

## A modified TASEP model for molecular motors

One considers a  $1D$  lattice of  $N$  sites. Each site is characterized by an occupation number  $n_i$  which is equal to 0 (empty) or 1 (occupied by one particle). Particles can jump on the right neighboring site if the site is empty, otherwise the particle does not move. In addition, the bulk sites are in contact to particle reservoirs, namely, particles can adsorb with a rate  $\omega_A$  and desorb with a rate  $\omega_D$ . At the boundaries, the situation is slightly different : on the site 1, the adsorption rate is  $\alpha$  and on the site  $N$ , the desorption rate is  $\beta$ . ( $0 < \alpha < 1$  and  $0 < \beta < 1$ )

1. Denoting the mean particle density  $\langle n_i \rangle$  on the site  $i$ , show that

$$\frac{d\langle n_i \rangle}{dt} = \langle n_{i-1}(1 - n_i) \rangle - \langle n_i(1 - n_{i+1}) \rangle + \omega_A \langle (1 - n_i) \rangle - \omega_D \langle n_i \rangle \quad (1)$$

for  $i \in [2, N - 1]$ .

**Solution:** The time derivative of the mean occupation number of the site  $i$  has four contributions

- hopping of a particle from site  $i - 1$  to  $i$   $\langle n_{i-1}n_i \rangle$  (gain term)
- hopping of a particle from site  $i$  to  $i + 1$   $\langle n_i n_{i+1} \rangle$  (loss term)
- adsorption on the site  $i$  if the site is empty  $\omega_A \langle (1 - n_i) \rangle$  (gain term)
- desorption of the site  $i$  if the site is occupied  $\omega_D \langle n_i \rangle$  (loss term)

2. Write the two kinetic equations for the boundaries,  $i = 1$  and  $i = N$ .

**Solution:** Boundary terms

- For the site 1, one has two terms : a gain term coming from the insertion of a particle and a loss term due to a hop of a particle from site 1 to site 2.

$$\frac{d\langle n_1 \rangle}{dt} = -\langle n_1(1 - n_2) \rangle + \alpha \langle (1 - n_1) \rangle \quad (2)$$

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- For the site  $N$ , one has two terms : a loss term coming from the exit of a particle and a gain term due to a hop of a particle from site  $N - 1$  to site  $N$ .

$$\frac{d\langle n_N \rangle}{dt} = \langle n_{N-1}(1 - n_N) \rangle - \beta \langle n_N \rangle \quad (3)$$

3. In order to simulate, this system, one proposes the following algorithm (for the bulk of the system) : One chooses randomly and uniformly a site  $i_0$

- if the site  $i_0$  is occupied, one chooses a uniform random number  $\eta$  between 0 and 1. If  $\eta < P_1$ , the particle is removed, else if the right neighboring site is empty, the particle is moved otherwise it stays here.
- if the site  $i_0$  is empty, one chooses a uniform random number  $\eta$  between 0 and 1. If  $\eta < P_2$ , a particle is adsorbed on the site  $i_0$ , else if the left neighboring site is occupied, the particle is moved otherwise nothing happens.

Give the values of  $P_1$  and  $P_2$  as a function of  $\omega_A$  and  $\omega_D$ .

**Solution:**

- If the site is occupied, we have two possible events, hopping and desorption with respective rates 1 and  $\omega_D$ . Therefore

$$P_1 = \frac{\omega_D}{1 + \omega_D}$$

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- If the site is empty, we have two possible events, hopping and adsorption with respective rates 1 and  $\omega_A$ . Therefore

$$P_2 = \frac{\omega_A}{1 + \omega_A}$$

4. Modify the previous algorithm to include the two boundary conditions.

**Solution:** By choosing at random the site  $i$ , the previous algorithm is modified for site 1 and  $N$  where

- For the site 1. If empty, one chooses a random number  $\eta$  between 0 and 1. if  $\eta < \alpha$  a site is inserted if not no insertion. If occupied, the particle hops on the left if the site is empty.
- For the site  $N$ . If empty and the site  $N - 1$  is occupied, the particle hops on  $N$ . If the site is occupied, one chooses a random number  $\eta$  between 0 and 1. if  $\eta < \beta$  the particle exits the lattice

