University of BRISTOL

Correlated Random Walks on the Lattice: First-Passage Problems on Square, Hexagonal and Honeycomb Lattices with Boundaries

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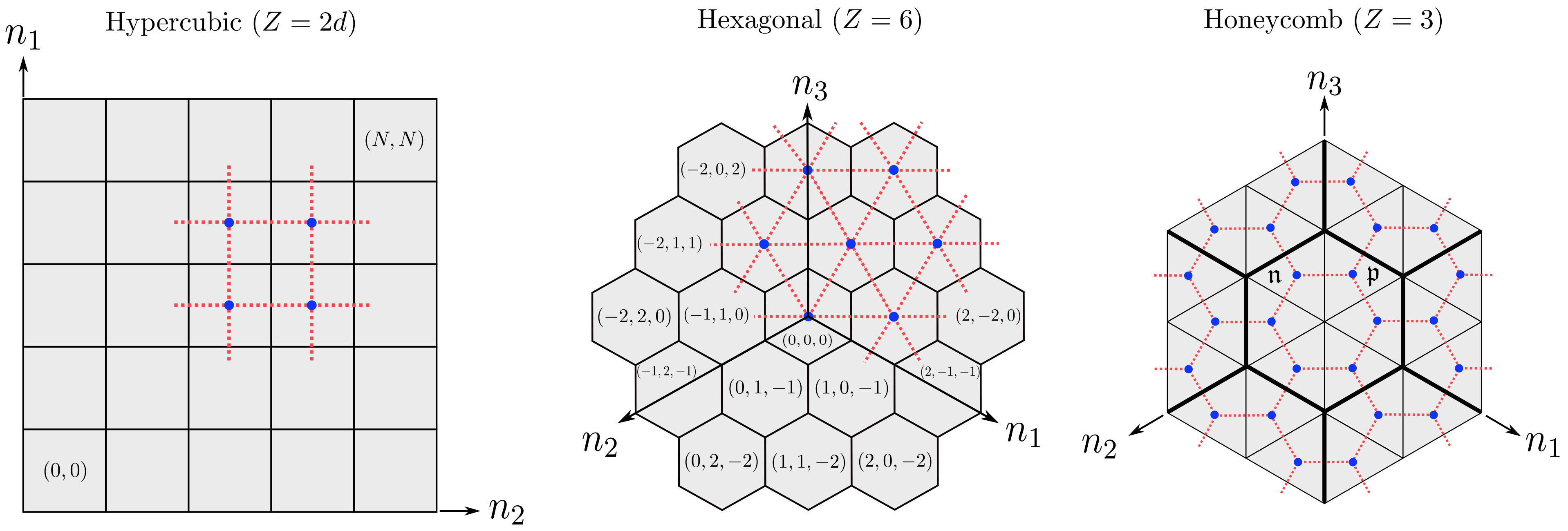
September 2024

Modelling and Applications of Anomalous Diffusions

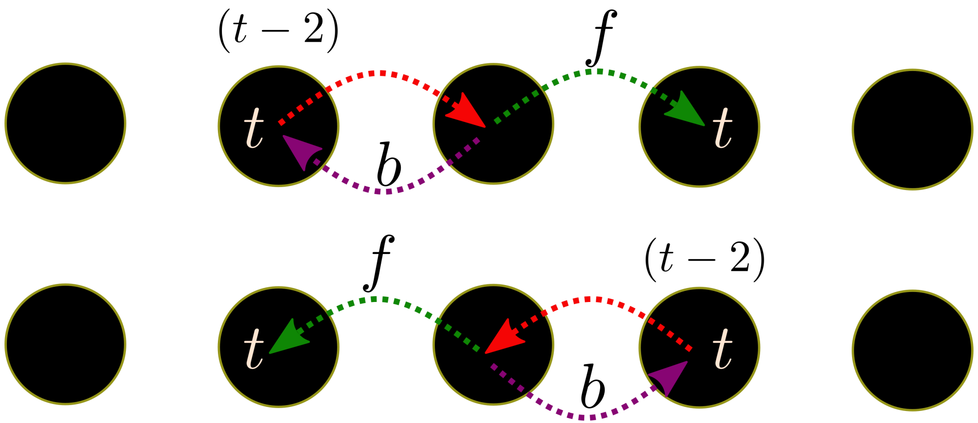
Preliminaries

The Three Lattices:



