APPC15

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# Multi species asymmetric simple exclusion process with impurity activated flips

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[Reference: *arXiv:2205.03082* (2022)]

# NON-EQUILIBRIUM SYSTEMS

"*net flow or current*"
of matter, energy etc.

"Transport phenomena"

- *vehicular traffic, pedestrian traffic*
- *intracellular protein transport*

"Phase transitions" in driven systems

- *jamming transition in traffic flow*
- *phase separation in active matter*
- *absorbing phase transition*

**Question:** How to analyze such qualitative features through analytical results **?**
Focus: non-equilibrium *steady state*

Equilibrium statitical mechanics

⇓

*starting point:* Hamiltonian *"H"*

⇓

*Key factor:* Probability distribution known $P(C) \propto e^{-\beta H(C)}$

*:Gibbs-Boltzmann distribution*

⇓

calculate average, fluctuation etc. observables

***In sharp contrast:***

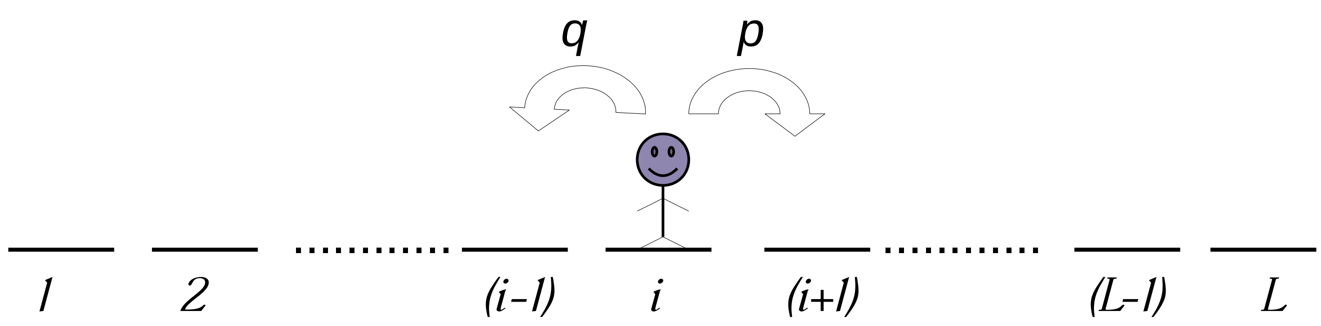
NON-EQUILIBRIUM statitical mechanics

⇓

no such generic form of probability distribution is known

**Question:** How to find steady state probability distribution for non-equilibrium systems ?

# A simple NON-EQUILIBRIUM system: a random walker on a 1-d periodic lattice




STEADY STATE: $L$ configurations: all equally likely $P(C) = \frac{1}{L}$

Broken detailed balance, current proportional to $(p-q)$

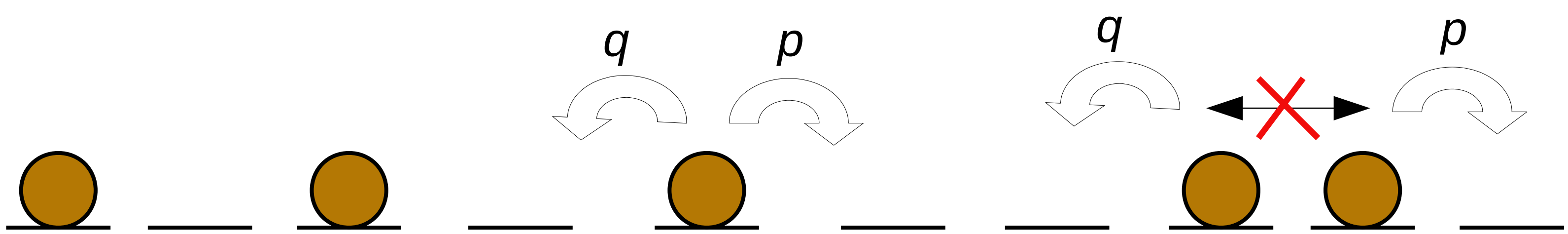
GENERALIZATION: **many interacting random walkers**

