RICE UNIVERSITY

THEORETICAL STUDIES OF COUPLED PARALLEL EXCLUSION PROCESSES

Anatoly B. Kolomeisky

Department of Chemistry

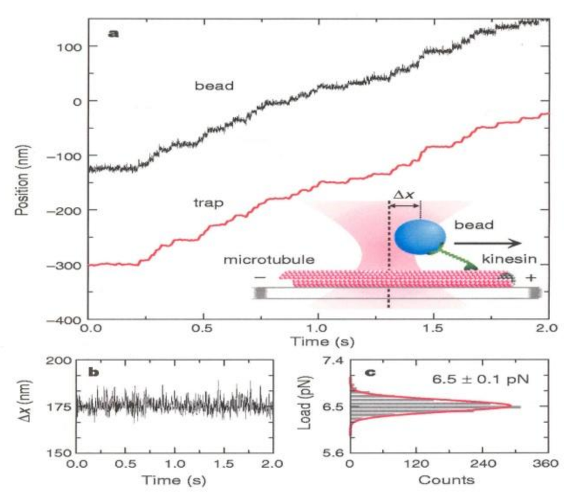
Houston, Texas, USA

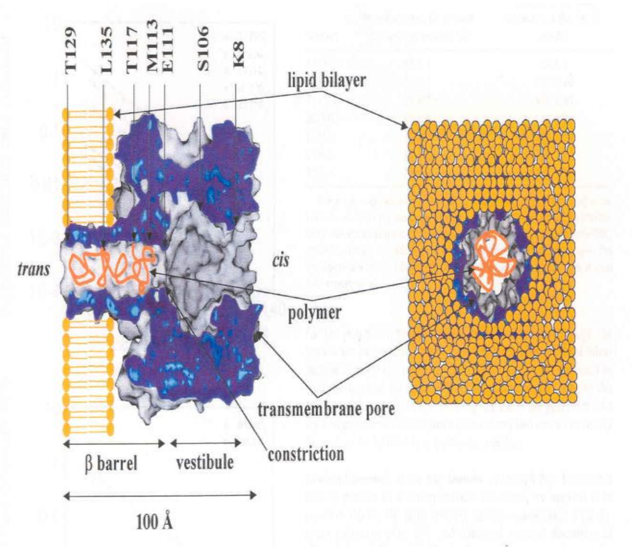
Asymmetric Simple Exclusion Processes

Applications:

To investigate 1D multi-particle, cooperative phenomena in chemistry, physics and biology

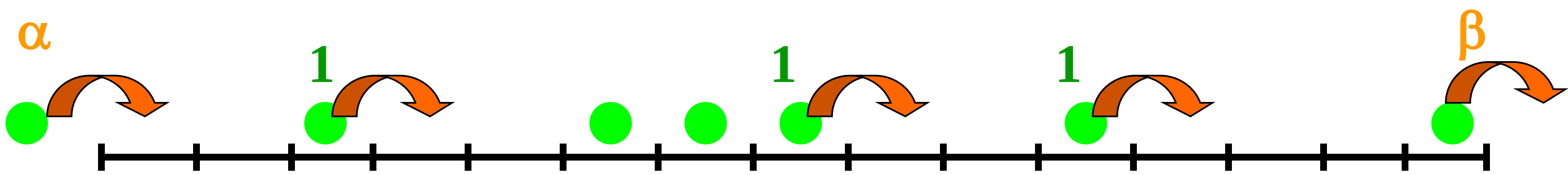
Biological transport, polymerization, protein synthesis	Gel electrophoresis, traffic problems, animal behavior, interface growth	Diffusion through biological channels, polymer dynamics