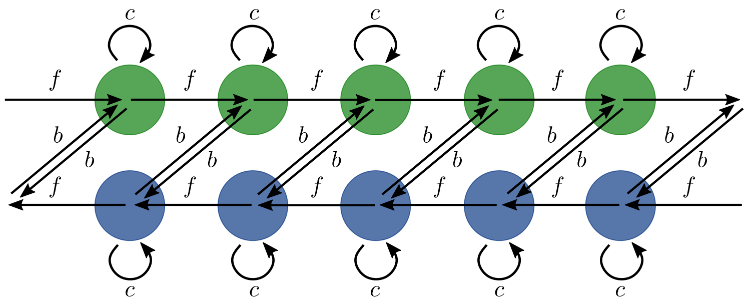
The Persistent Random Walk:

- One-step memory dependence.
- Walker is assigned a probability to *continue* in the direction last travelled.
- Outgoing probability from a site depends on how the walker entered the site.



The Mapping to a Higher Order Markov Chain:

A Note on Notation: $\mathcal{Q}_{n_0}(n,t) = \left[\mathcal{Q}_{n_0}(n,1,t), \mathcal{Q}_{n_0}(n,2,t)\right]^T, \ \mathcal{Q}_{n_0}(n,t) = \mathcal{Q}_{n_0}(n,1,t) + \mathcal{Q}_{n_0}(n,2,t) = \sum_i \boldsymbol{\mathcal{Q}}_{n_0}(n,z)_i.$



$\mathcal{Q}_{n_0}(n,t)$: Occupation Probability of being at n at time t given $\mathcal{Q}(n,0) = \delta_{n,n_0}$

f : Prob. of moving in same direction as last movement.

b : Prob. of switching direction from last movement.

c : Prob. of waiting in the current state.

Master Equation (2 States):

$$\mathcal{Q}(n,1,t+1) = f\mathcal{Q}(n-1,1,t) + b\mathcal{Q}(n-1,2,t) + c\mathcal{Q}(n,1,t)$$

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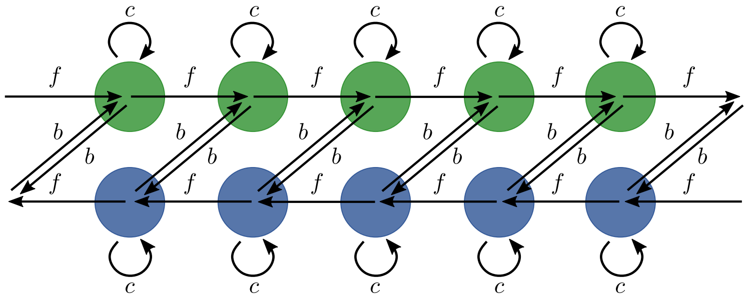

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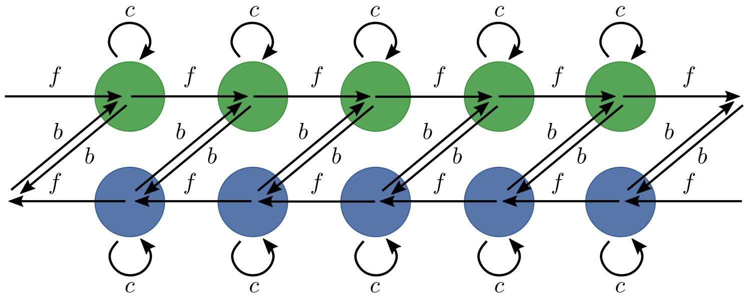

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$$\Downarrow\Downarrow\Downarrow$$

$$\boldsymbol{\mathcal{Q}}(n,t+1) = \mathbb{A}\cdot\boldsymbol{\mathcal{Q}}(n-1,t) + \mathbb{B}\cdot\boldsymbol{\mathcal{Q}}(n+1,t) + \mathbb{C}\cdot\boldsymbol{\mathcal{Q}}(n,t)$$

$$\mathbb{A} = \begin{bmatrix} f & b \\ 0 & 0 \end{bmatrix}, \qquad \mathbb{B} = \begin{bmatrix} 0 & 0 \\ b & f \end{bmatrix}, \qquad \mathbb{C} = \begin{bmatrix} c & 0 \\ 0 & c \end{bmatrix}.$$