5. To obtain an approximate treatment of this model, one performs a mean-field approximation ( $\langle n_i n_{i+1} \rangle = \langle n_i \rangle \langle n_{i+1} \rangle$ ). Moreover, one considers the large  $N$  limit ( $\Omega_A = N\omega_A$  and  $\Omega_D = N\omega_D$  are constants) to have a continuous description of the model. One sets  $\langle n_i \rangle = \rho(x, t)$  where  $x = i/N$ . Keeping the leading order terms in  $1/N$ ,

$$\langle n_{i\pm 1} \rangle = \rho(x, t) \pm \frac{1}{N} \frac{\partial \rho(x, t)}{\partial x} \quad (4)$$

Show that the bulk kinetic equation obeys

$$\frac{\partial \rho(x, \tau)}{\partial \tau} = A(\rho) \frac{\partial \rho(x, \tau)}{\partial x} + (C - D\rho) \quad (5)$$

where  $\tau = t/N$ ,  $A(\rho)$  is a function of  $\rho$  and  $C$  and  $D$  two constants to be determined.

**Solution:** Expanding the discrete equations at first order gives

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$$\frac{d\langle n_i \rangle}{dt} \rightarrow \frac{\partial \rho(x, t)}{\partial t}$$

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$$\langle (n_i(1 - n_{i+1})) \rangle \rightarrow \rho(x, t)(1 - \rho(x, t) + \frac{1}{N} \frac{\partial \rho}{\partial x})$$

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$$\langle (n_{i-1}(1 - n_i)) \rangle \rightarrow (\rho(x, t) - \frac{1}{N} \frac{\partial \rho}{\partial x})(1 - \rho(x, t))$$

—

$$\omega_A \langle 1 - n_i \rangle \rightarrow \omega_A(1 - \rho(x, t))$$

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$$\omega_D \langle n_i \rangle \rightarrow \omega_D \rho(x, t)$$

Combining all terms give

$$\frac{\partial \rho}{\partial t} = \frac{1}{N} \frac{\partial \rho}{\partial x} (2\rho - 1) + \omega_A - (\omega_A + \omega_D) \rho(x, t) \quad (6)$$

By using the change of variable  $\tau = \frac{t}{N}$ , one obtains Eq. with  $C = \Omega_A$  and  $D = \Omega_A + \Omega_D$ .

6. One considers the case where  $\Omega_D = \Omega_A = \Omega$ . Show that the steady-state of mean-field kinetic equation is given by

$$(2\rho - 1) \left( \frac{\partial \rho}{\partial x} - \Omega \right) = 0 \quad (7)$$

**Solution:** By using that the time derivative cancels and that  $\Omega_D = \Omega_A = \Omega$  one obtains Eq.7

7. Determine two simple solutions of Eq.(7).

**Solution:**

- First solution  $\rho = 1/2$
- second solution  $\rho = \Omega x + \rho_0$ .

In the following, we restrict the study to the region of the phase space where  $\alpha < 1/2$  and  $\beta < 1/2$ .

8. At the boundaries, the densities are given by  $\rho(0) = \alpha$  and  $\rho(1) = 1 - \beta$ . Show there exists a value  $\Omega_c$ , for which a continuous solution for  $\rho(x)$  is possible.

**Solution:**

- On the left, one has  $\rho = \alpha + \Omega x$  (because  $\rho(0) = \alpha$ )
- On the right, one has  $1 - \beta = \alpha + \Omega$  which gives

$$\Omega_C = 1 - \alpha - \beta$$

9. In general, one expects a shock formation in the system. Moreover, in order to observe a shock in a stationary state, it is necessary that the shock velocity vanishes, namely the mass currents through the shock must be equal. Denoting  $\rho_l(x_s)$  the local density on the left of the shock and  $\rho_r(x_s)$  the local density on the right (where  $x_s$  is the position of the shock), show that the mass current conservation gives

$$(\rho_l(x_s) - \rho_r(x_s))(1 - \rho_l(x_s) - \rho_r(x_s)) = 0 \quad (8)$$

**Solution:** The flux on the left is given by  $\rho_l(1 - \rho_l)$  and on the right  $\rho_r(1 - \rho_r)$ . Equating the two terms gives Eq.8