MODEL: **asymmetric simple exclusion process (ASEP)**

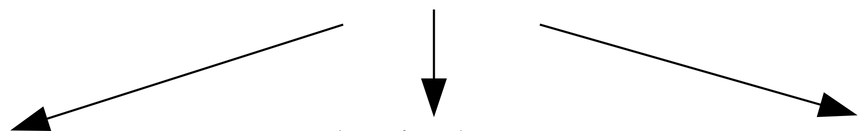
*(paradigmatic model for driven non-equilibrium systems in 1-d)*

# Asymmetric Simple Exclusion Process (ASEP)

many particle system with "*hardcore exclusion*" interaction




Importance:



*mathematical:*

**exactly solvable model**

*physical:*

**phase transitions in one-dimension with local dynamics**

*applications:*

**toy model for:**
**traffic flow**
**motor protein transport**

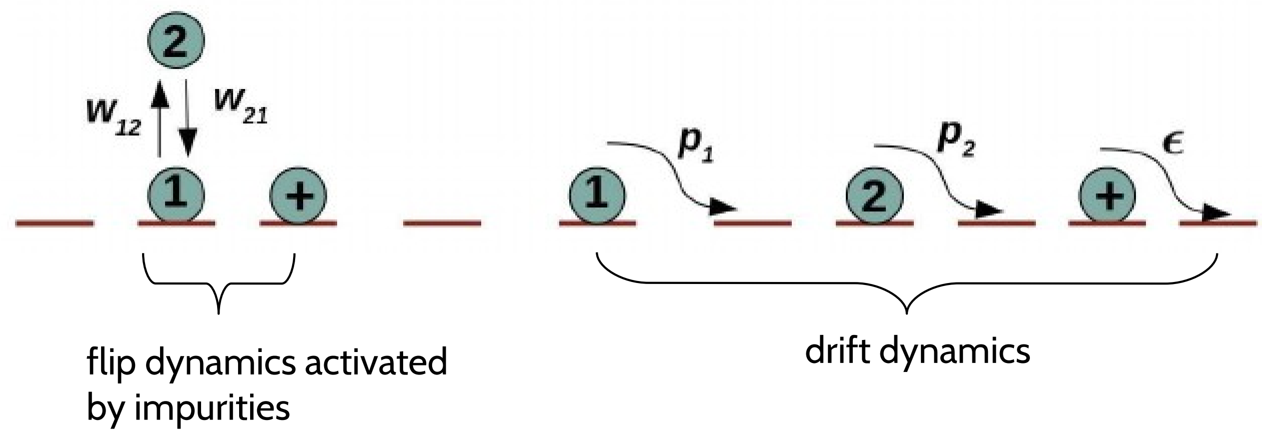
**Steady state:**

*periodic boundary condition*: all configurations equally likely, uncorrelated, no phase transition

*open boundary condition*: interesting **matrix product state**, correlated, three different phases

# *Our model:* Multi species TASEP with impurity activated flips

Model: Two species TASEP with impurities




one dimensional periodic lattice

Dynamics for the multi species model:

$$\begin{aligned} \text{drift (species)}: \quad & I0 \xrightarrow{p_I} 0I, \qquad I = 1, 2, ..., \mu, \\ \text{drift (impurity)}: \quad & +0, \xrightarrow{\epsilon} 0+ \\ \text{flip}: \quad & I+ \underset{w_{KI}}{\overset{w_{IK}}{\rightleftharpoons}} K+, \qquad I, K = 1, ..., \mu \end{aligned}$$

Generic features :