Closed-Form Expressions for the Bounded Occupation Probability

Unbounded Solution:

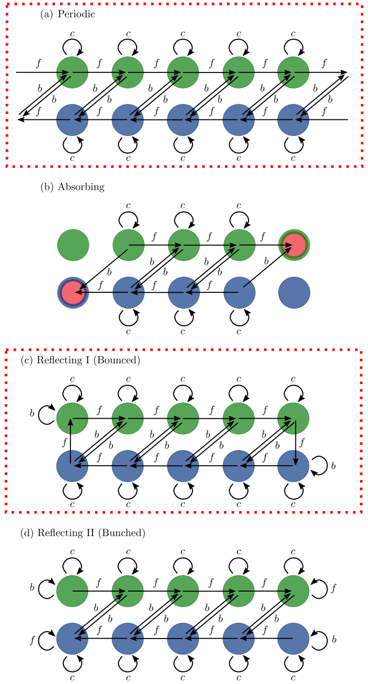
$$\tilde{\mathcal{Q}}_{n_0}(n,z) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\mathrm{e}^{-i\xi(n-n_0)}}{1-2cf+(f^2-b^2+c^2)z^2-2zf(1-cz)} \begin{bmatrix} 1-z(f\mathrm{e}^{i\xi}+c) & -zb\mathrm{e}^{i\xi} \\ -zb\mathrm{e}^{-i\xi} & 1-z(f\mathrm{e}^{-i\xi}+c) \end{bmatrix} \cdot \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \mathrm{d}\xi, \qquad \text{where} \qquad \tilde{Q}_{n_0}(n,z) = \sum_i \mathcal{Q}_{n_0}(n,z)_i.$$

$$\tilde{Q}_{n_0}(n,z) = \frac{1}{(1-2zc)\sqrt{(1+\delta z^2)^2 - 4\varepsilon^2 z^2}} \left(\frac{(1-zc)}{r_+(z)^{|n-n_0|}} + \frac{\alpha_1(b-f)}{r_+(z)^{|n-n_0+1|}} + \frac{\alpha_2(b-f)}{r_+(z)^{|n-n_0-1|}} \right),$$

$$r_+(z) = \frac{1+\delta z^2}{2z\varepsilon}\left(1+\sqrt{1-\frac{4z^2\varepsilon^2}{1+\delta z^2}}\right), \qquad \delta = \frac{f^2-b^2+c^2}{1-2cz}, \qquad \varepsilon = \frac{f(1-cz)}{1-2cz}.$$

$f > b \implies$ Persistence, $f < b \implies$ Anti-Persistence, and $f = b \implies$ Diffusion.

Bounded One Dimensional Domains:



Impose Periodic Boundaries via the Method of Images:

$$\boldsymbol{P}^{(p)}_{n_0}(n,t) = \sum_{\kappa=-\infty}^{\infty} \boldsymbol{Q}_{n_0+N\kappa}(n,t)$$

$$\boldsymbol{P}^{(p)}_{n_0}(n,t) = \frac{1}{N}\int_{-\pi}^{\pi} \sum_{\kappa_1=-\infty}^{\infty} \mathrm{e}^{-i\kappa(n-n_0)}\delta\left(\xi - \frac{2\pi}{N}\kappa\right)\boldsymbol{\lambda}(\boldsymbol{\xi})^t \cdot \boldsymbol{\mathcal{U}}_{\boldsymbol{m_0}}\mathrm{d}\xi$$

B. Hughes. *Random Walks and Random Environments Vol 1.* (1995).

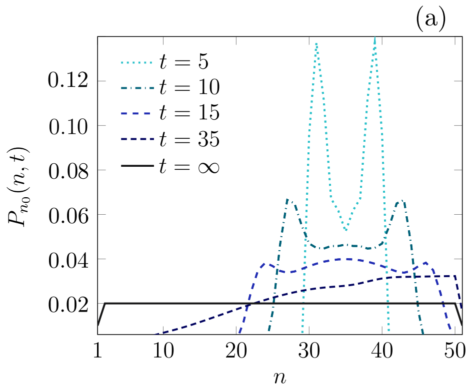
Impose Reflective Boundaries via *Squeezing* Method:

