Markovian and non-Markovian Transport on the Lattice: A Random Walk with Internal Degrees of Freedom Approach

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Our General Framework:

We introduce here a general procedure to find the first-passage distribution of random walks with internal states. Below we give some important use cases.

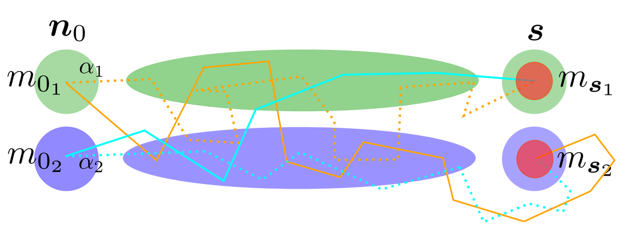
The idea is to place absorbing traps on individual internal states. We then write a Master equation (1) governing the state level dynamics. Insertion of the initial condition (2) and considering the trajectories that begin and end in each state as mutually exclusive leads to the formal solution for absorbing occupation probability (3). Some algebra leads to the first passage probabiltiy (red box), where we have expressed it in terms of the occupation probability.

$$P(\boldsymbol{n},m,t+1)=\sum_{\boldsymbol{n}'}\sum_{m'}\left[A(\boldsymbol{n},m,\boldsymbol{n}',m')P(\boldsymbol{n}',m',t)+\sum_{i=1}^{S}\delta_{\boldsymbol{n},\boldsymbol{s}_i}\delta_{m,m_{\boldsymbol{s}_i}}(1-\rho_{m_{\boldsymbol{s}_i}})A(\boldsymbol{s}_i,m_{\boldsymbol{s}_i},\boldsymbol{n}',m')P(\boldsymbol{n}',m',t)\right] \quad (1)$$

$$P(\boldsymbol{n},m,0)=\delta_{\boldsymbol{n},\boldsymbol{n}_0}\sum_{m=1}^{M}\delta_{m,m_0}\alpha_{m_0}\left[(1-\rho_{m_s})\delta_{(\boldsymbol{n}_0,m_0)\in\mathcal{S}}+\delta_{(\boldsymbol{n}_0,m_0)\notin\mathcal{S}}\right] \quad (2)$$

The pink terms are defect-free while the blue terms represent the dynamics at a trap.

$$\widetilde{P}_{\boldsymbol{n}_0,m_0}(\boldsymbol{n},m,z)=\sum_{m=1}^{M}\sum_{m_0=1}^{M}\left\{\alpha_{m_0}\widetilde{P}^{(\gamma)}_{\boldsymbol{n}_0,m_0}(\boldsymbol{n},m,z)-\sum_{i=1}^{S}\frac{\rho_{m_{s_i}}}{1-\rho_{m_{s_i}}}\alpha_{m_{s_i}}\widetilde{P}^{(\gamma)}_{\boldsymbol{s}_i,m_{s_i}}(\boldsymbol{n},m,z)\widetilde{P}_{\boldsymbol{n}_0,m_0}(\boldsymbol{s}_i,m_{s_i},z)\right\} \quad (3)$$



Each trajectory must have a unique start and end state. We weight the contribution of each according to its initial distribution.

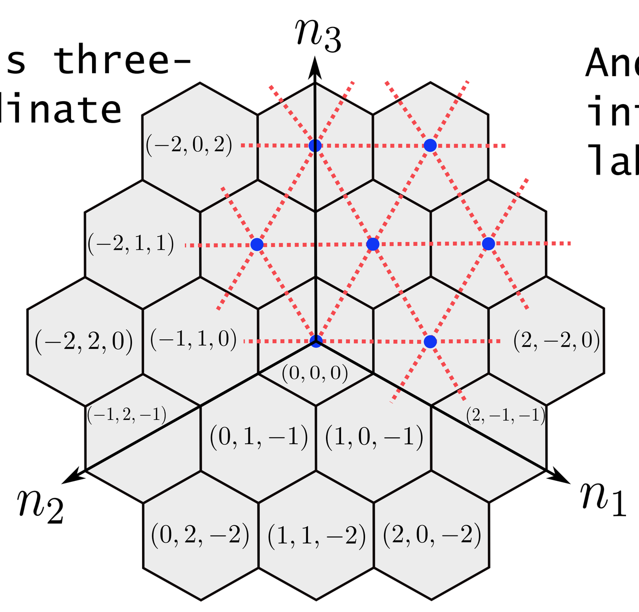
$$\boxed{\widetilde{F}_{\boldsymbol{n}_0}(\mathcal{S},z)=\sum_{j=1}^{M}\sum_{i=1}^{S}\alpha_{m_{s_i}}\frac{\det\left[\mathbb{H}^{(i)}(\boldsymbol{n}_0,m_{0_j},z)\right]}{\det\left[\mathbb{H}(z)\right]}}$$