Asymmetric Simple Exclusion Processes

1D Lattice Gas Models with Hard-Core Exclusions

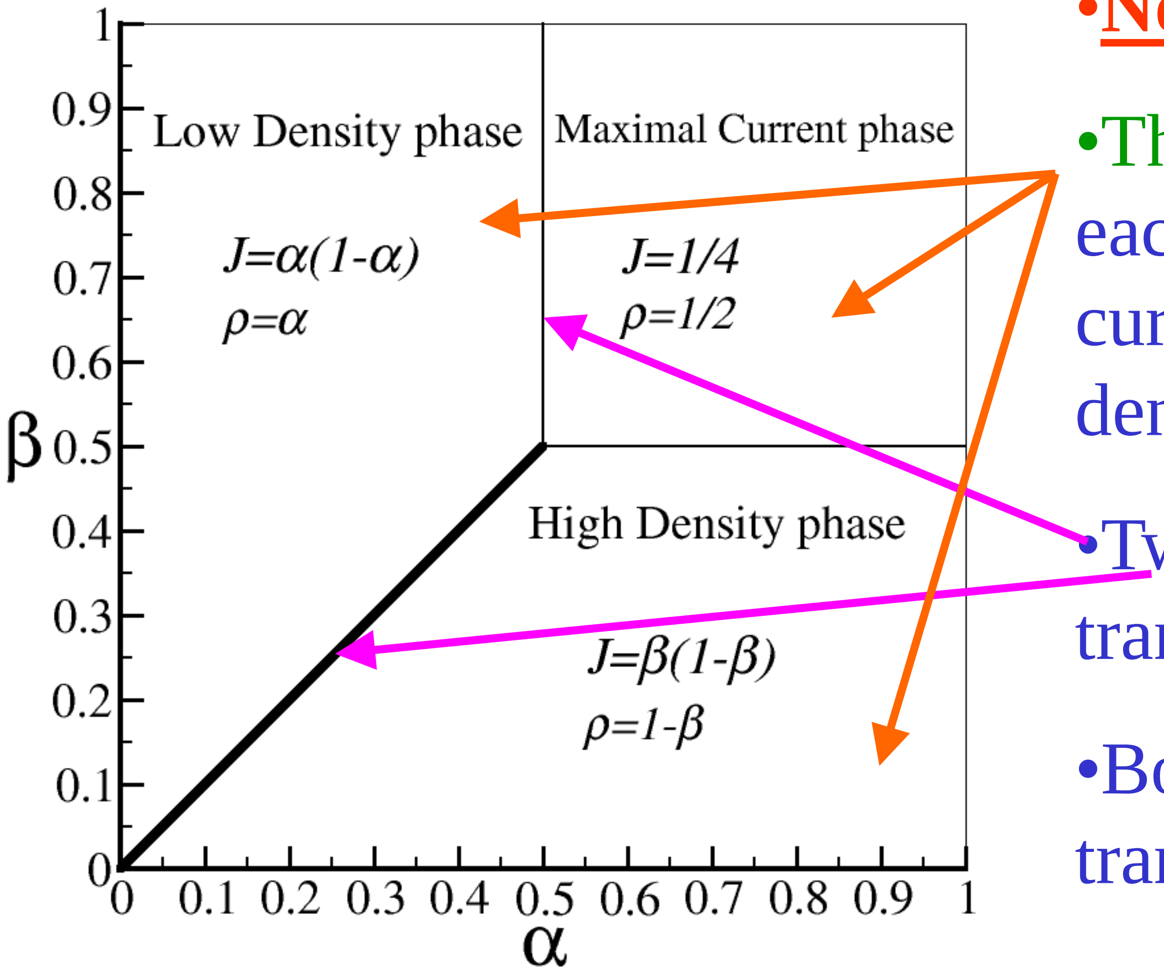


The simplest model: **Totally Asymmetric Simple Exclusion Process (TASEP)**

- Nonequilibrium process
- Particles enter from the left with rate $0 \leq \alpha \leq 1$ if the first site is unoccupied
- Inside the lattice particles hop to the next site with rate 1 if there is no particle at this site – hard-core exclusion
- Particles leave from to the right with rate $0 \leq \beta \leq 1$

Exact Solutions of TASEP

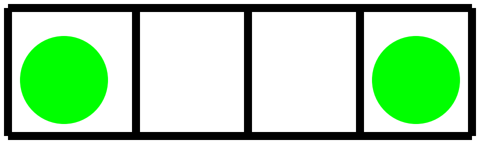
Derrida *et al.*, *J. Phys. A: Math Gen.* **26** 1493 (1993), G. Schutz et al., *J. Stat. Phys.* (1992)