**(i) disordered system**

*[ distinct hopping rates ]*

**(ii) non-conserved system**

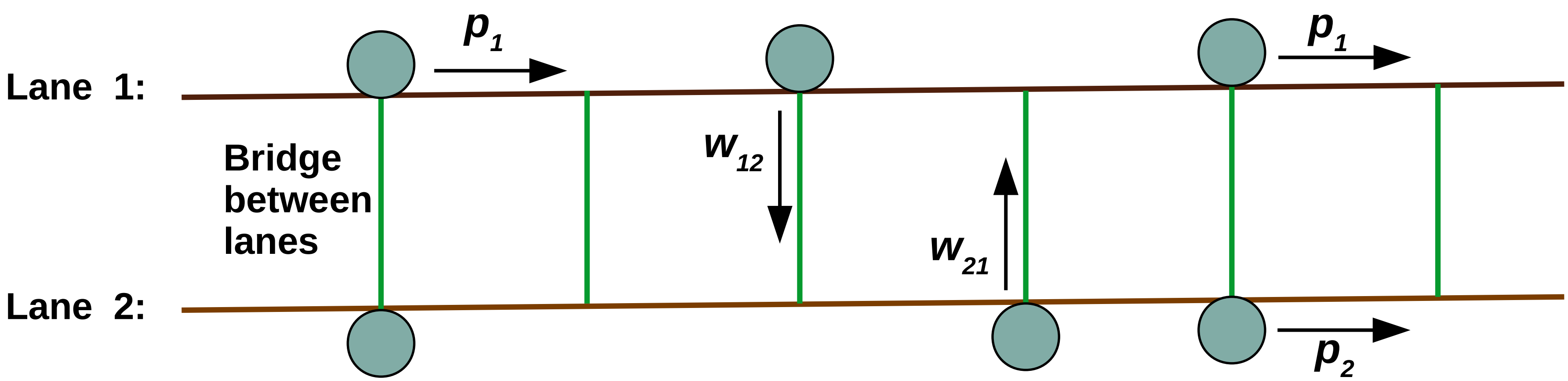
*[ Flip between species]*

**(iii) non-ergodic system**

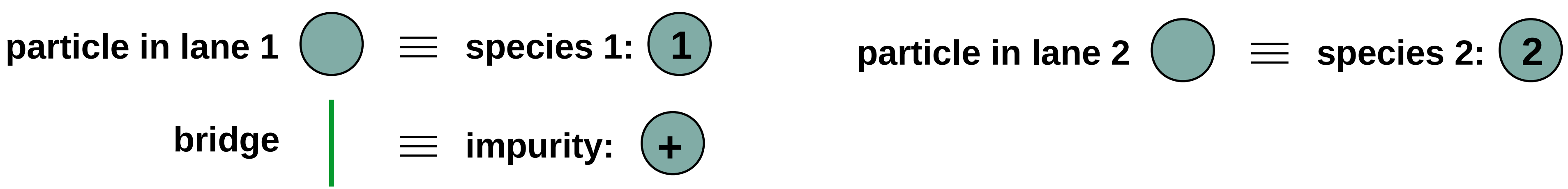
*[Not all configurations accessible fom a particular initial configuration]*

**Motivation 1:** Exact solution of steady state probability distribution and observables ?

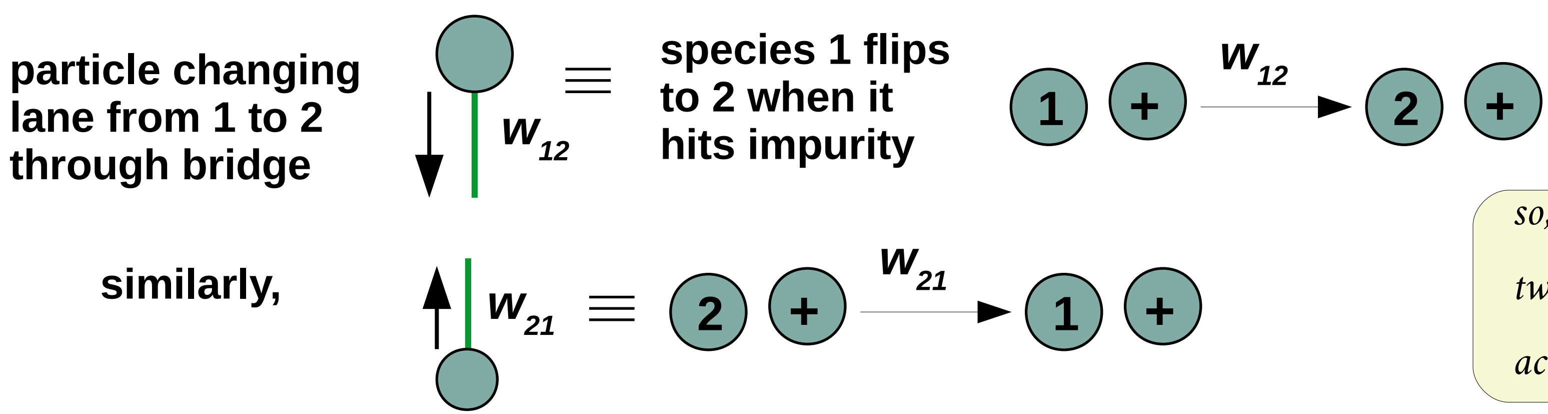
## Motivation 2: Connection to simplistic two-lane traffic flow