10. By using Eq.(8), show that the shock position is given

$$x_s = \frac{1}{2} + \frac{\beta - \alpha}{2\Omega} \quad (9)$$

**Solution:**

- On the left, one has  $\rho = \alpha + \Omega x$  (because  $\rho(0) = \alpha$ )
- On the right, one has  $= 1 - \beta + \Omega(x - 1)$  (because  $\rho(1) = 1 - \beta$ )

At the shock location  $\rho_l = 1 - \rho_r$  which gives

$$x_s = \frac{1}{1} + \frac{\beta - \alpha}{2\Omega} \quad (10)$$

11. Show that the discontinuity of the density at the shock,  $\Delta = \rho_r(x_s) - \rho_l(x_s)$ , is given by

$$\Delta = \Omega_c - \Omega \quad (11)$$

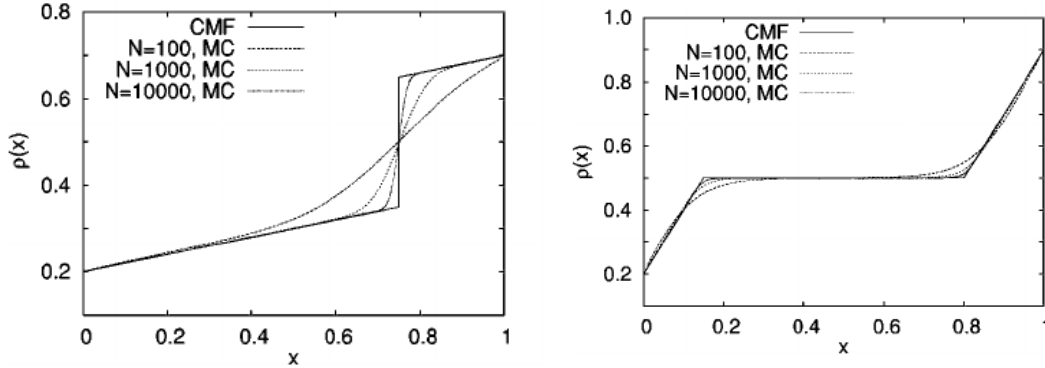


FIGURE 1 – Simulation results and mean-field predictions :  $\alpha = 0.2, \beta = 0.1$  (left)  $\Omega = 0.1$  (right)  $\Omega = 2$

**Solution:** The discontinuity is

$$\Delta = \rho_R - \rho_L = \Omega_C - \Omega \quad (12)$$

12. Fig.(1) shows that for  $\Omega > \Omega_c$ , there is no shock, but the density profile is a continuous piece wise function where the central region has a density equal to  $1/2$ . Determine the positions  $x_l$  and  $x_r$  as function of  $\alpha, \beta$  and  $\Omega$  corresponding to the bounds of the interval where the density is constant.

**Solution:** Following the simulation results, one has  $\rho_L = \alpha + \Omega x$  and  $\rho_L = 1/2$ , which gives

$$x_L = \left(\frac{1}{2} - \alpha\right) \frac{1}{\Omega}$$

Similarly, on the right, one obtains

$$x_R = 1 - \left(\frac{1}{2} - \beta\right) \frac{1}{\Omega}$$

13. What happens when  $\Omega = \Omega_c$  ? .

**Solution:** When  $\Omega = \Omega_c$ ,  $x_L = x_R$ , one recovers the continuous solution

14. In Fig.(1), mean-field prediction seems in a very good agreement with simulation results. Is it always the case for a phase transition? Justify your answer by giving some

examples.

**Solution:** Generally, the mean-field approximation overestimates the critical temperature for systems at equilibrium (For instance Ising model on a square lattice  $T_{mf} = 4J$  and  $T_{ex} = 2.26..$ , on a cubic lattice  $T_{mf} = 6$  and  $T_{ex} = 4.51$ ). For this model, the mean-field is based on the mass conservation which explains that the critical phenomenon is not overestimated