Exact solution of two non-crossing partially directed walks with contact interaction

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AUSTRALIAN RESEARCH COUNCIL
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Motivation

We want to model

- the process of *unzipping* two strands of DNA

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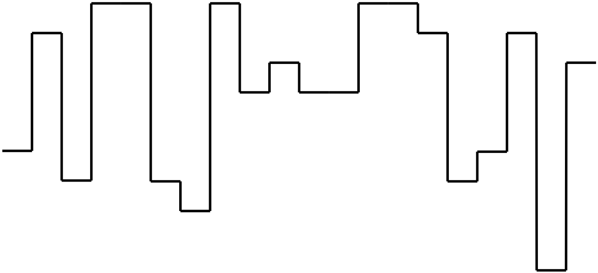
We want to model

- the process of *unzipping* two strands of DNA
- using a pair of partially directed walks

A Partially directed Walk



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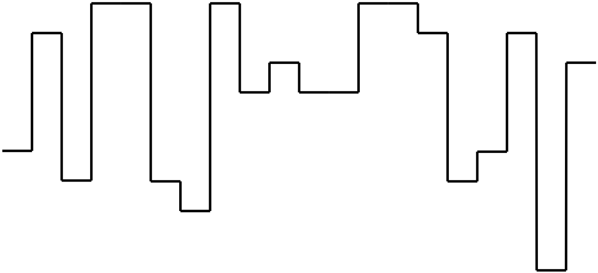

- Steps allowed: North, South, East

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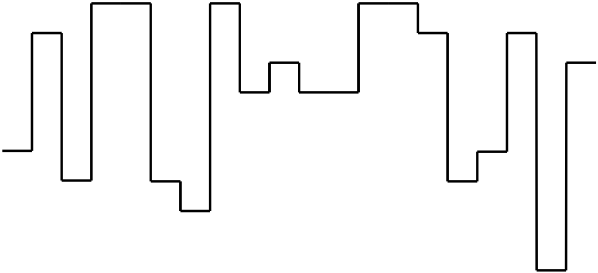

- Steps allowed: North, South, East
- subject to self-avoiding constraint

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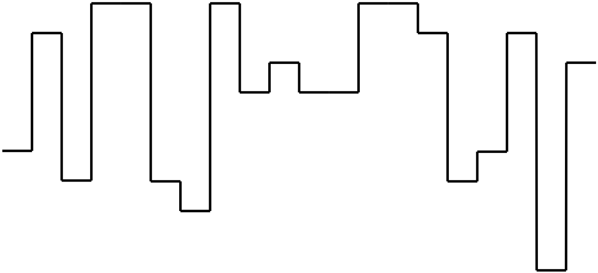
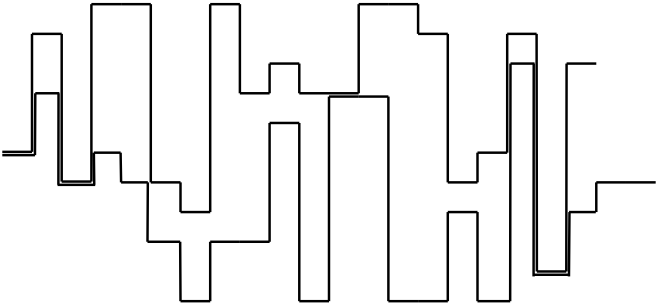


- Steps allowed: North, South, East
- subject to self-avoiding constraint
- Our walks start and end with a step East