### Equivalent 1-d model with two species and impurity:




*Then the lane change dynamics becomes:*




*so, we have a 1-d model of two species TASEP with flips activated by impurities*

# Motivation 3: Connection to enzymatic chemical reactions



$$E + S \underset{k_b}{\overset{k_f}{\rightleftharpoons}} ES \underset{\bar{k}_b}{\overset{\bar{k}_f}{\rightleftharpoons}} E + P$$

simplified version →

$$S + E \underset{k_P}{\overset{k_S}{\rightleftharpoons}} P + E$$

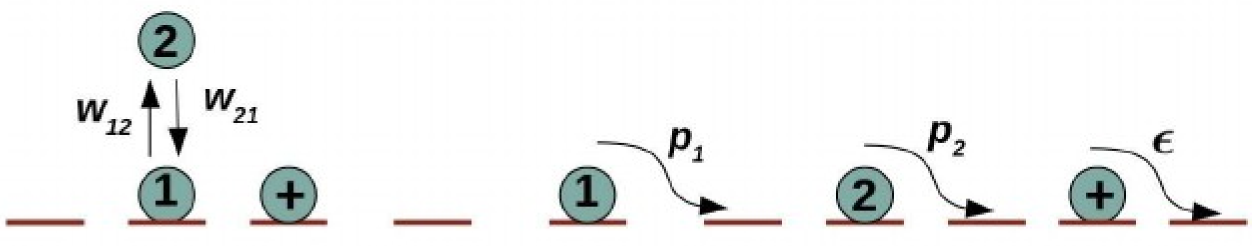
| *Enzymatic chemical reaction:* | | | *2-TASEP-IAF* | |
|---|---|---|---|---|
| Substrate: | *S* | $\equiv$ | Species: | 1 |
| Product: | *P* | $\equiv$ | Species: | 2 |
| Enzyme: | *E* | $\equiv$ | Impurity: | + |

| | | | |
|---|---|---|---|
| Substrate diffusion: | $S \xrightarrow{p_1}$ | $\equiv$ | $10 \xrightarrow{p_1} 01$ |
| Product diffusion: | $P \xrightarrow{p_2}$ | $\equiv$ | $20 \xrightarrow{p_2} 02$ |
| Enzyme diffusion: | $E \xrightarrow{\epsilon}$ | $\equiv$ | $+0 \xrightarrow{\epsilon} 0+$ |
| Forward reaction: | $S + E \xrightarrow{k_S} P + E$ | $\equiv$ | $1+ \xrightarrow{w_{12}} 2+$ |
| Backward reaction: | $P + E \xrightarrow{k_P} S + E$ | $\equiv$ | $2+ \xrightarrow{w_{21}} 1+$ |

# Multi species TASEP with impurity activated flips

($\mu$-TASEP-IAF)

Model: Two species TASEP with impurities




one dimensional periodic lattice

Dynamics for the multi species model:

$$\begin{array}{lllll} \text{drift (species)}: & I0 & \xrightarrow{p_I} & 0I, & I = 1, 2, ..., \mu, \\ \text{drift (impurity)}: & +0, & \xrightarrow{\epsilon} & 0+ & \\ \text{flip}: & I+ & \underset{w_{KI}}{\overset{w_{IK}}{\rightleftharpoons}} & K+, & I, K = 1, ..., \mu \end{array}$$

Input parameters: $\{p_I, \epsilon, w_{IK}, \rho_0, \rho_+\}$ $\rho_0$: vacancy density $\rho_+$: impurity density

Question: *can we solve the exact steady state probability distribution for this system ?*

Answer: *Yes, we can, using MATRIX PRODUCT ANSATZ.*

# Exact steady state: Totally asymmetric motion

matrix product ansatz:

$$P(\{s_i\}) \propto \mathrm{Tr}\left[\prod_{i=1}^{L} X_i\right],$$

$$X_i = E\,\delta_{s_i,0} + A\,\delta_{s_i,+} + \sum_{K=1}^{\mu} D_K\,\delta_{s_i,K}$$

*component at each site represented by a matrix*

*species "K"* → $D_K$

*impurity* → $A$

*vacancy* → $E$

...012+... ≡ ...$ED_1D_2A$...

