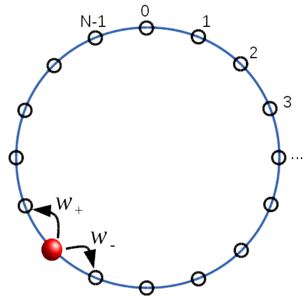
Sample Solutions Exercise 8

Exercise 8.1: Random walk on a ring (12P)

Consider a ring with N sites enumerated by $i = 0, 1, \ldots, N-1$. A particle (the red bullet) moves on the ring by jumping randomly to the neighboring sites. The random walk of the particle is biased, i.e., it hops to the right and to the left with generally different constant rates w_+ and w_- (see figure).



(a) Compute the matrix elements $\mathcal{L}_{ij}$ of the time evolution operator $\mathcal{L}$ for general N (using Kronecker-δ's). Write down the explicit matrix for $N = 4$ and check whether the columns add up to 0. (2P)

(b) Guess the stationary state $|P_{stat}\rangle = |P_\infty\rangle$ for general N guided by physical arguments. Verify your result and compute the entropy of the stationary state. (2P)

(c) Because of translational invariance the eigenvectors $|\psi^{(k)}\rangle$ of $\mathcal{L}$ can be determined for general N by means of an exponential ansatz

$$\psi_j^{(k)} = \langle j|\psi^{(k)}\rangle = e^{ikj}\,.$$

How are the values of k constrained by the periodicity of the ring and what is the allowed range of k in which all solutions are unique? (2P)

(d) Compute the corresponding eigenvalues λ_k and their real part $Re[\lambda_k]$. (2P)

(e) Determine the dominating relaxation time τ_{max}. (1P)

(f) How does the largest relaxation time scale with N if N is very large? Why is the result reasonable with respect to the central limit theorem? (2P)

(g) Under which conditions does the stationary state obey detailed balance? (1P)

Note: In all parts of the exercise, if not stated otherwise, N is assumed to be arbitrary.

Sample Solution

(a) Since we have only a single particle, the microscopic configurations of the system can be labeled by the position of the particle on the ring, i.e. $\Omega = \{1,, \ldots, N\}$. In the canonical basis the Liouville operator is given by the matrix elements

$$\mathcal{L}_{ij} = -w_+\delta_{i,j+1} - w_-\delta_{i,j-1} + (w_+ + w_-)\delta_{i,j} \qquad (*)$$

where $j \pm 1$ is understood cyclically on the ring, i.e., modulo N (this should be at least mentioned). The explicit matrix for $N = 4$ reads

$$\mathcal{L} = \begin{pmatrix} w_- + w_+ & -w_- & 0 & -w_+ \\ -w_+ & w_+ + w_- & -w_- & 0 \\ 0 & -w_+ & w_+ + w_- & -w_- \\ -w_- & 0 & -w_+ & w_+ + w_- \end{pmatrix}$$

As one can see, the sum over all columns vanishes.

(b) The dynamics is translational invariant along the ring, hence the stationary state has to be translational invariant as well. This means that all probabilities have to be equal:

$$|P_\infty\rangle = \begin{pmatrix} 1/n \\ 1/n \\ \dots \\ 1/n \end{pmatrix} .$$

In fact, one can easily check that $\mathcal{L}|P_\infty\rangle = 0$ since not only the column sum but also the row sum of $\mathcal{L}$ vanishes.
Since the stationary probability distribution is flat the entropy $H = \ln|\Omega| = \ln N$ is maximal.

(c) The exponential ansatz is like a plane wave in quantum mechanics. Obviously this wave has to be periodic on the ring, i.e.

$$\psi^{(k)}_{j+N} \equiv \psi^{(k)}_j \; ,$$

giving the condition

$$e^{ikN} = 1 \quad \Rightarrow \quad k = \frac{2\pi n}{N} \text{ with } n \in \mathbb{N} \, .$$

Since the solution $\psi^{(k)}_j = \exp\big(\frac{2\pi i n j}{N}\big)$ does not change under the replacement $n \to n + N$, the index n can be restricted to the range $0, 1, 2, \dots, N-1$.

(d) The eigenvalue problem reads

$$\mathcal{L}|\psi^{(k)}\rangle = \lambda_k|\psi^{(k)}\rangle \qquad \Rightarrow \qquad \sum_{j=0}^{N-1} \mathcal{L}_{ij}\psi^{(k)}_j = \lambda_k \psi^{(k)}_i$$

Inserting (*) this turns into

$$\sum_{j=0}^{N-1} \Big(-w_+\delta_{i,j+1} - w_-\delta_{i,j-1} + (w_+ + w_-)\delta_{i,j} \Big) \psi^{(k)}_j = \lambda_k \psi^{(k)}_i$$

Evaluating the Kronecker-δ's and renaming $i \to j$ gives

$$+(w_+ + w_-)\psi^{(k)}_j - w_+\psi^{(k)}_{j-1} - w_-\psi^{(k)}_{j+1} = \lambda_k \psi^{(k)}_j$$

Now we insert the solution of (c) and divide both sides of the equation by $\psi^{(k)}_i$:

$$\lambda_k \;=\; w_+ + w_- - w_+ \exp\big(-\frac{2\pi i n}{N}\big) - w_- \exp\big(+\frac{2\pi i n}{N}\big)$$

Therefore the eigenvalues are complex numbers. The real part of an oscillating exponential function is $Re[e^{i\phi}] = \cos\phi$. Thus the real part of the eigenvalue is given by

$$Re[\lambda_k] \;=\; (w_+ + w_-)\Big(1 - \cos\big(\frac{2\pi n}{N}\big)\Big)$$

Remark: Complex eigenvalues are okay in stochastic processes as long as they occur in complex-conjugate pairs.

(e) The largest relaxation time is the reciprocal of the smallest real part of the eigenvalues of $\mathcal{L}$. Since the cosine in the above formula varies from 1 (for $n = 0$) to -1 (for $n = N/2$) and then back to 1, the eigenvalues with the smallest real part are those for $n = 1$ and $n = N - 1$ (the corresponding eigenvalues form a complex conjugate pair). Hence the largest relaxation time is

$$\tau_{max} = \frac{1}{(w_+ + w_-)\big(1 - \cos(\frac{2\pi}{N})\big)} \, .$$

(f) Using $\cos x \approx 1 - \frac{1}{2}x^2 + \mathcal{O}(x^4)$ we expand τ to lowest order, obtaining

$$\tau_{max} \approx \frac{1}{(w_+ + w_-)\frac{2\pi^2}{N^2} + \mathcal{O}(N^{-4})} \, ,$$

meaning that τ_{max} scales as N^2. Regarding the CLT, which for a random walk starting at a given site predicts a variance growing as $\sigma^2 \sim t$, we expect the system to become stationary (equally distributed) when σ becomes of the order of the system size N. Therefore it is reasonable that $\tau \sim N^2$.

(g) The stationary state is uniform, meaning that all probabilities equal $1/N$, we have

$$J_{i \to i+1} - J_{i+1 \to i} = (w_+ - w_-)\frac{1}{N}.$$

Detailed balance means that the probability currents cancel pairwise, hence detailed balance holds if and only if the rates are symmetric, i.e. $w_+ = w_-$.

(Σ = 12P)