Pair of non-crossing Partially directed Walks



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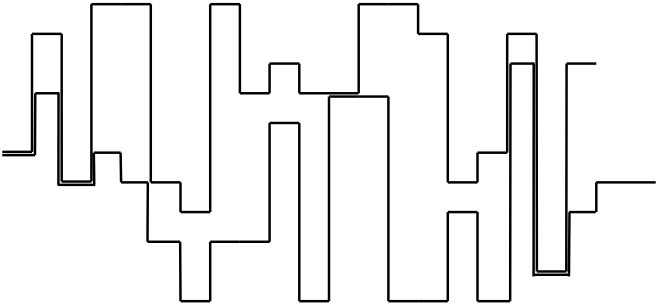
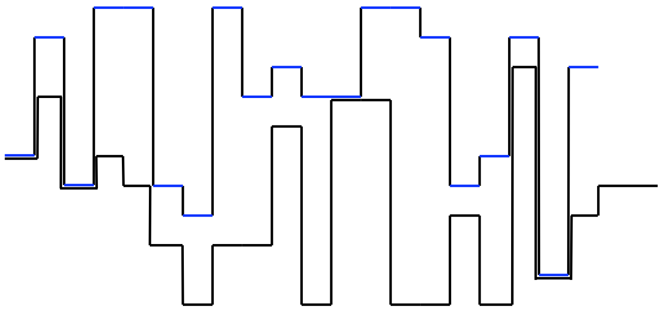


- Top walk: $N_1 = 20,\ M_1 = 63,\ L_1 = 83$
- Bottom walk: $N_2 = 22,\ M_2 = 61,\ L_2 = 83$

Pair of non-crossing Partially directed Walks



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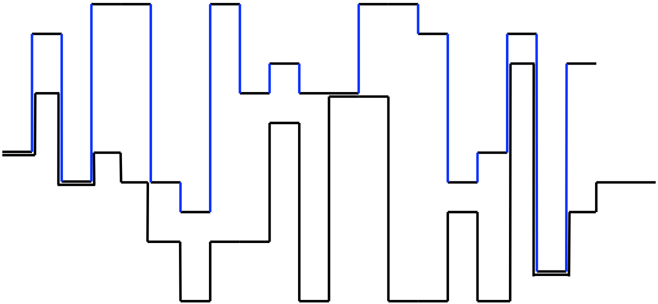

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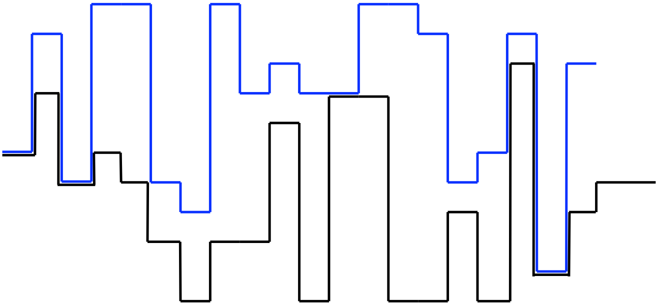

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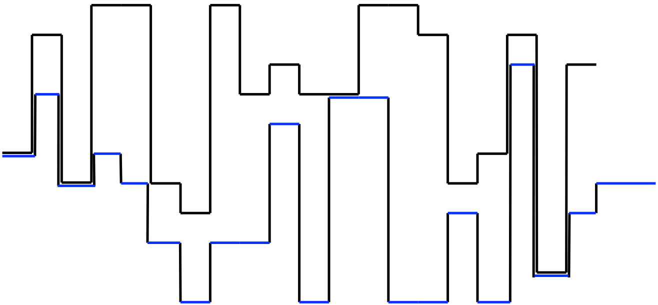

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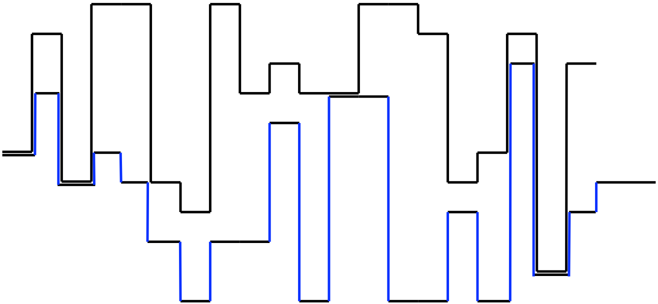

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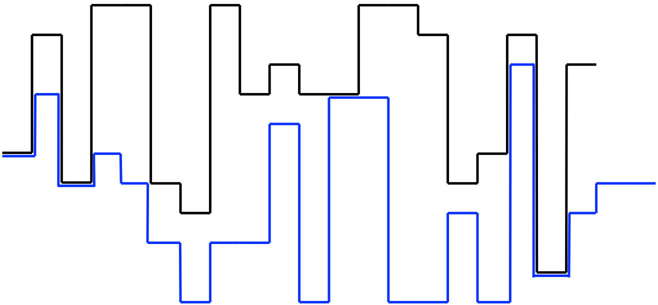