Matrix representation : $\mu = 3$

Finite dimensional representations:

$$D_1 = d_1 \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad D_2 = d_2 \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad D_3 = d_3 \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$E = \begin{pmatrix} \frac{1}{\epsilon} & 0 & 0 & 0 \\ \frac{1}{p_1} - \frac{1}{\epsilon} & \frac{1}{p_1} & 0 & 0 \\ \frac{1}{p_2} - \frac{1}{\epsilon} & 0 & \frac{1}{p_2} & 0 \\ \frac{1}{p_3} - \frac{1}{\epsilon} & 0 & 0 & \frac{1}{p_3} \end{pmatrix} \quad A = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\begin{aligned} d_1 &= w_{21}w_{31} + w_{23}w_{31} + w_{32}w_{21} \\ d_2 &= w_{12}w_{32} + w_{13}w_{32} + w_{31}w_{12} \\ d_3 &= w_{13}w_{23} + w_{12}w_{23} + w_{21}w_{13} \end{aligned}$$

## Exact steady state: Partially asymmetric motion :

Dynamics :

$$\begin{array}{rcccl} \text{drift (species)}: & I0 & \underset{q_I}{\overset{p_I}{\rightleftharpoons}} & 0I & I=1,2,...,\mu \\ \text{drift (impurity)}: & +0 & \xrightarrow{\epsilon} & 0+ & \\ \text{flip}: & I+ & \underset{w_{KI}}{\overset{w_{IK}}{\rightleftharpoons}} & K+ & I,K=1,...,\mu \end{array}$$

Matrix representation : $\mu = 3$

Infinite dimensional representations:

$$D_I = \begin{pmatrix} d_I^{1,1} & d_I^{1,2} & d_I^{1,3} & d_I^{1,4} & . & . \\ 0 & d_I^{2,2} & d_I^{2,3} & d_I^{2,4} & . & . \\ 0 & 0 & d_I^{3,3} & d_I^{3,4} & . & . \\ 0 & 0 & 0 & d_I^{4,4} & . & . \\ . & . & & & . & \\ . & . & & & & . \end{pmatrix}$$

$$d_I^{m,m+r} = \frac{(m)_r}{r!\,p_I^r}\left(\frac{q_I}{p_I}\right)^{m-1} d_I^{1,1}$$

$$I = 1,2,3$$

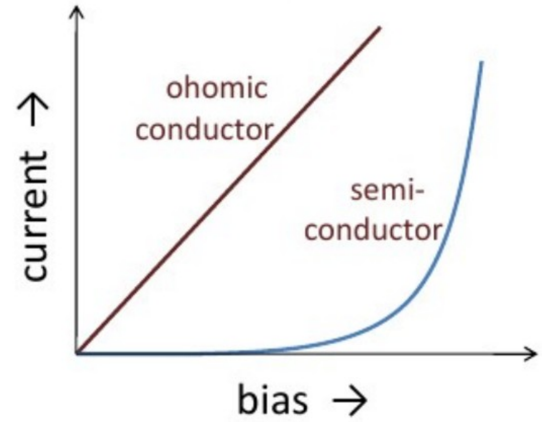
$$E = \begin{pmatrix} 0 & 0 & 0 & 0 & . & . \\ 1 & 0 & 0 & 0 & . & . \\ 0 & 1 & 0 & 0 & . & . \\ 0 & 0 & 1 & 0 & . & . \\ 0 & 0 & 0 & 1 & & \\ . & . & & & . & \\ . & . & & & & . \end{pmatrix}$$

$$A = \begin{pmatrix} 1 & \frac{1}{\epsilon} & \frac{1}{\epsilon^2} & \frac{1}{\epsilon^3} & . & . \\ 0 & 0 & 0 & 0 & . & . \\ 0 & 0 & 0 & 0 & . & . \\ . & . & . & . & . & . \\ . & . & . & . & . & . \end{pmatrix}$$

$$\begin{aligned} d_1^{1,1} &= w_{21}w_{31} + w_{23}w_{31} + w_{32}w_{21} \\ d_2^{1,1} &= w_{12}w_{32} + w_{13}w_{32} + w_{31}w_{12} \\ d_3^{1,1} &= w_{13}w_{23} + w_{12}w_{23} + w_{21}w_{13} \end{aligned}$$