This is a general expression for the first-passage probability for any random walk with internal states. It allows any (finite) number of targets and an arbitrary initial weighting distribution.

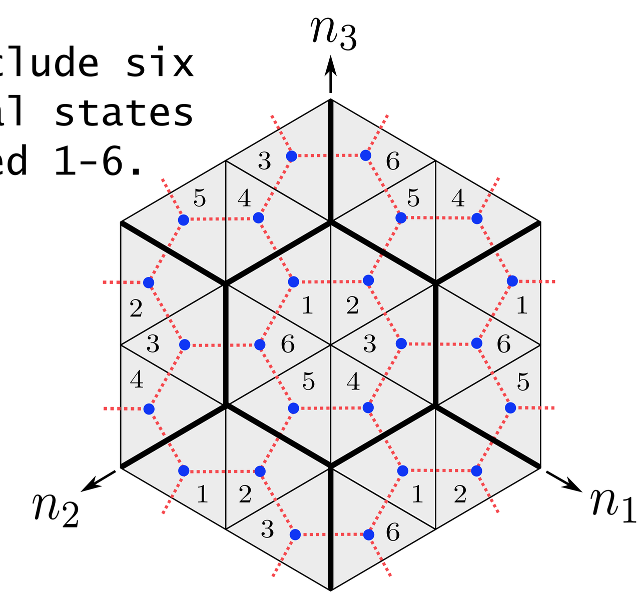
Walks on Non-Bravais Lattices:

- A lattice is non-Bravais if it has different site types.
- This makes the analytics of random walks on these lattices harder as translational invariance is broken.
- We use internal states to regain translational invariance with different site types as states grouped into homogenous sites.
- We may apply this reasoning to many different lattice tessellations e.g., square-octogon and tri-hexagonal (Kagome) but we focus here on the honeycomb lattice.

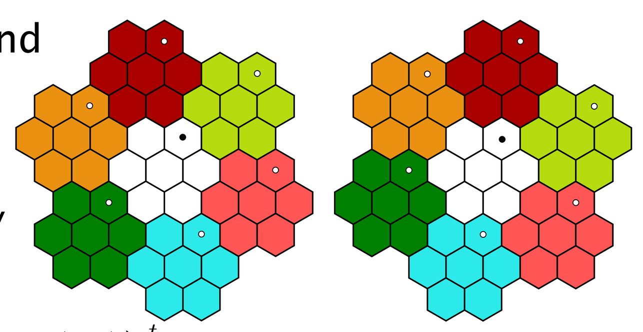
We use Her's three-axis cooridinate system



And include six internal states labelled 1-6.



We modify the method of images to this geometry and show there are **two ways to costruct it**, which we call the **left and right shift.**



This allows us to find the occupation probability as

$$\boldsymbol{\mathcal{P}}_{\boldsymbol{n}_0,m_0}(\boldsymbol{n},t)=\frac{\boldsymbol{\lambda}^{(\mathcal{H})}(0,0)^t\cdot\boldsymbol{U}_{m_0}}{\Omega}+\frac{1}{\Omega}\sum_{r=0}^{R-1}\sum_{s=0}^{3r+2}\left\{\mathrm{e}^{\frac{-2\pi i(\boldsymbol{n}-\boldsymbol{n}_0)\cdot\boldsymbol{k}(r,s)}{\Omega}}\boldsymbol{\lambda}^{(\mathcal{H})}\left(\frac{2\pi k_1(r,s)}{\Omega},\frac{2\pi k_2(r,s)}{\Omega}\right)^t+\mathrm{e}^{\frac{2\pi i(\boldsymbol{n}-\boldsymbol{n}_0)\cdot\boldsymbol{k}(r,s)}{\Omega}}\boldsymbol{\lambda}^{(\mathcal{H})}\left(\frac{-2\pi k_1(r,s)}{\Omega},\frac{-2\pi k_2(r,s)}{\Omega}\right)^t\right\}\cdot\boldsymbol{U}_{m_0}$$