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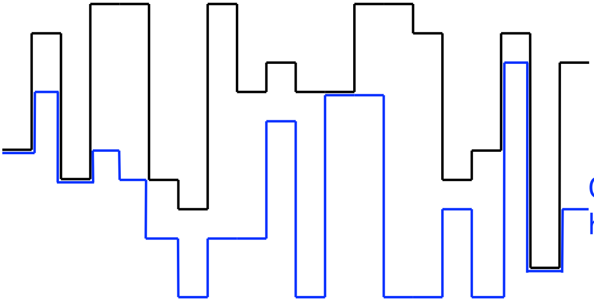
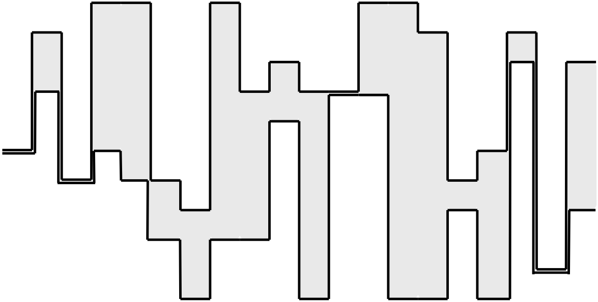


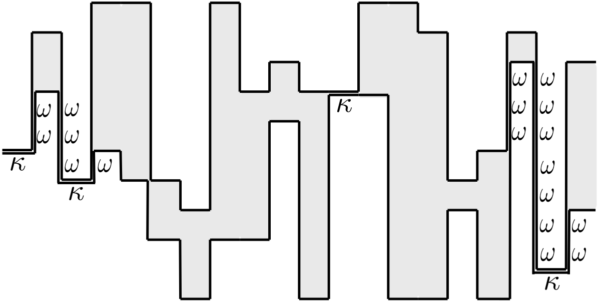
- Top walk: $N_1 = 20, \; M_1 = 63, \; L_1 = 83$
- Bottom walk: $N_2 = 20, \; M_2 = 60, \; L_2 = 80$

Pair of non-crossing Partially directed Walks



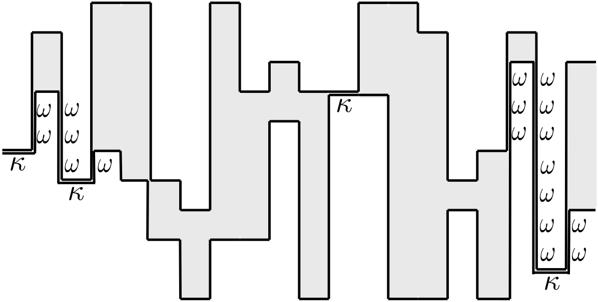
- is easier to generate combinatorially

Pair of non-crossing Partially directed Walks



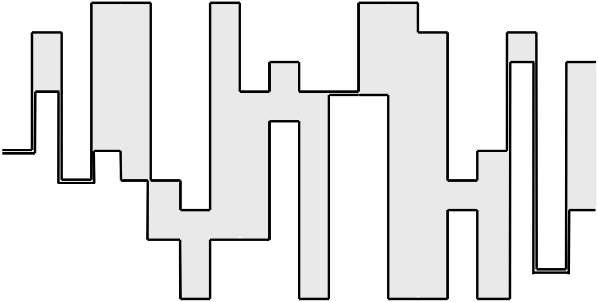
- We really want the version with contact weights

Pair of non-crossing Partially directed Walks



- We really want the version with contact weights
- This example has weight $x^{40} y_1^{63} y_2^{60} \kappa^4 \omega^{18} \mu^5$

Pair of non-crossing Partially directed Walks



- We really want the version with contact weights
- but will do unweighted version first to show method