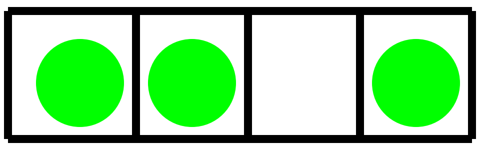
- **<u>Nonequilibrium process</u>**
- Three stationary states each with its own particle current (J) and bulk density(ρ)
- Two types of phase transitions
- Boundary-induced phase transitions

Solutions of TASEP

Exact Solutions: Matrix Product Anzats



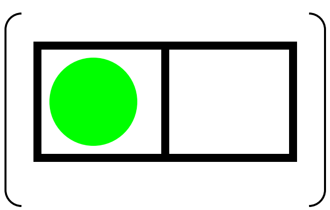
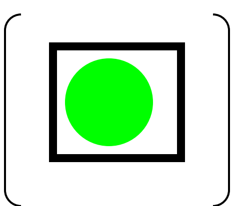
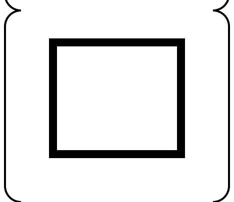
D*E*E*D



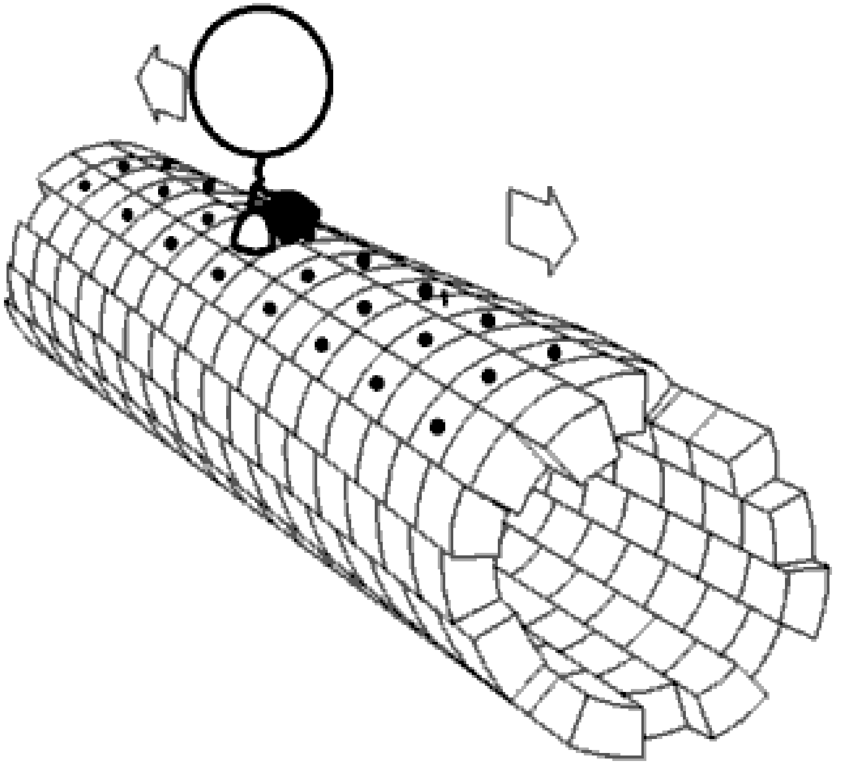
D*D*E*D

Every configuration of N sites is assigned with the product of N matrices of 2 types: ***D***-for occupied site, ***E***-for empty site

Approximate Solutions: Mean field methods

Probability  = Probability  * Probability 

TRANSPORT PROCESSES



More realistic description of biological transport, traffic problems, etc., requires coupling of exclusion processes

Animations are courtesy of Marie Curie Research Institute, Molecular Motors Group

OUR GOALS:

1) **Investigate parallel coupled exclusion processes, specifically how it affects non-equilibrium phase diagrams, particle currents and density profiles.**
2) **What is the effect of symmetry in the coupling, is the most optimal transport achieved for symmetric or asymmetric cases?**
3) **Homogeneous coupling *vs* inhomogeneous coupling.**
4) **What are mechanisms controlling dynamics of the system that couples asymmetric and symmetric exclusion processes**