# Negative differential mobility :

what we generally observe:




*current increases with increasing bias*

**Decreasing current with increasing bias** ⟹ ***negative differential mobility***

**Model:** Three species ASEP with impurity activated flips

**Dynamics:** $10 \underset{q_1}{\overset{p_1}{\rightleftharpoons}} 01$ $\quad 20 \underset{q_2}{\overset{p_2}{\rightleftharpoons}} 02$ $\quad 30 \underset{q_3}{\overset{p_3}{\rightleftharpoons}} 03$ $\quad +0 \xrightarrow{\epsilon} 0+$ $\quad 1+ \underset{w_{21}}{\overset{w_{12}}{\rightleftharpoons}} 2+$

**Set up:**

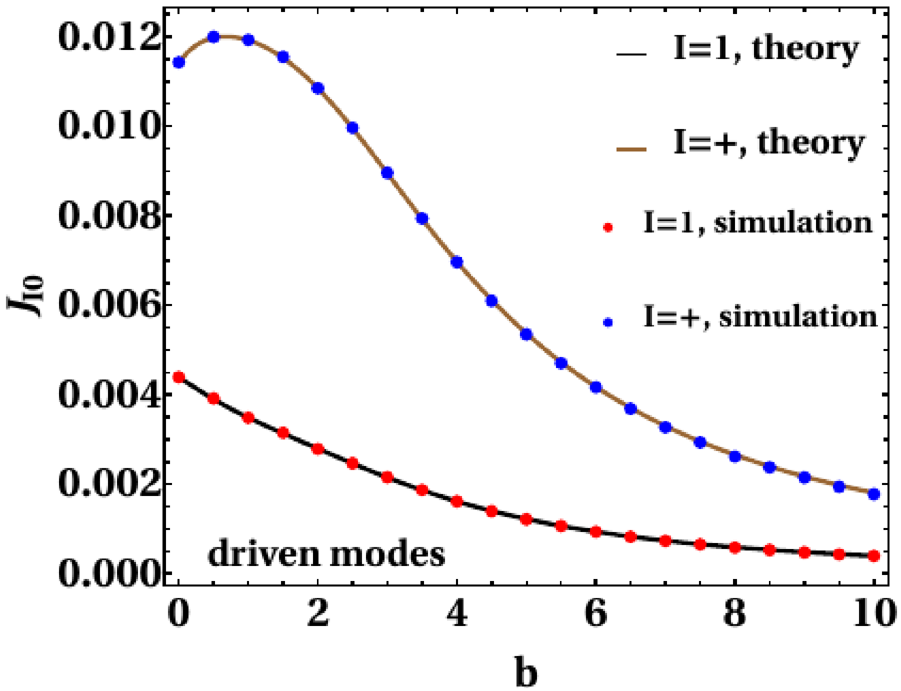
$p_1 = 1, q_1 = e^{-b}$ — *species 1 is driven mode with bias* $\ln(p_1/q_1) = b$