Functional Equation

$$G(\mu) = \sum_{N,M_1,M_2,H\geq 0} c_{N,M_1,M_2,H}\, x^{2N} y_1^{M_1} y_2^{M_2} \mu^H$$

$$\begin{aligned}
G(\mu) =& x^2 \\
&+x^2 \left(\frac{y_1\mu}{1-y_1\mu} + 1 + \frac{y_1/\mu}{1-y_1/\mu} \right) \left(\frac{y_2\mu}{1-y_2\mu} + 1 + \frac{y_2/\mu}{1-y_2/\mu} \right) G(\mu) \\
&-x^2 \frac{y_1/\mu}{1-y_1/\mu} \left(\frac{y_2 y_1}{1-y_2 y_1} + 1 + \frac{y_2/y_1}{1-y_2/y_1} \right) G(y_1) \\
&-x^2 \left(\frac{y_1 y_2}{1-y_1 y_2} + 1 + \frac{y_1/y_2}{1-y_1/y_2} \right) \frac{y_2/\mu}{1-y_2/\mu} G(y_2)
\end{aligned}$$

Kernel Formulation

- $G(\mu) := G(x, y_1, y_2; \mu)$

$$K(\mu)G(\mu) = x^2\left(1 - A_1(\mu)G(y_1) - A_2(\mu)G(y_2)\right)$$

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where *kernel*

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and

$$A_1(\mu) = \frac{y_1/\mu}{1 - y_1/\mu} \left(\frac{y_2 y_1}{1 - y_2 y_1} + 1 + \frac{y_2/y_1}{1 - y_2/y_1} \right),$$

$$A_2(\mu) = \frac{y_2/\mu}{1 - y_2/\mu} \left(\frac{y_1 y_2}{1 - y_1 y_2} + 1 + \frac{y_1/y_2}{1 - y_1/y_2} \right).$$

Classic Kernel Method (in a simpler context)

- Classic kernel method. Suppose $G(\mu) := G(y;\mu)$, and:

$$K(\mu)G(\mu) = 1 + A(\mu)G(y)$$

  - Set $K(\mu) = 0$

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  - Therefore
$$G(y) = \frac{-1}{A(\mu_0)}$$
  - Back-substituting gives full solution:
$$G(\mu) = \frac{1 - A(\mu)/A(\mu_0)}{K(\mu)}.$$

Kernel Method for our situation

- $G(\mu) := G(x, y_1, y_2; \mu)$

$$K(\mu)G(\mu) = x^2(1 - A_1(\mu)G(y_1) - A_2(\mu)G(y_2))$$

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$$A_1(\mu_1)G(y_1) + A_2(\mu_1)G(y_2) = 1$$
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- Solve the set of simultaneous equations for $G(y_1)$ and $G(y_2)$.
- Back-substituting gives full solution for $G(\mu)$.

Exact Solution

$$G(\mu) = \frac{x^2}{K(\mu)} \left(1 - \frac{A_1(\mu)\Big(A_2(\mu_1) - A_2(\mu_2)\Big) - A_2(\mu)\Big(A_1(\mu_1) - A_1(\mu_2)\Big)}{A_1(\mu_2)A_2(\mu_1) - A_2(\mu_2)A_1(\mu_1)} \right)$$

where

$$K(\mu) = 1 - x^2 \left(\frac{y_1\mu}{1 - y_1\mu} + 1 + \frac{y_1/\mu}{1 - y_1/\mu} \right) \left(\frac{y_2\mu}{1 - y_2\mu} + 1 + \frac{y_2/\mu}{1 - y_2/\mu} \right)$$

and

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$$A_2(\mu) = \frac{y_2/\mu}{1 - y_2/\mu} \left(\frac{y_1 y_2}{1 - y_1 y_2} + 1 + \frac{y_1/y_2}{1 - y_1/y_2} \right)$$

Exact Solution simplifies to:

$$G(\mu) = x^2 \frac{(\mu - 1/y_1)(\mu - 1/y_2)}{(\mu - 1/\mu_1)(\mu - 1/\mu_2)}$$

$G(\mu)$ is not as simple as it looks

We can write the kernel:

$$K(\mu) = \frac{(\mu - \mu_1)(\mu - 1/\mu_1)(\mu - \mu_2)(\mu - 1/\mu_2)}{(\mu - y_1)(\mu - 1/y_1)(\mu - y_2)(\mu - 1/y_2)}$$