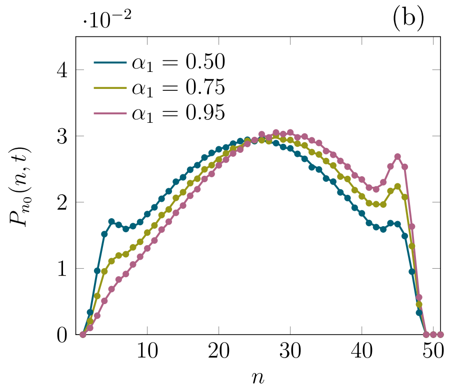
$$\boldsymbol{P}^{(r)}_{n_0}(n,t) = \boldsymbol{P}^{(p)}_{n_0}(n,t) + \mu(n)\boldsymbol{P}^{(p)}_{n_0}(M+2-n,t)$$

K. Kalay. Effects of confinement on the statistics of encounter times: exact analytical results for random walks in a partitioned lattice. *J. Phys. A: Math. Theor.*, 45(21), (2012).

S. Chandrasekhar Stochastic problems in physics and astronomy. *Rev. Mod. Phys.*, 15(1), (1943).

Occupation Probability with Reflection:





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

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

Higher Dimensional Propagators:

$$\boldsymbol{\mathcal{Q}}(\boldsymbol{n}, t+1) = \sum_{i=1}^{d} \mathbb{A}_{2d}^{(i)} \cdot \boldsymbol{\mathcal{Q}}(\boldsymbol{n}-\boldsymbol{e}_i, t) + \mathbb{B}_{2d}^{(i)} \cdot \boldsymbol{\mathcal{Q}}(\boldsymbol{n}+\boldsymbol{e}_i, t)\} + \mathbb{C}_{2d} \cdot \boldsymbol{\mathcal{Q}}(\boldsymbol{n}, t)$$

$$\Downarrow\Downarrow\Downarrow$$

$$\boldsymbol{P}_{\boldsymbol{n_0}}^{(\gamma)}(\boldsymbol{n}, t) = \frac{1}{N^d} \sum_{\kappa_1=0}^{N_1-1} \cdots \sum_{\kappa_d=0}^{N_d-1} \left[\prod_{i=1}^{d} g_{\kappa_i}^{(\gamma)}\left(n_i, n_{0_i}\right) \right] \boldsymbol{\lambda}\left(\pi \mathcal{N}_1^{(\gamma)}, \ldots, \pi \mathcal{N}_{2d}^{(\gamma)}\right)^t \cdot \boldsymbol{\mathcal{U}}_{\boldsymbol{m_0}}$$

$g_{\kappa_i}^{(\gamma)}\left(n_i, n_{0_i}\right)$ known in L. Giuggioli *Phys. Rev. X* (2020)

Higher Dimensional Propagators:

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What does $\boldsymbol{\lambda}\left(\pi\mathcal{N}_1^{(\gamma_1)}, ..., \pi\mathcal{N}_d^{(\gamma_d)}\right)$ look like?

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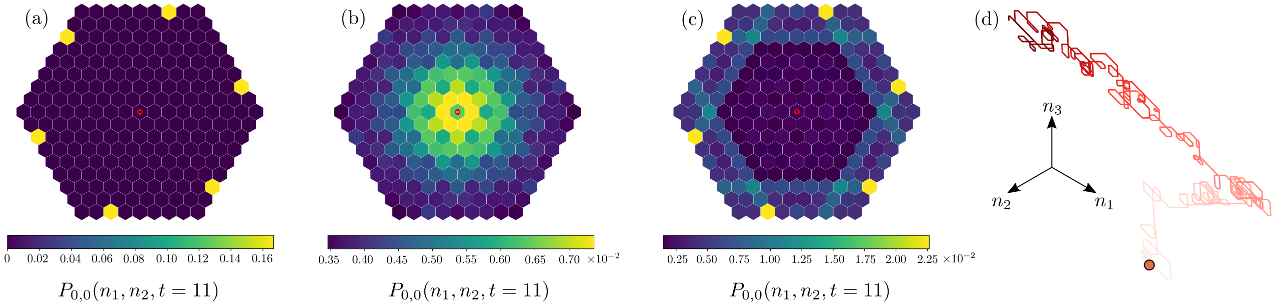
- For Bravais lattices it is of size $Z \times Z$
- Diagonal elements represent remaining in the previous state,
- Alternating off-diagonals represent back-tracking,
- Other elements in row represent sideways movement.

