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 ω_A and desorb with a rate ω_D. At the boundaries, the situation is slightly different : on the site 1, the adsorption rate is α and on the site N, the desorption rate is β. ($0 < \alpha < 1$ and $0 < \beta < 1$)

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

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

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

2. Write the two kinetic equations for the boundaries, $i = 1$ and $i = N$.
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 η 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 η between 0 and 1. If $\eta < P2$, 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 ω_A and ω_D.
4. Modify the previous algorithm to include the two boundary conditions.
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 $1/N$,

$$\langle n_{i\pm1} \rangle = \rho(x, t) \pm \frac{1}{N} \frac{\partial \rho(x, t)}{\partial x} \tag{2}$$

   Show that the bulk kinetic equation obeys

$$\frac{\partial \rho(x, \tau)}{\partial \tau} = A(\rho) \frac{\partial \rho(x, \tau)}{\partial x} + (C - D\rho) \tag{3}$$

   where $\tau = t/N$, $A(\rho)$ is a function of ρ and C and D two constants to be determined.
6. One considers the case where $\Omega_D = \Omega_A = \Omega$. Show that the steady-state of mean-field kinetic equation is given by

$$(2\rho - 1) \left(\frac{\partial \rho}{\partial x} - \Omega \right) = 0 \tag{4}$$

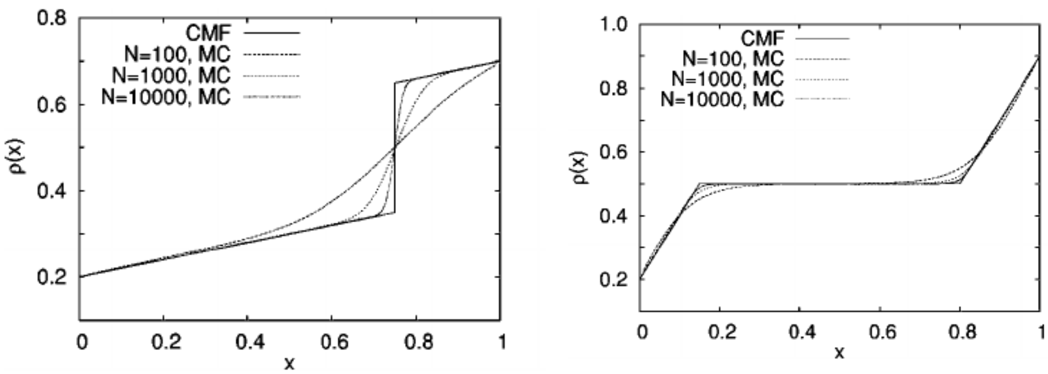

FIGURE 1 – Simulation results and mean-field predictions : $\alpha = 0.2$, $\beta = 0.1$ (left) $\Omega = 0.1$ (right) $\Omega = 2$

7. Determine two simple solutions of Eq.(4).

   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 exits a value Ω_c, for which a continuous solution for $\rho(x)$ is possible.
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

$$(\rho_l(x_s) - \rho_r(x_s))(1 - \rho_l(x_s) - \rho_r(x_s)) = 0 \tag{5}$$

10. By using Eq.(5), show that the shock position is given

$$x_s = \frac{1}{2} + \frac{\beta - \alpha}{2\Omega} \tag{6}$$

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

$$\Delta = \Omega_c - \Omega \tag{7}$$

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 α, β and Ω corresponding to the bounds of the interval where the density is constant.
13. What happens when $\Omega = \Omega_c$?.

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.