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where the numerator is the quartic:

$$\mu^4 - \left(\frac{\alpha}{y_1 y_2}\right)\mu^3 + \left(\frac{\gamma}{y_1 y_2}\right)\mu^2 - \left(\frac{\alpha}{y_1 y_2}\right)\mu + 1$$

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with

$$\alpha = (y_1 + y_2)(1 + y_1 y_2)$$
$$\gamma = 2y_1 y_2 - x^2(y_1^2 - 1)(y_2^2 - 1) + (y_1^2 + 1)(y_2^2 + 1)$$

Explicit Generating Function is:

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where

$$\mu_1^{\pm 1} = \frac{\alpha - \sqrt{\beta} \mp \sqrt{(\alpha^2 + \beta - 16 y_1^2 y_2^2) - 2\alpha\sqrt{\beta}}}{4 y_1 y_2}$$

$$\mu_2^{\pm 1} = \frac{\alpha + \sqrt{\beta} \mp \sqrt{(\alpha^2 + \beta - 16 y_1^2 y_2^2) + 2\alpha\sqrt{\beta}}}{4 y_1 y_2}$$

for

$$\alpha = (y_1 + y_2)(1 + y_1 y_2)$$
$$\beta = (y_1 - y_2)^2 (y_1 y_2 - 1)^2 + 4x^2 y_1 y_2 (y_1^2 - 1)(y_2^2 - 1)$$

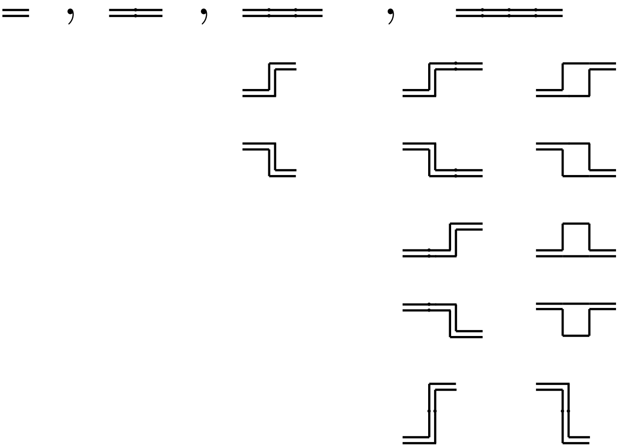
Specializing $G(x, y_1, y_2; \mu)$

Setting $x = y_1 = y_2 = t$ and $\mu = 0$ counts pairs of paths with combined total length t, which end at a common height.

$$
\begin{aligned}
G(t,t,t;0) &= \frac{1}{4t^2}\left(1+t+t^2-t^3-\sqrt{1+2t-t^2-t^4-2t^5+t^6}\right) \\
&\quad \times \left(1-t+t^2+t^3-\sqrt{1-2t-t^2-t^4+2t^5+t^6}\right) \\
&= t^2+t^4+3t^6+11t^8+46t^{10}+\dots \\
&=: \sum_L Z_L t^L
\end{aligned}
$$

Checking ...

$$t^2 + t^4 + 3t^6 + 11t^8 \quad \cdots$$



A critical value of t

$$G(t,t,t;0)$$
$$= \frac{1}{4t^2}\left(1+t+t^2-t^3-\sqrt{(t^4-1)(t+(1+\sqrt{2}))(t-(1-\sqrt{2}))}\right)$$
$$\times\left(1-t+t^2+t^3-\sqrt{(t^4-1)(t-(-1+\sqrt{2}))(t-(-1-\sqrt{2}))}\right)$$

- Smallest root under the square-root sign is $t_c = \sqrt{2}-1$

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- Hence number of configurations, Z_L, grows like $L^{-3/2} \times t_c^{-L}$, i.e.