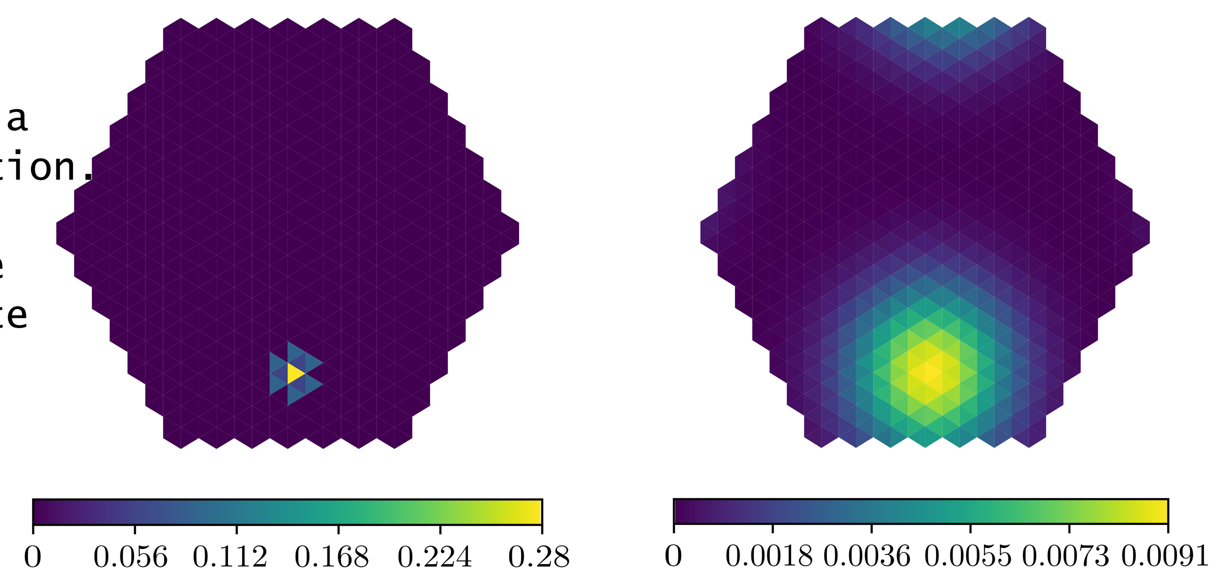
The propagator is an $\mathfrak{n}\times 1$ column vector where $\mathfrak{n}$ is the number of internal states, making it straightforward to access the state occupation probability.

The possible movement steps are encoded into the **structure function** which is a matrix of size $\mathfrak{n}\times\mathfrak{n}$. For the honeycomb LRW, we have:

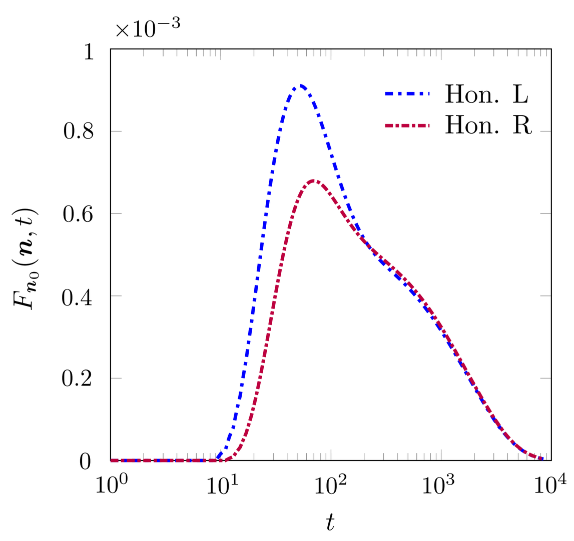
The parameter q controls the speed of diffusion over the lattice and may be considered as a rescaling of the diffusion constant.