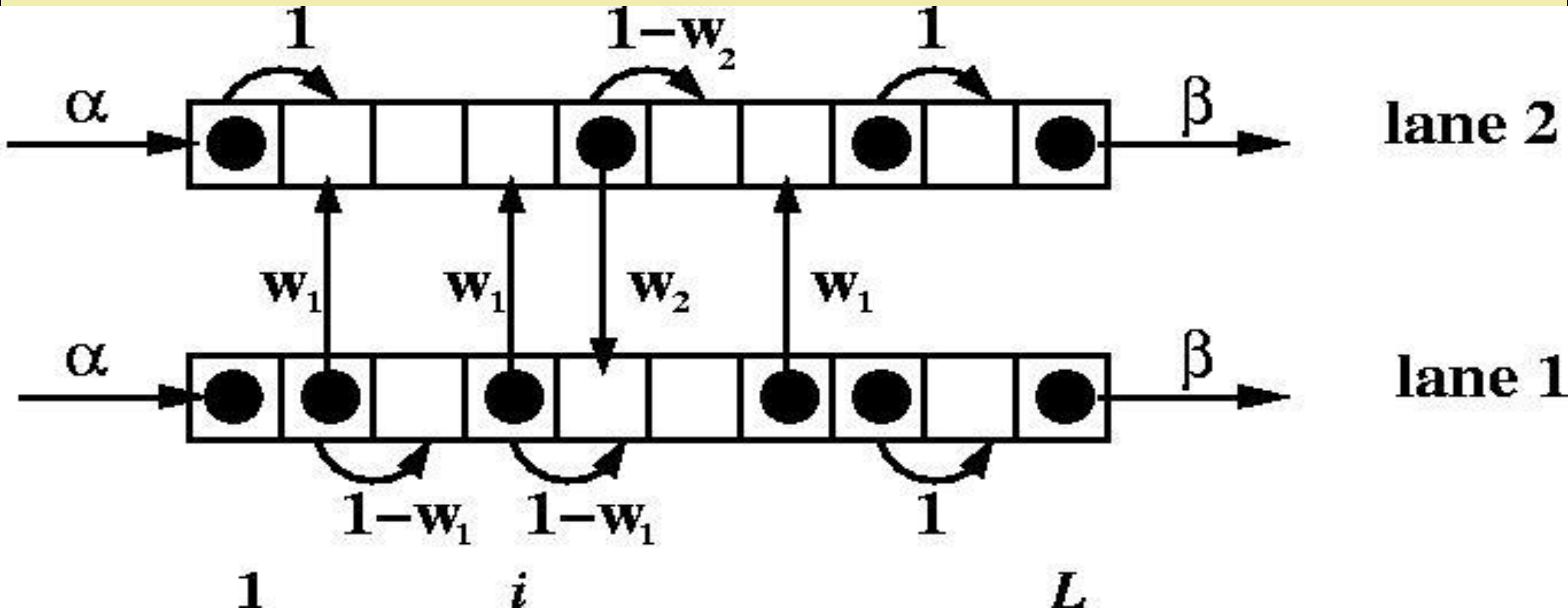
Our Methods: exact solutions, smart mean-field approach and extensive Monte Carlo computer simulations

Many contributors in the field: G. Schutz, R. Stinchcomb, V. Popkov, T. Chou, S. Klumpp, R. Lipowsky, D. Chowdhury,..