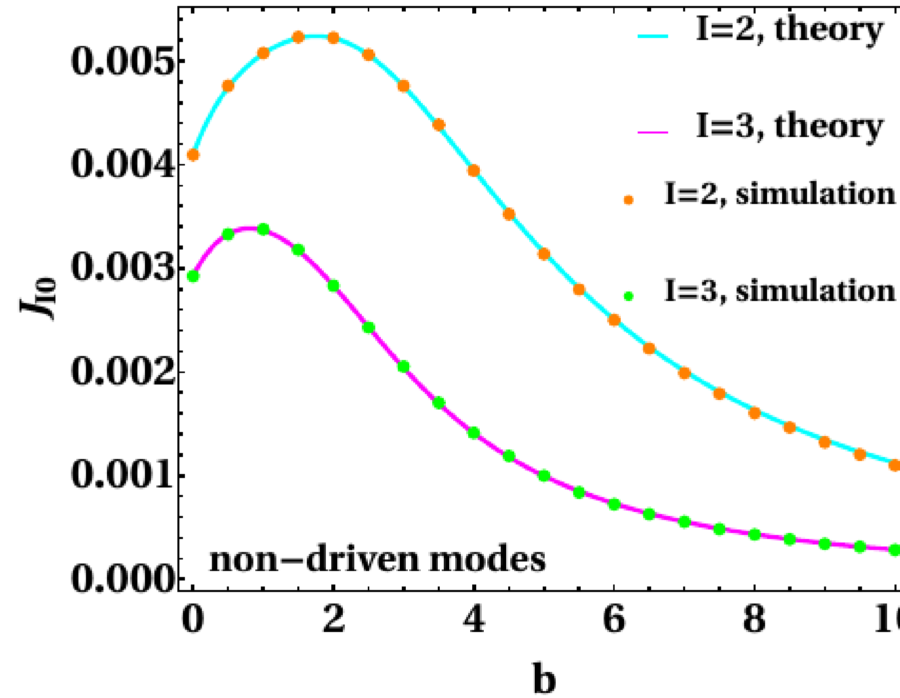
$p_2 = \frac{1}{1+b^2} = q_2$ — ***species 2 is non-driven mode, but its hop rates decreases with increasing b [key ingredient]***

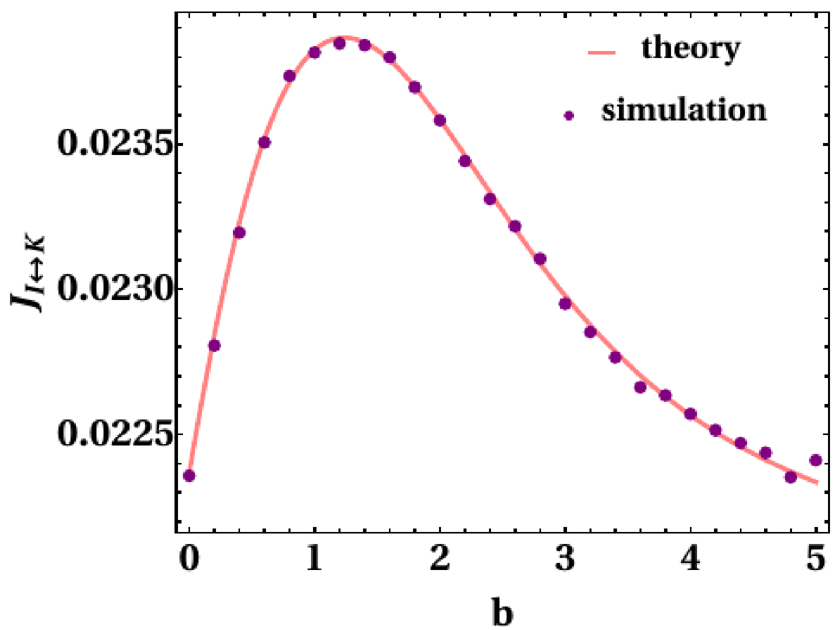
$p_3 = 1 = q_3$ — *species 3 is non-driven mode with hop rates independent of b*

$\epsilon > 0$ — *impurity is driven mode with hop rate independent of b*

Drift currents for both *driven modes* and *non-driven modes* decrease with increasing bias ($b$) for large values of $b$ :




The flip current also exhibits negative differential mobility

The hard core exclusion helps in causing negative differential mobility

# Conclusions

- we have obtained an exact matrix product steady state for
  "*multi-species (totally) asymmetric simple exclusion process with impurity activated flips*"
  ---- a *disordered, nonconserved, nonergodic* system.

- we get *finite dimensional matrices* for the *totally asymmetric case* and
  *infinite dimensional matrices* for the *partially asymmetric case.*

- The model provides interesting mappings to *(i) simplistic multi lane traffic flow ,*
  *(ii) enzymatic chemical reactions.*

- We observe *negative differential mobility*, where both the drift current and flip current can decrease with increasing bias .

✸ The model exhibits *clustering phenomenon* induced by counter flow.
(transition between *free flowing phase* and *clustering phase*).

[Reference: *arXiv:2208.03297* (2022)]

**THANK YOU**