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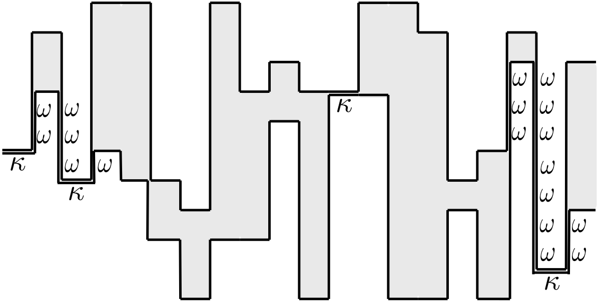
- Hence number of configurations, Z_L, grows like $L^{-3/2} \times t_c^{-L}$, i.e.
$$L^{-3/2}(\sqrt{2}+1)^L$$
- Quartic is:

$$\begin{aligned}0 = {} & t^8(1-t)^8 - t^6(1-t)^8(1+t^2)(1-2t-t^2)G \\ & - 2t^5(1-t)^6(1-t+t^2)(1+t^2)(1-2t-t^2)G^2 \\ & + t^4(1-t)^6(1+t^2)^2(1-2t-t^2)^2G^3 \\ & + t^4(1-t)^4(1+t^2)^2(1-2t-t^2)^2G^4\end{aligned}$$

Contact weights



Functional Equation, with contact weights

$$
\begin{aligned}
G(\mu) =& x^2 + x^2 \left(\frac{y_1\mu}{1-y_1\mu} + 1 + \frac{y_1/\mu}{1-y_1/\mu} \right) \left(\frac{y_2\mu}{1-y_2\mu} + 1 + \frac{y_2/\mu}{1-y_2/\mu} \right) G(\mu) \\
&- x^2 \frac{y_1/\mu}{1-y_1/\mu} \left(\frac{y_2 y_1}{1-y_2 y_1} + 1 + \frac{y_2/y_1}{1-y_2/y_1} \right) G(y_1) \\
&- x^2 \left(\frac{y_1 y_2}{1-y_1 y_2} + 1 + \frac{y_1/y_2}{1-y_1/y_2} \right) \frac{y_2/\mu}{1-y_2/\mu} G(y_2) \\
&+ (\kappa-1)x^2 \left(\frac{y_2 y_1}{1-y_2 y_1} + 1 + \frac{y_2/y_1}{1-y_2/y_1} \right) G(y_1) \\
&+ (\kappa-1)x^2 \left(\frac{y_1 y_2}{1-y_1 y_2} + 1 + \frac{y_1/y_2}{1-y_1/y_2} \right) G(y_2) \\
&+ x^2 \left(\frac{\omega y_1 y_2}{1-\omega y_1 y_2} - \frac{y_1 y_2}{1-y_1 y_2} \right) \left(\frac{y_2\mu}{1-y_2\mu} + 1 \right) G(y_1) \\
&+ x^2 \left(\frac{y_1\mu}{1-y_1\mu} + 1 \right) \left(\frac{\omega y_2 y_1}{1-\omega y_2 y_1} - \frac{y_2 y_1}{1-y_2 y_1} \right) G(y_2) \\
&+ (\kappa-1)x^2 \left(\frac{\omega y_1 y_2}{1-\omega y_1 y_2} - \frac{y_1 y_2}{1-y_1 y_2} \right) G(y_1) \\
&+ (\kappa-1)x^2 \left(\frac{\omega y_1 y_2}{1-\omega y_1 y_2} - \frac{y_1 y_2}{1-y_1 y_2} \right) G(y_2) \, .
\end{aligned}
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G(\mu) =& x^2 + x^2 \left(\frac{y_1 \mu}{1 - y_1 \mu} + 1 + \frac{y_1/\mu}{1 - y_1/\mu} \right) \left(\frac{y_2 \mu}{1 - y_2 \mu} + 1 + \frac{y_2/\mu}{1 - y_2/\mu} \right) G(\mu) \\
& - x^2 \frac{y_1/\mu}{1 - y_1/\mu} \left(\frac{y_2 y_1}{1 - y_2 y_1} + 1 + \frac{y_2/y_1}{1 - y_2/y_1} \right) G(y_1) \\
& - x^2 \left(\frac{y_1 y_2}{1 - y_1 y_2} + 1 + \frac{y_1/y_2}{1 - y_1/y_2} \right) \frac{y_2/\mu}{1 - y_2/\mu} G(y_2) \\
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\end{aligned}$$

2-roots Kernel Method again:

- $G(\mu) := G(x, y_1, y_2, \kappa, \omega; \mu)$

$$K(\mu)G(\mu) = x^2(1 - A_1(\mu)G(y_1) - A_2(\mu)G(y_2))$$

- Set $K(\mu) = 0$ to find 'correct' roots $\mu = \mu_1, \mu_2$
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- Back-substituting gives full solution for $G(\mu)$, where functions A_1 and A_2 now depend on κ and ω.