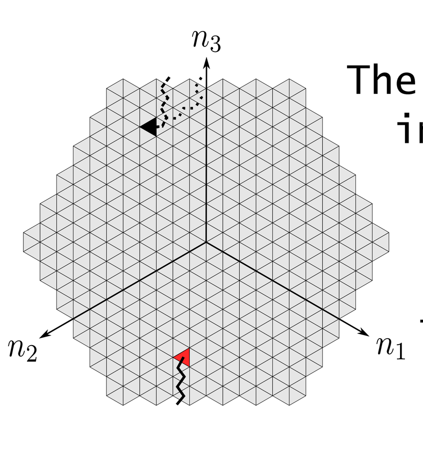
$$\boldsymbol{\lambda}^{(\mathcal{H})}(\xi_1,\xi_2)=\begin{bmatrix}1-q & \frac{q}{3} & 0 & \frac{q}{3}\mathrm{e}^{i\xi_1} & 0 & \frac{q}{3}\\ \frac{q}{3} & 1-q & \frac{q}{3} & 0 & \frac{q}{3}\mathrm{e}^{i\xi_2} & 0\\ 0 & \frac{q}{3} & 1-q & \frac{q}{3} & 0 & \frac{q}{3}\mathrm{e}^{-i(\xi_1-\xi_2)}\\ \frac{q}{3}\mathrm{e}^{-i\xi_1} & 0 & \frac{q}{3} & 1-q & \frac{q}{3} & 0\\ 0 & \frac{q}{3}\mathrm{e}^{-i\xi_2} & 0 & \frac{q}{3} & 1-q & \frac{q}{3}\\ \frac{q}{3} & 0 & \frac{q}{3}\mathrm{e}^{i(\xi_1-\xi_2)} & 0 & \frac{q}{3} & 1-q\end{bmatrix}$$

Diffusive spread out of a localised initial condition. Due to the finite space will eventually saturate to a uniform steady state



$\mathcal{P}_{\boldsymbol{n}_0,m_0}(n_1,n_2,m,t=2)$ $\quad$ $\mathcal{P}_{\boldsymbol{n}_0,m_0}(n_1,n_2,m,t=50)$





The choice of left or right shift impacts the FP distribution in the timeframe dominated by indirect trajectories as the periodic boundary alters their path in different ways.

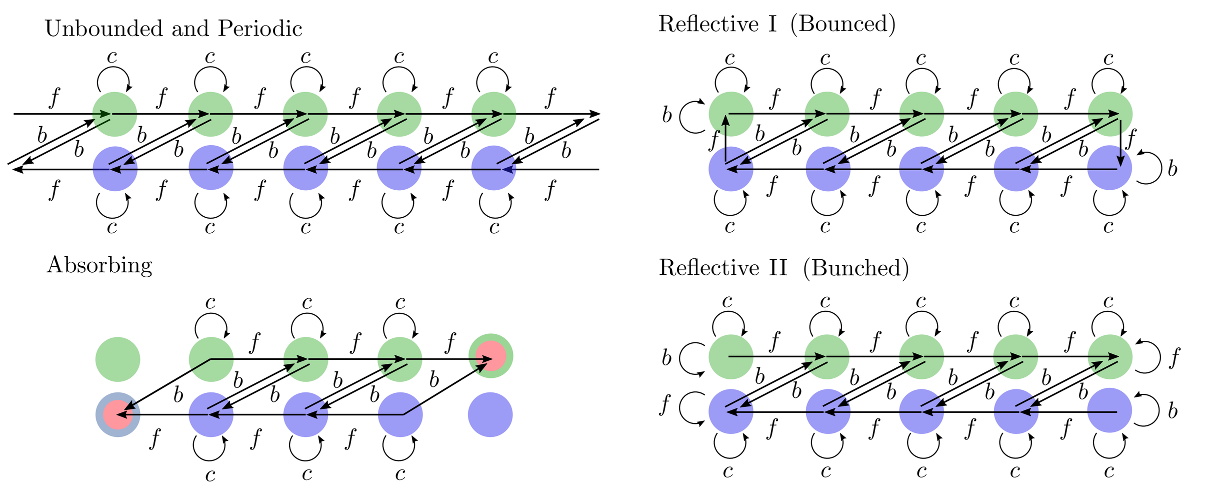
D.M., S. Sarvaharman and L. Giuggioli, *Phys. Rev. E* (2023) ->

The Persistent Random Walk:

- The persistent random walk is a one-step non-Markov process.
- We encode the direction the walker entered the site as an internal state. Therefore in 1d we require two internal states, in 2d we requrie four etc.
- The coupled random variable of position and direction last travlled may be considered as Markovian.