Correlation in the Hexagonal Lattice:



Ballistic

Slightly Persistent

Chiral

$$\boldsymbol{P}_{\boldsymbol{n}_0}^{(\mathcal{H})}(n_1,n_2,t) = \left\{ \frac{\boldsymbol{\lambda}^{(\mathcal{H})}(0,0)^t}{\Omega} + \frac{1}{\Omega}\sum_{r=0}^{R-1}\sum_{w=0}^{3r+2} \mathrm{e}^{\frac{2\pi i \boldsymbol{\kappa}\cdot(\boldsymbol{n}-\boldsymbol{n}_0)}{\Omega}} \boldsymbol{\lambda}^{(\mathcal{H})}\left(\frac{2\pi\kappa_1}{\Omega},\frac{2\pi\kappa_2}{\Omega}\right)^t + \mathrm{e}^{\frac{-2\pi i\boldsymbol{\kappa}\cdot(\boldsymbol{n}-\boldsymbol{n}_0)}{\Omega}}\boldsymbol{\lambda}^{(\mathcal{H})}\left(\frac{-2\pi\kappa_1^{[i]}}{\Omega},\frac{-2\pi\kappa_2}{\Omega}\right)^t\right\}\cdot\boldsymbol{\mathcal{U}}_{\boldsymbol{m}_0},$$

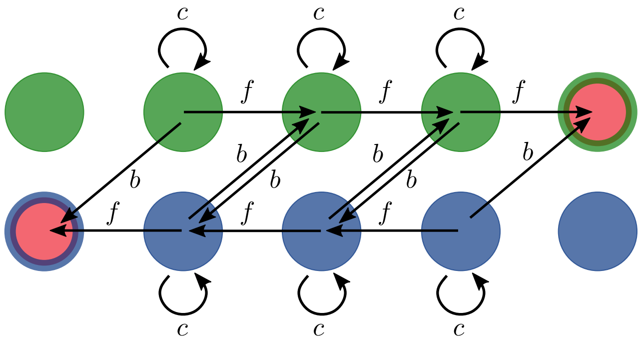
$\boldsymbol{\kappa} = [\kappa_1(r,w), \kappa_2(r,w)],\ \kappa_1(r,w) = R(w+1) + w - r,\ \kappa_2(r,w) = R(2 - w + 3r) + r + 1.$ (**D.M.**, S. Sarvaharman, L. Giuggioli. *Phys. Rev. E*, 2023)

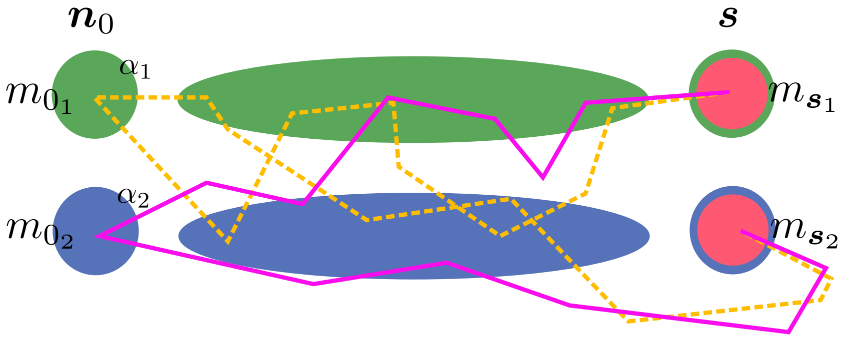
The First-Passage Probability

The First-Passage via the Defect Technique:

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

We place traps on individual *states*:





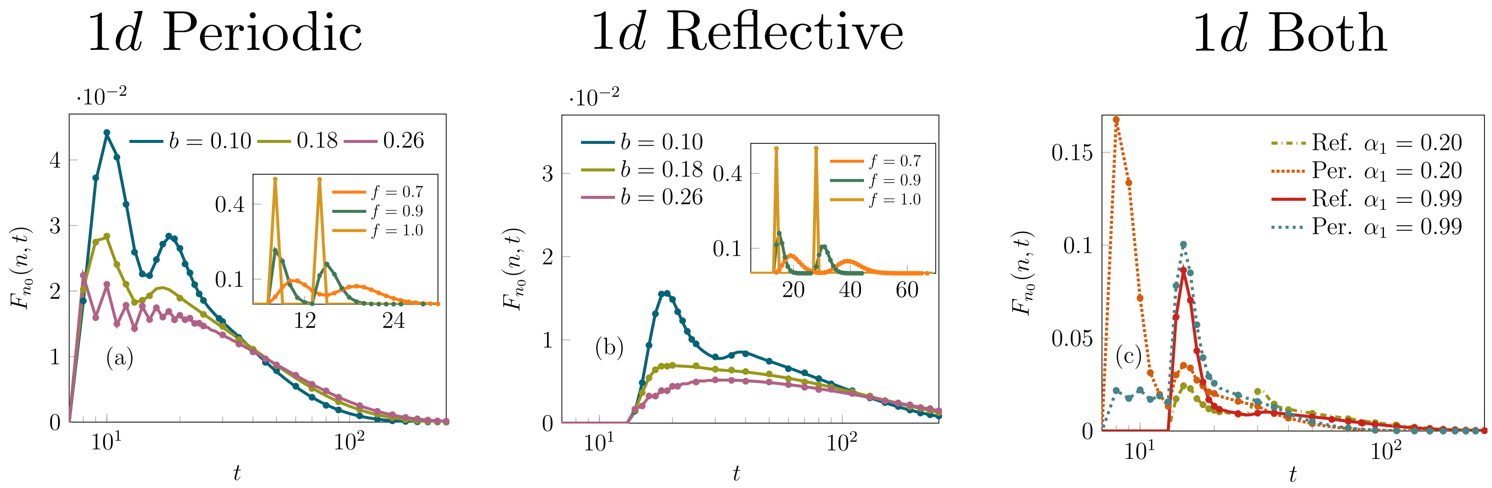
The First-Passage via the Defect Technique:

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

- $A(\boldsymbol{n},m,\boldsymbol{n}',m')P(\boldsymbol{n}',m',t)\Rightarrow$ Transitions into *defect-free* states
- $\sum_{i=1}^{S}\delta_{\boldsymbol{n},\boldsymbol{s}}\delta_{m,m_{\boldsymbol{s}_i}}\left(1-\rho_{\boldsymbol{s},m_{\boldsymbol{s}_i}}\right)A\left(\boldsymbol{s}_i,m_{\boldsymbol{s}_i},\boldsymbol{n}',m'\right)P(\boldsymbol{n}',m',t)\Rightarrow$ Transitions into *defective* states
- With initial condition: $P(\boldsymbol{n},0)=\delta_{\boldsymbol{n},\boldsymbol{n}_0}\sum_{m=1}^{M}P(\boldsymbol{n},m,0)$, where $P(\boldsymbol{n},m,0)=\delta_{m,m_0}\alpha_{m_0}\left[\left(1-\rho_{\boldsymbol{s},m_{\boldsymbol{s}_i}}\right)\delta_{(\boldsymbol{n}_0,m_0)\in\mathcal{S}}+\delta_{(\boldsymbol{n}_0,m_0)\notin\mathcal{S}}\right]$.

$$\tilde{F}_{\boldsymbol{n}_0}(\mathcal{S},z)=\sum_{m_0=1}^{M}\sum_{i=1}^{S}\alpha_{m_{s_i}}\frac{\det\left(\mathbb{H}^{(i)}(\boldsymbol{n}_0,m_0,z)\right)}{\det(\mathbb{H}(z))}\Leftarrow$$ Matrices comprised of occupation probabilities shown earlier in the talk