TWO-CHANNEL TASEP

Definition of Model

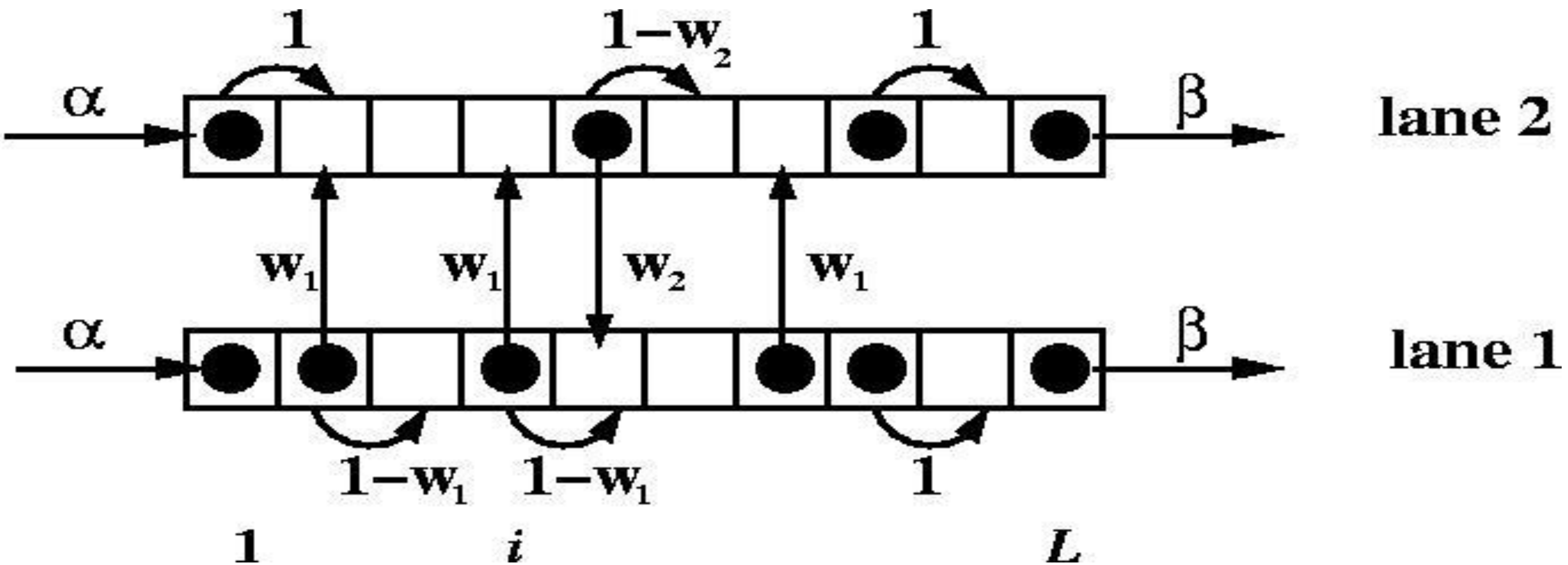
-Two parallel 1D lattices of size L
- Both channels have entrance rate α and exit rate β
- Probability to hop between channels is w_1 and w_2, respectively
- Coupled non-equilibrium process