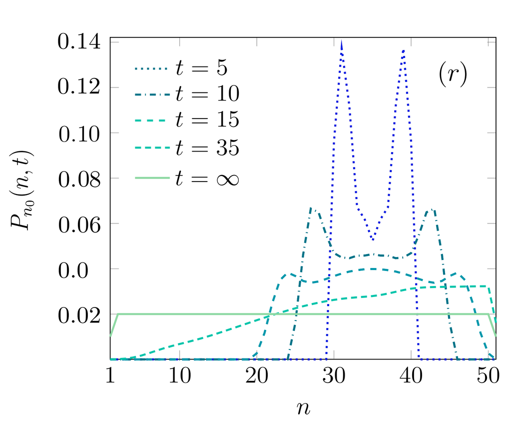
One Dimension:

The green state represents entering the site from the left and the blue state represents entering from the right.

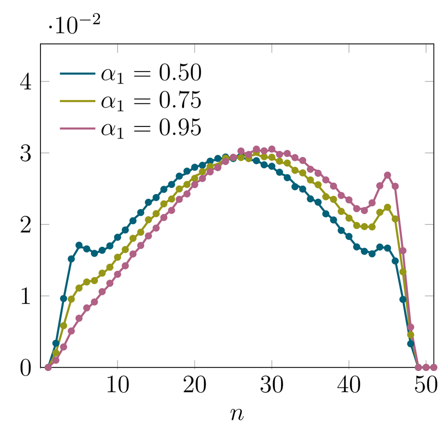


Just like the non-Bravais case, the connections are encoded **into the structure function ---> ** $\boldsymbol{\lambda}(\xi)=\begin{bmatrix}f\mathrm{e}^{i\xi}+c & b\mathrm{e}^{i\xi}\\ b\mathrm{e}^{-i\xi} & f\mathrm{e}^{-i\xi}+c\end{bmatrix}$ and pertain into **the occupation probability:**

f: persist forward
b: turn back
c: remain still



Spread starts as persistent then becomes diffusive in longer times.

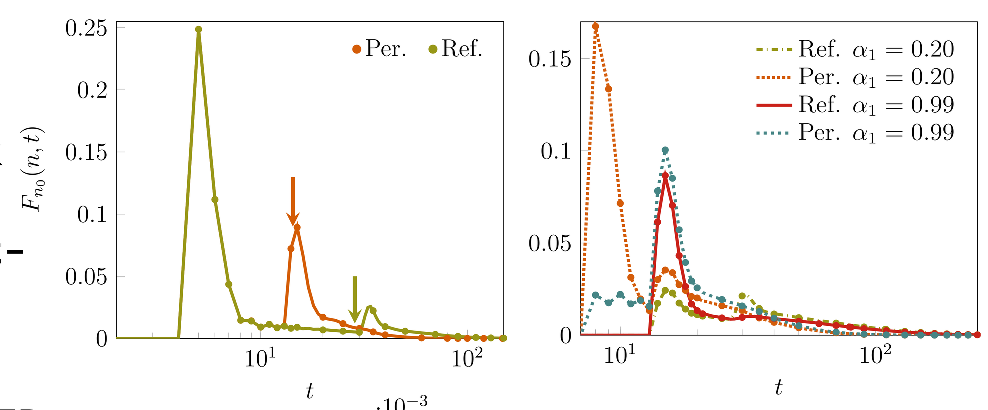


$$\mathbf{P}^{(p)}_{n_0}(n,t)=\frac{1}{N}\sum_{\kappa=0}^{N-1}\mathrm{e}^{\frac{-2\pi i\kappa(n-n_0)}{N}}\boldsymbol{\lambda}\left(\frac{2\pi\kappa}{N}\right)^t\cdot\boldsymbol{U}_{m_0}$$