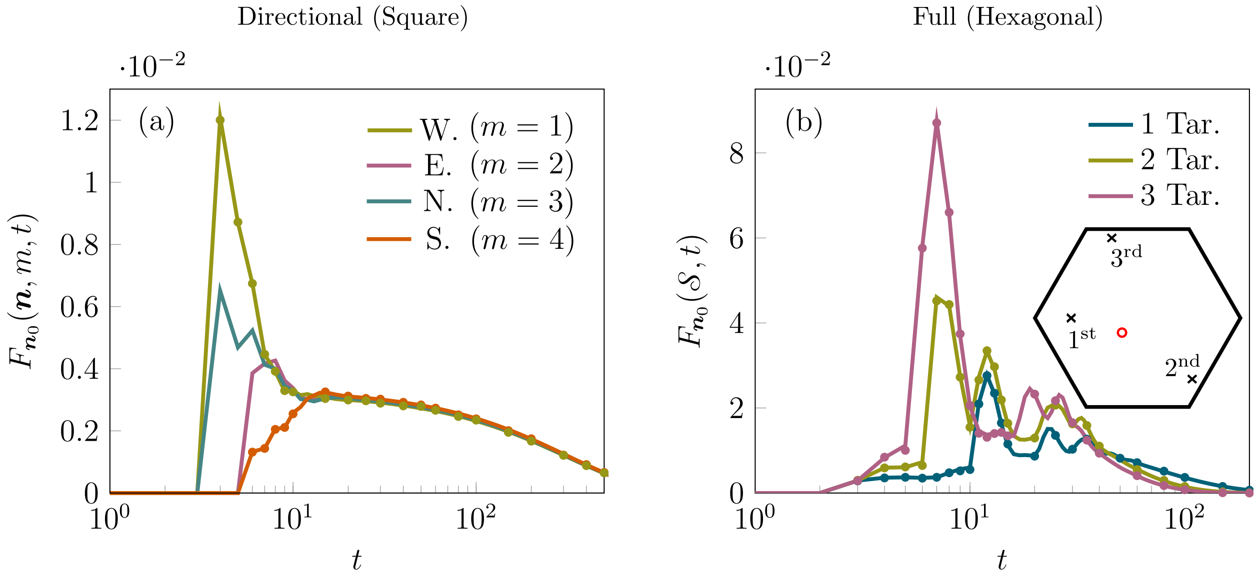
First-Passage Probabilities:



$n_0 = 8, \quad n = 22$ (Dots represent the results from stochastic simulations)

(**D.M.**, L. Giuggioli. *New J. Phys*, 2024)

First-Passage Probabilities:

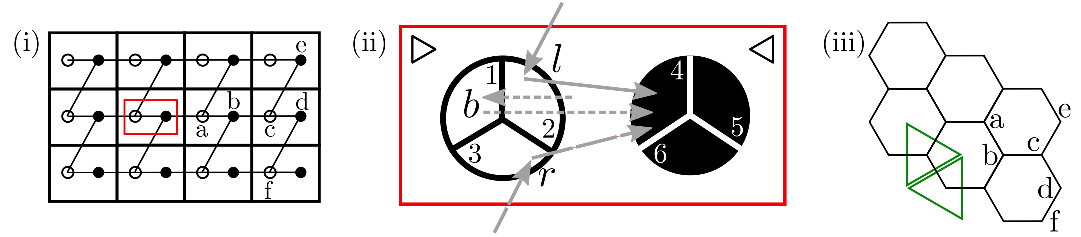


(Dots represent the results from stochastic simulations)

(**D.M.**, L. Giuggioli. *New J. Phys*, 2024)

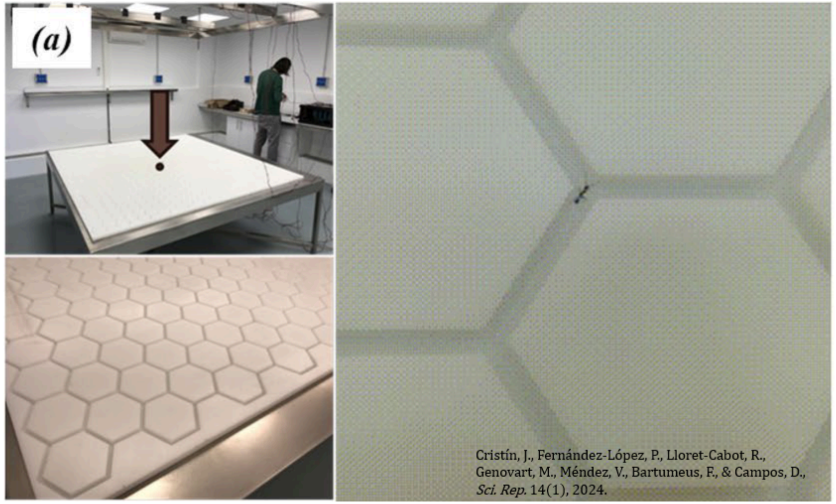
A model for Foraging Behaviour in *Aphaenogaster senilis*

