A solvable model of weighted SAWs in a box

Nicholas Beaton & Aleks Owczarek

School of Mathematics and Statistics, University of Melbourne, Australia

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Self-avoiding walks

A self-avoiding walk (SAW) on a lattice (e.g. $\mathbb{Z}^d$) is a sequence of vertices

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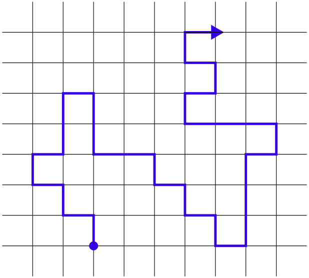
such that ω_i, ω_{i+1} are adjacent on the lattice and $\omega_i \neq \omega_j$ for $i \neq j$.



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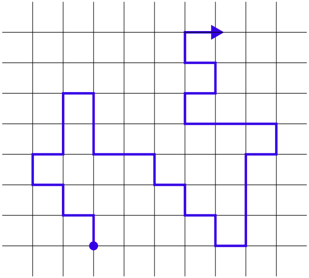

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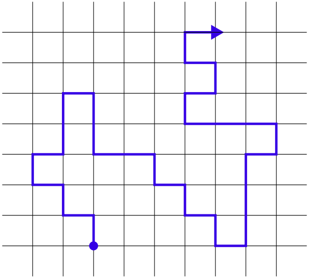

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Also interesting to study in their own right.

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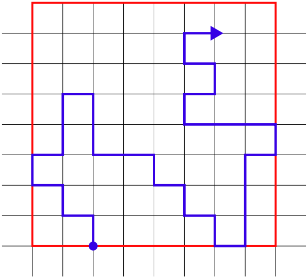

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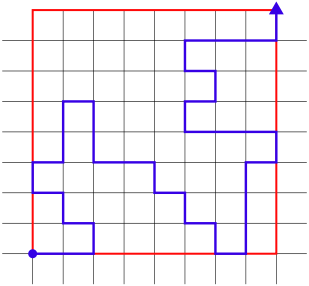

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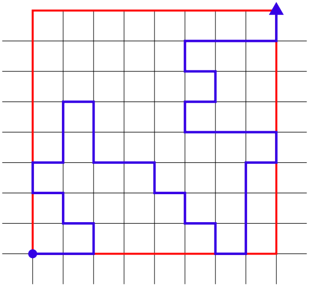

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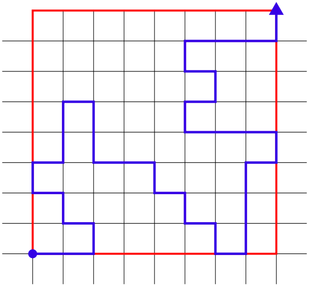

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exists. Conjectured that

$$c_L \sim \lambda_2^{L^2+bL+c} \cdot L^g$$

with (on the square lattice) $\lambda_2 \approx 1.7445498$, $b \approx -0.04354$, $c \approx 0.5624$, $g \approx 0$ [Guttmann & Jensen 2022].

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Elaborate on this by introducing variable t to weight each SAW according to its length. Then the count c_L becomes a partition function $C_L(t)$, with $c_L = C_L(1)$.

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$\lambda_1(t)$: finite and < 1 for $0 < t < \mu^{-1}$, $= 1$ at $t = \mu^{-1}$, and infinite for $t > \mu^{-1}$

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Nothing else rigorous known about the functions λ_1, λ_2 or the subdominant behaviour.

A solvable version

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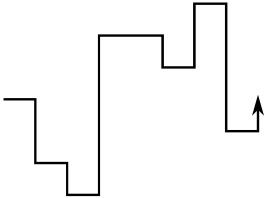

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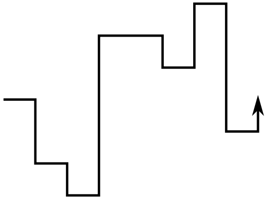

Let $P_L(t)$ be the partition function for PDWs which cross an $L \times L$ square:

$$P_1(t) = 2t^2$$
$$P_2(t) = 6t^4 + 2t^6 + t^8$$
$$P_3(t) = 20t^6 + 18t^8 + 16t^{10} + 10t^{12}$$
$$P_4(t) = 70t^8 + 112t^{10} + 145t^{12} + 150t^{14} + 113t^{16} + 20t^{18} + 10t^{20} + 4t^{22} + t^{24}$$

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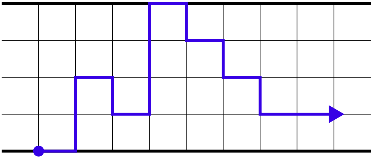
So the asymptotic behaviour is neither λ_1^L nor $\lambda_2^{L^2}$, but instead something in between.

$t < 1$: Generating function approach

Take PDWs in a strip of height L.