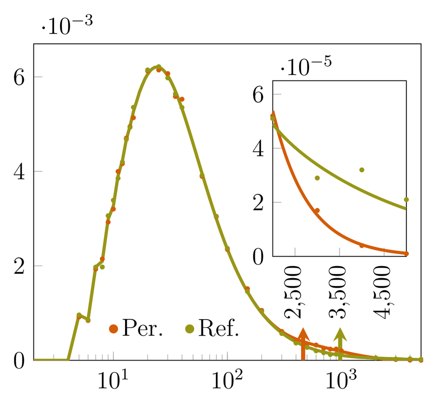
$$\mathbf{P}^{(r)}_{n_0}(n,t)=\frac{1}{2N-2}\sum_{\kappa=0}^{2N-3}\left[\mathrm{e}^{\frac{-\pi i\kappa(n-n_0)}{N}}+\mathrm{e}^{\frac{-\pi i\kappa(2N-n-n_0)}{N}}\right]\boldsymbol{\lambda}\left(\frac{\pi\kappa}{N-1}\right)^t\cdot\boldsymbol{U}_{m_0}$$

Non-uniform initial memory weighting leads to asymmetric propagation.

Knowledge of the occupation probability allows us to evaluate our general **first-passage** framework above. We show here the **effects of confinement on the first-passage distribution.**



As shown in the top two plots, the FP probability for a PRW in confinement may be **bimodal**. We plot via the arrows the **Mean First-Passage Time (MFPT)** and show that it **may fall in a region with a very low probability of a FP event occuring.**



In the bottom plot we show the anti-persistent case. Here with more **indirect trajectories, the bimodality is suppressed** and the MFPT is a more represetative quantity.

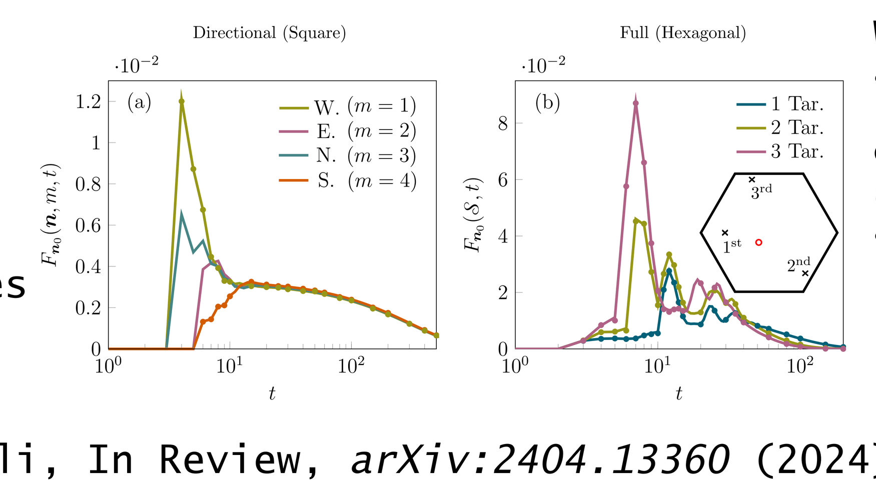
Higher Dimensions:

We have derived the propagator in arbitrary dimension for both boundary conditons ->

Argument of structure function and the spatial dependency are dependent on boundary condition

$$\mathbf{P}^{(\gamma)}_{\boldsymbol{n}_0}(\boldsymbol{n},t)=\frac{1}{N^d}\sum_{\kappa_1=0}^{N_1-1}\cdots\sum_{\kappa_d=0}^{N_d-1}\left[\prod_{i=1}^{d}g^{(\gamma)}_{\kappa_i}(n_i,n_{0_i})\right]\boldsymbol{\lambda}\left(\pi\mathcal{N}^{(\gamma)}_{\kappa_1},\ldots,\pi\mathcal{N}^{(\gamma)}_{\kappa_d}\right)^t\cdot\boldsymbol{U}_{m_0}$$

In higher dimensions we may study the directional FP. At short times, direction plays more of a role. When indirect trajectories takeover each direction is equally likely



We may have an arbitrary (finite) number of targets. Their spatial distribution affects the FP.

D.M. and L. Giuggioli, In Review, *arXiv:2404.13360* (2024) ->

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