Persistence over the Honeycomb Lattice:



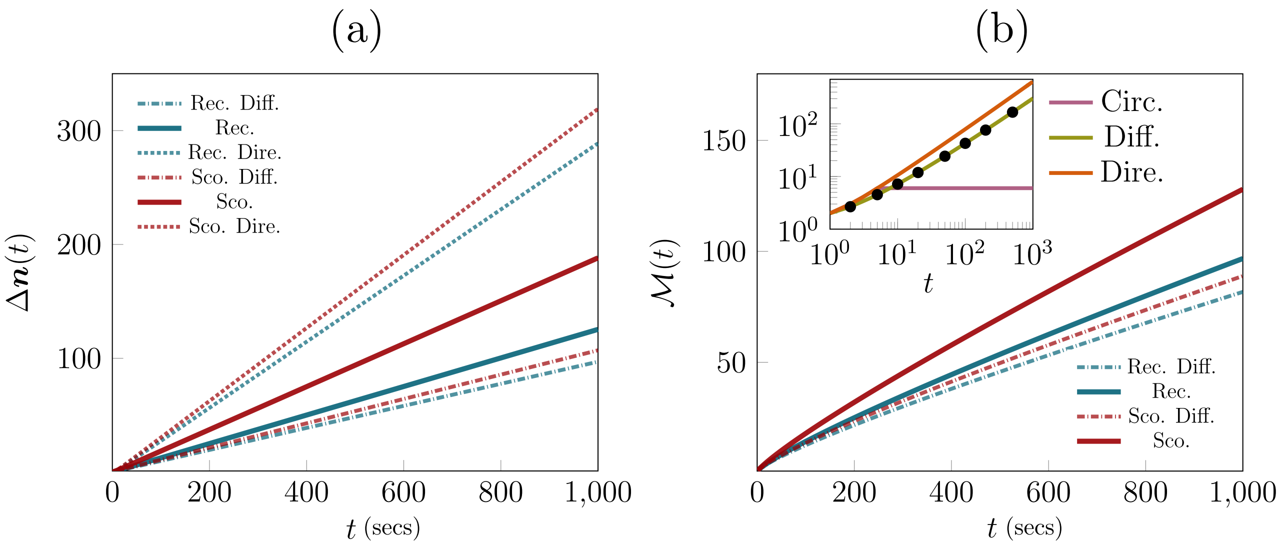
E. Montroll *J. Math. Phys*, (1969)

$$\lambda(\xi_1,\xi_2) = \begin{array}{c} \nwarrow \\ \swarrow \\ \longrightarrow \\ \searrow \\ \nearrow \\ \longleftarrow \end{array} \overset{\begin{array}{cccccc} \nwarrow & \swarrow & \longrightarrow & \searrow & \nearrow & \longleftarrow \end{array}}{\begin{bmatrix} c & 0 & 0 & b & l & r \\ 0 & c & 0 & re^{-i\xi_2} & be^{-i\xi_2} & le^{-i\xi_2} \\ 0 & 0 & c & le^{i\xi_1} & re^{i\xi_1} & be^{i\xi_1} \\ b & l & r & c & 0 & 0 \\ re^{i\xi_2} & be^{i\xi_2} & le^{i\xi_2} & 0 & c & 0 \\ le^{-i\xi_1} & re^{-i\xi_1} & be^{-i\xi_1} & 0 & 0 & c \end{bmatrix}}$$



Cristín, J., Fernández-López, P., Lloret-Cabot, R., Genovart, M., Méndez, V., Bartumeus, F., & Campos, D., *Sci. Rep.* 14(1), 2024.

Persistence over the Honeycomb Lattice:



Black dots from iterative results in G. Zumofen, and A. Blumen, A., *J. Chem. Phys.* (1982)

Thank-you

References and Acknowledgements

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