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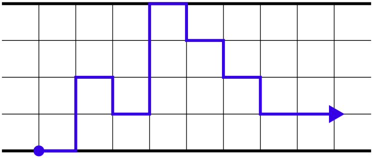

Grow walks step-by-step, using three generating functions $H(t, s, v)$, $U(t, s, v)$, $D(t, s, v)$ according to the direction of the final step, where

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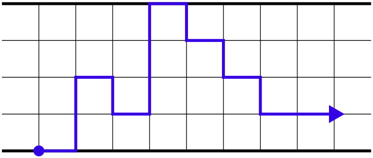

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Then

$$H(v) = 1 + ts\left(H(v) + U(v) + D(v)\right),$$
$$U(v) = tv\left(H(v) + U(v)\right) - tv\left(v^L[v^L]H(v) + v^L[v^L]U(v)\right),$$
$$D(v) = t\overline{v}\left(H(v) + D(v)\right) - t\overline{v}\left([v^0]H(v) + [v^0]D(v)\right).$$

Eliminate all the U and D terms to get

$$\left(1 - ts + \frac{t^2 s}{t - v} - \frac{t^2 s v}{1 - tv}\right) H(v) = 1 - \frac{t}{t - v} + \frac{t}{t - v} H_0 - \frac{t v^{L+1}}{1 - tv} H_L$$

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where

$$V = \frac{1 - ts + t^2 + t^3 s - \sqrt{(1 - ts + t^2 + t^3 s)^2 - 4t^2}}{2t}$$

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A bit of approximation and the saddle point method (steepest descent) yields

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So

$$\lambda_1(t) = \frac{4t^2}{1 - t^2}$$

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Then

$$\begin{aligned} P_L(t) &= (1, t, t^2, \ldots, t^L) \cdot T_L(t)^L \cdot (0, 0, \ldots, 0, 1)^\mathsf{T} \\ &= \frac{1}{t}(1, 0, 0, \ldots, 0) \cdot T_L(t)^{L+1} \cdot (0, 0, \ldots, 0, 1)^\mathsf{T}. \end{aligned}$$

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Want to diagonalise T_L, so consider the eigen-equation

$$T\mathbf{g} = \lambda\mathbf{g} \qquad \Longleftrightarrow \qquad \sum_{j=1}^{L+1} t^{|i-j|+1} g_j = \lambda g_i$$

Bethe ansatz approach gives the eigenvalue

$$\lambda = -\frac{z(1-t^2)}{(1-tz)(1-\frac{z}{t})} = \frac{t(1-t^2)}{1-t(z+\frac{1}{z})+t^2}$$

where $z = z_{L,k}$ is a root of

$$A_{L,k}(t,z) = 1 - tz + (-1)^k z^{L+1}(t-z)$$

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Actually $2L+2$ valid roots but they come in $z \leftrightarrow \frac{1}{z}$ pairs with each pair giving the same eigenvalue/vector.

Then diagonalising (using the fact that T_L is real symmetric) eventually gives

$$P_L(t) = \frac{(1-t^2)^{L+1}}{2t} \sum_{k=1}^{L+1} \frac{(-1)^{k+1}(1+(-1)^{k+1} z_{L,k}^L)^2 (1-z_{L,k}^2) z_{L,k}^{L+1}}{(1+(-1)^{k+1}(L+1) z_{L,k}^L (1-z_{L,k}^2) - z_{L,k}^{2L+2})(z_{L,k}-t)^{L+1}(\frac{1}{t}-z_{L,k})^{L+1}}$$

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Lemma

For $t > 1$ and $L > \frac{2}{t-1}$, $L-1$ of the reciprocal pairs of roots $z_{L,k}$ are on the unit circle, and two pairs (one for even k and one for odd k) are real, positive and not on the unit circle.

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Now because $A_{L,k}$ is palindromic (odd k) or antipalindromic (even k) its roots have nice properties.

Lemma

For $t > 1$ and $L > \frac{2}{t-1}$, $L-1$ of the reciprocal pairs of roots $z_{L,k}$ are on the unit circle, and two pairs (one for even k and one for odd k) are real, positive and not on the unit circle.

This follows from a lemma due to Vieira:

Lemma (Vieira 2017)

Let $p(z) = a_0 + a_1 z + \cdots + a_n z^n$ be a palindromic or antipalindromic polynomial of degree n. If

$$|a_{n-\ell}| > \frac{1}{2} \sum_{\substack{k=0 \\ k\neq \ell, n-\ell}}^{n} |a_k|, \qquad \ell < \frac{n}{2},$$

then $p(z)$ has at least $n-2\ell$ roots on the unit circle.

Taking $\ell = 1$ and getting from "at least" to "exactly" only requires a bit of elementary calculus.

The two reciprocal pairs which are not on the u.c. turn out to be real and positive. Take $z_{L,1}$ to be the representative which is inside the u.c. for odd k, and likewise $z_{L,2}$ for even k.

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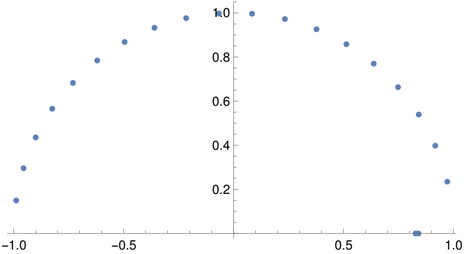
Then easy to show that $z_{L,1}, z_{L,2} \to \frac{1}{t}$ as $L \to \infty$.