Exact Solution, with contact weights

$$G(\mu) = \frac{x^2}{K(\mu)} \left(1 - \frac{A_1(\mu)\Big(A_2(\mu_1) - A_2(\mu_2)\Big) - A_2(\mu)\Big(A_1(\mu_1) - A_1(\mu_2)\Big)}{A_1(\mu_2)A_2(\mu_1) - A_2(\mu_2)A_1(\mu_1)} \right)$$

where

$$A_1(\mu) = \left(\frac{1}{1 - y_1/\mu} - \kappa\right) \frac{1 - y_2^2}{(1 - y_2 y_1)(1 - y_2/y_1)} + \left(\frac{y_2\mu}{1 - y_2\mu} + \kappa\right)\left(\frac{y_1 y_2}{1 - y_1 y_2} - \frac{\omega y_1 y_2}{1 - \omega y_1 y_2}\right)$$

and

$$A_2(\mu) = \left(\frac{1}{1 - y_2/\mu} - \kappa\right) \frac{1 - y_1^2}{(1 - y_1 y_2)(1 - y_1/y_2)} + \left(\frac{y_1\mu}{1 - y_1\mu} + \kappa\right)\left(\frac{y_2 y_1}{1 - y_2 y_1} - \frac{\omega y_2 y_1}{1 - \omega y_2 y_1}\right).$$

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- Moral:
  - same singularities as non-interacting case, and
  - other singularities arising as poles from A, B, C

Specializing $G(x, y_1, y_2, \kappa, \omega; \mu)$, keeping interactions

- Setting $x = y_1 = y_2 = t$ and $\mu = 0$ counts pairs of paths with combined total length t, which end at a common height.

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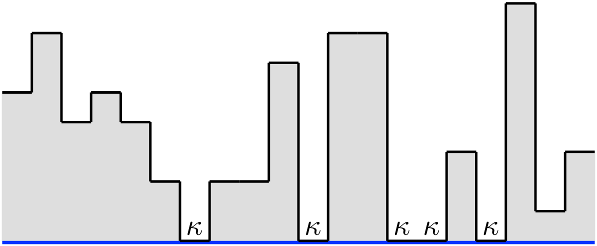
- Look at $G(t, t, t, \kappa, \omega; 0) = \sum_L Z_L(\kappa, \omega) t^L$
- Use insight from "one sticky walk above a wall"



solved previously: $G(t, t, 0, \kappa, \cdot; 0)$

Singularities

- We expect significant singularities of $G(t, t, t, \kappa, \omega; 0)$ to be
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- 'Sit on algebraic singularity' by substituting $t=\sqrt{2}-1$. Get $G(t,t,t,\kappa,\omega;0)\big|_{t=\sqrt{2}-1} =$

$$\frac{(-1/47)\left(-4+4\sqrt{2}+(4+3\sqrt{2})\sqrt{10-7\sqrt{2}}\right)\left(-47\omega+73+50\sqrt{2}+(136+88\sqrt{2})\sqrt{10-7\sqrt{2}}\right)}{4\omega(\sqrt{2}+1+\kappa)-28-20\sqrt{2}+4\kappa+8\kappa\sqrt{2}+(24\omega+17\omega\sqrt{2}-100-71\sqrt{2}+32\kappa+24\kappa\sqrt{2})\sqrt{10-7\sqrt{2}}}$$

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- This finite generating function must diverge: denominator $=0$

