d} p_{i,j}^{(n)} u^i v^j.$$

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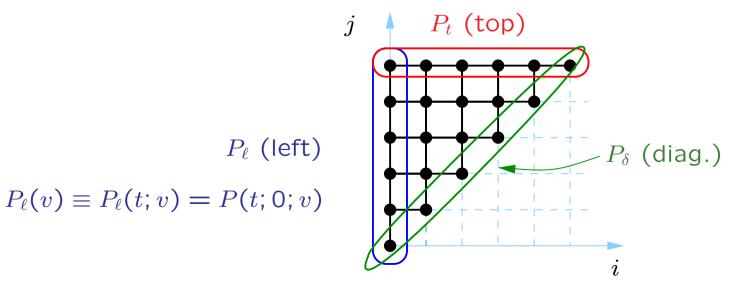
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The above recursion translates as

$$\left( 1 - t + \frac{t}{d} (4 - u - \bar{u} - v - \bar{v}) \right) P(u, v) = \frac{t}{d} \left( \frac{1 - u^d v^d}{(1 - uv)(1 - t)} - (\bar{u} - 1) P_\ell(v) - (v - 1) v^{d - 1} P_t(u) - (u + \bar{v}) P_\delta(uv) \right),$$

where  $\bar{u} = 1/u$ ,  $\bar{v} = 1/v$ , and the series  $P_{\ell}$ ,  $P_t$  and  $P_{\delta}$  describe the numbers  $p_{i,j}^{(n)}$  on the boundaries of the graph:



### Back to the inversion number

We are interested in

$$I_d(t) = \sum_{n \ge 0} I_{d,n} t^n = P(t; 1, 1),$$

which, according to the functional equation, may be rewritten

$$\mathsf{I}_{d}(t) = \frac{t}{(1-t)^{2}} - \frac{2tP_{\delta}(1)}{d(1-t)}.$$
$$\triangleleft \, \triangleleft \, \diamond \, \triangleright \, \triangleright$$

$$P(t; u, v) \equiv P(u, v) := \sum_{n \ge 0} t^n \sum_{0 \le i \le j < d} p_{i,j}^{(n)} u^i v^j.$$

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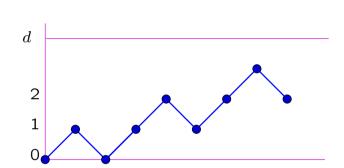
# What a beautiful equation!

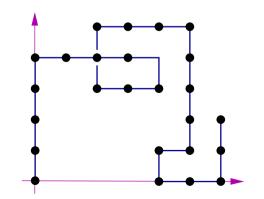
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Analogies with:

• Walks with steps  $\pm 1$  in a strip of height d:

$$(1 - t(u + \bar{u}))P(u) = 1 - t\bar{u}P_0 - tu^{d+1}P_d$$





• Walks in the quarter plane

$$(1 - t(u + \overline{u} + v + \overline{v}))P(u, v) =$$
  
$$1 - t\overline{u}P(0, v) - t\overline{v}P(u, 0)$$

• and others...

$$\begin{pmatrix} 1 - t + \frac{t}{d}(4 - u - \bar{u} - v - \bar{v}) \end{pmatrix} P(u, v) = \\ \frac{t}{d} \left( \frac{1 - u^d v^d}{(1 - uv)(1 - t)} - (\bar{u} - 1)P_\ell(v) - (v - 1)v^{d - 1}P_t(u) - (u + \bar{v})P_\delta(uv) \right)$$

• Cancel the kernel  $\left(1-t+\frac{t}{d}(4-u-\bar{u}-v-\bar{v})\right)$  by coupling u and v

$$\left( 1 - t + \frac{t}{d} (4 - u - \bar{u} - v - \bar{v}) \right) P(u, v) =$$

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- Cancel the kernel  $\left(1 t + \frac{t}{d}(4 u \bar{u} v \bar{v})\right)$  by coupling u and v
- Exploit the symmetries of this kernel, which is invariant by  $(u, v) \mapsto (\bar{u}, v)$  $(u, v) \mapsto (u, \bar{v}), (u, v) \mapsto (\bar{u}, \bar{v})$  (the reflection principle)

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One obtains an explicit expression of  $P_{\delta}(q)$  at every  $q \neq -1$  such that  $q^{d+1} = -1$ , and this is enough to reconstruct the whole polynomial  $P_{\delta}(u)$  (and in particular,  $P_{\delta}(1)$ ) by interpolation.

# The final result

The generating function  $I_d(t) = \sum_{n \ge 0} I_{d,n} t^n$  is

$$\mathsf{I}_d(t) = \frac{d(d+1)}{4(1-t)} - \frac{1}{8(d+1)^2} \sum_{k,j=0}^d \frac{(c_j + c_k)^2}{s_j^2 s_k^2} \frac{1}{1 - t x_{jk}}$$

with

$$c_k = \cos \alpha_k, \quad s_k = \sin \alpha_k, \quad \alpha_k = \frac{(2k+1)\pi}{2d+2},$$

and

$$x_{jk} = 1 - \frac{4}{d}(1 - c_j c_k).$$

## Perspectives

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• Other groups: mostly, finite irreducible Coxeter groups, with the length as the distance statistics ([Troili 02]: the case of  $I_2(d)$ ). When the generators are all reflections, see [Sjöstrand 10]!