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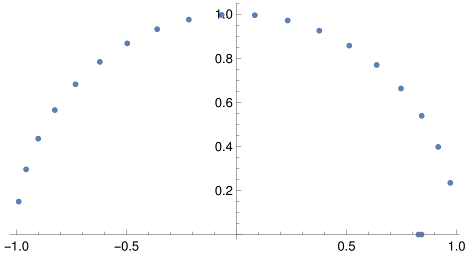

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Then the two roots not on the u.c. turn out to be the only ones which contribute to the dominant asymptotics:

$$P_L(t) \sim \frac{(1-t^2)^{L+1}}{2t} \sum_{k=1}^{2} \frac{(-1)^{k+1}(1+(-1)^{k+1} z_{L,k}^L)^2 (1-z_{L,k}^2) z_{L,k}^{L+1}}{(1+(-1)^{k+1}(L+1) z_{L,k}^L (1-z_{L,k}^2) - z_{L,k}^{2L+2})(z_{L,k}-t)^{L+1}(\frac{1}{t}-z_{L,k})^{L+1}}$$

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$$A_{L,k}(t,z) = 1 - tz + (-1)^k z^{L+1}(t-z) = 0$$

Rearrange to get

$$\begin{aligned}\log\left[(-1)^{k+1}(\tfrac{1}{t} - z)\right] &= (L+1)\log z + \log t + \log(t-z) \\ &\sim -(L+1)\log t + \log t + \log(t - \tfrac{1}{t}) \\ &= \log\left(\frac{t^2-1}{t^{L+3}}\right).\end{aligned}$$

Hence to first order

$$z_{L,k} \sim z^*_{L,k} = \frac{1}{t} + (-1)^k \left(\frac{t^2-1}{t^3}\right) t^{-L}, \qquad k = 1,2$$

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This can be iterated to get to second order

$$z_{L,k} \sim z^{**}_{L,k} = \frac{1}{t} + (-1)^k t^{-L} \left(\frac{t^2-1}{t^3}\right) \left(1 + (-1)^k t^{-L} L \frac{t^2-1}{t^2}\right)$$

Finally we substitute this in and simplify lots to get the dominant asymptotics for $t > 1$:

$$P_L(t) \sim \begin{cases} \left(\dfrac{t^4}{t^2-1}\right)^L t^{L^2} & L \text{ even} \\ \dfrac{t^2-1}{t^2} \cdot L^2 \cdot \left(\dfrac{t^3}{t^2-1}\right)^L \cdot t^{L^2} & L \text{ odd.} \end{cases}$$

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So $\lambda_2(t) = t$. The parity effects arise because PDWs (and SAWs for that matter) can fill every vertex for even L but not for odd L.

Average length & phase transition

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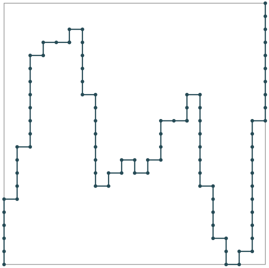
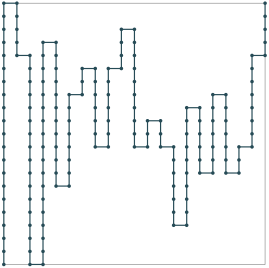
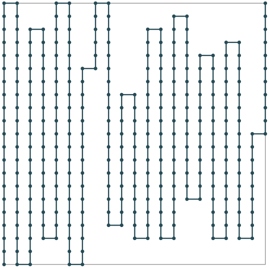


(a)



(b)



(c)

PDWs in a box of size $L = 20$ sampled from the Boltzmann distribution, at (a) $t = 0.8$, (b) $t = 1$ and (c) $t = 1.2$. The respective lengths are 92, 170 and 326.

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$$\langle n \rangle_L = \frac{t \frac{d}{dt} P_L(t)}{P_L(t)}$$

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$$\langle n \rangle_L \sim \begin{cases} L^2 + \dfrac{2(t^2-2)L}{t^2-1} & L \text{ even} \\ L^2 + \dfrac{(t^2-3)L}{t^2-1} + \dfrac{2}{t^2-1} & L \text{ odd.} \end{cases}$$

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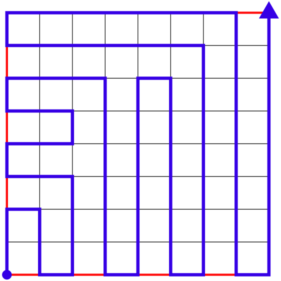
A possible generalisation might be prudent walks which do have some entropy even at high density



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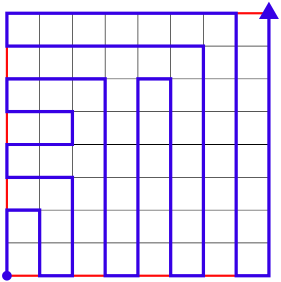

https://arxiv.org/abs/2212.09200

Thank you!