Singularities

- Denominator $\left(G(t,t,t,\kappa,\omega;0)|_{t=\sqrt{2}-1} \right)$ is $\frac{1}{188} \times$

$$\kappa\omega + \left(1 + 2\sqrt{2} + (6\sqrt{2} + 8)\sqrt{10 - 7\sqrt{2}}\right)\kappa$$
$$+ \left(1 + \sqrt{2} + (6 + 17\sqrt{2}/4)\sqrt{10 - 7\sqrt{2}}\right)\omega$$
$$- 7 - 5\sqrt{2} - (25 + 71\sqrt{2}/4)\sqrt{10 - 7\sqrt{2}}$$

Curve of Singularities

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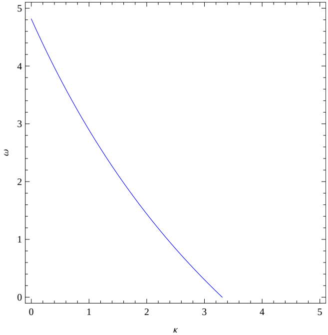
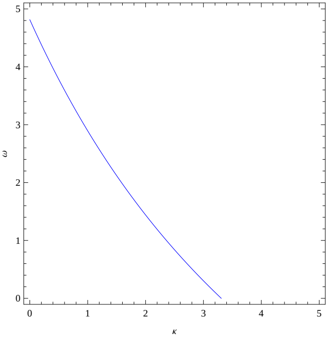
$$\kappa\omega + 9.05468\kappa + 6.22182\omega - 29.9548 = 0$$



Thermal Unbinding



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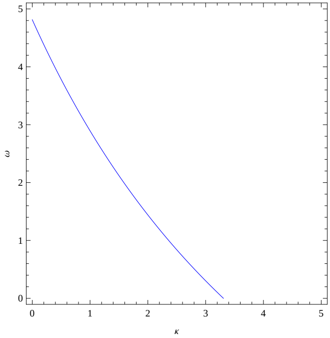
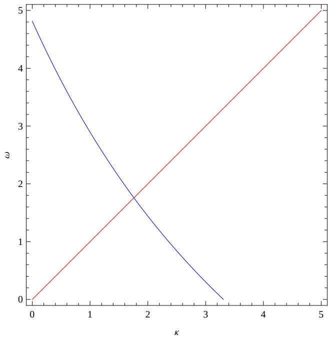


- Below curve: unbound state and $t_c = \sqrt{2} - 1$
- Above curve: bound state and $t_c =$ "complicated" (κ, ω)

Interested in case: $\kappa = \omega$



- Unbinding occurs below:

$$\kappa = \omega = 1.75843$$

Curious Observation:

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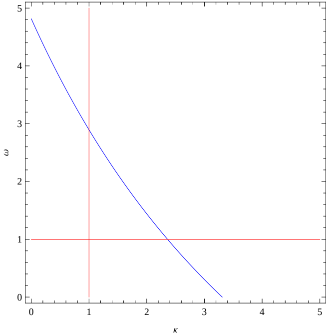

Curious Observation:

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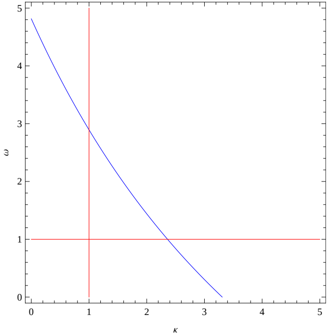

- Why would this be?

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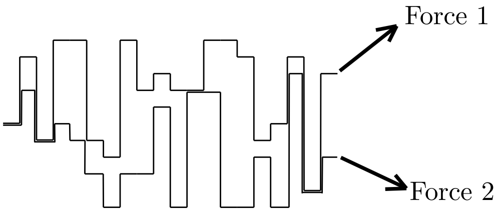
- Kernel method works, with care!
- Thermal unbinding as expected
- Full solution allows pulling to be analyzed ...

Outlook

- We are in the process of completing analysis of the full model with pulling:



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- J. Osborn and T. Prellberg, *'Forcing Adsorption of a Tethered Polymer by Pulling'* J. Stat. Mech. (2010) P09018
- E. Orlandini and S. G. Whittington *Adsorbing polymers subject to an elongational force: the effect of pulling direction* J. Phys. A: Math. Theor. **43** (2010)

THE END
(for now)