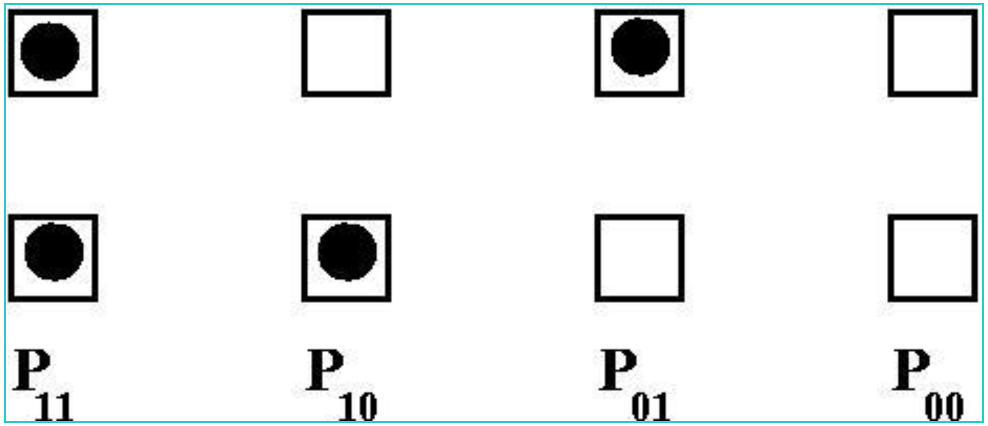
TWO-CHANNEL TASEP

Consider symmetric coupling

$$w_1 = w_2 = w$$

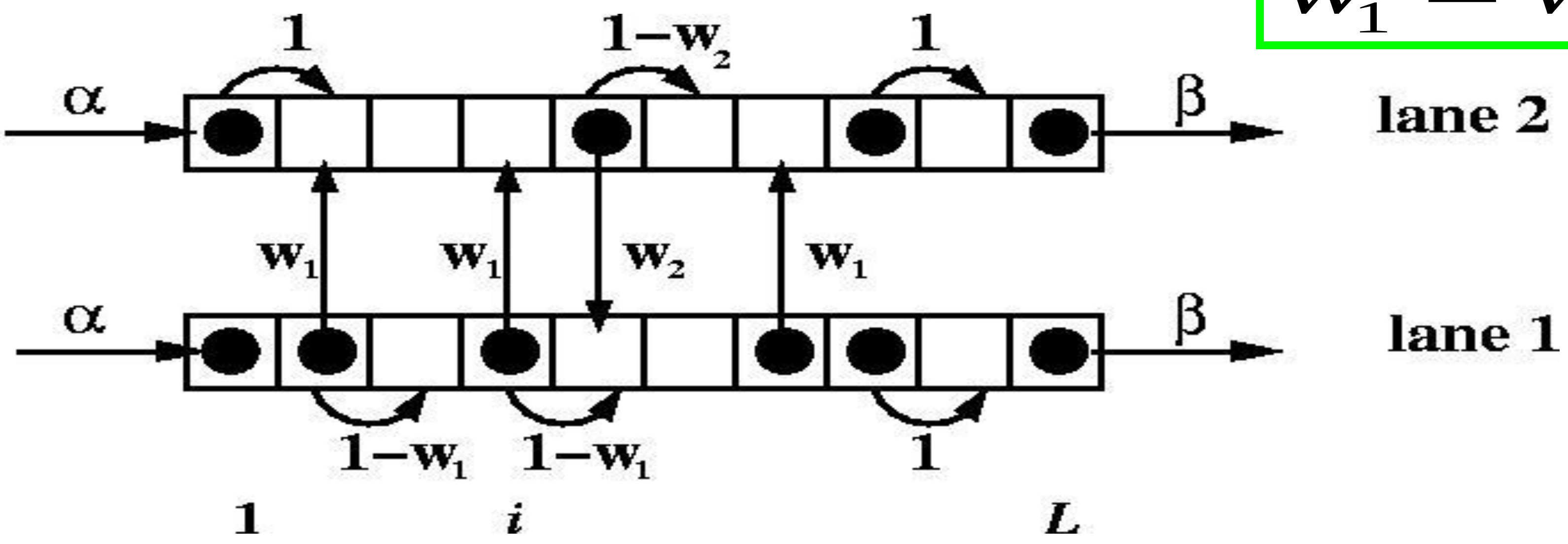


4 possible states for a vertical cluster of lattice sites



TWO-CHANNEL TASEP: EXACT SOLUTIONS

$$w_1 = w_2 = w$$



1) w=0 – no coupling ⇨ Two one-channel TASEP with known exact solutions

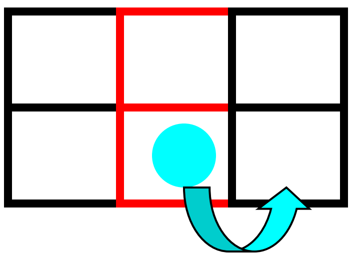
2) w=1 – strong coupling ⇨ Exact solutions are possible

TWO-CHANNEL TASEP: STRONG COUPLING

w=1 case

How to get P_{00}?

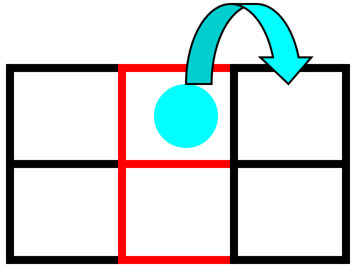
P_{10}



1-w=0

1-w=0

P_{01}



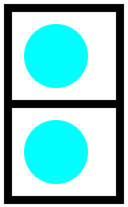
$P_{00}=0$

$P_{10}=P_{01}$ – by symmetry

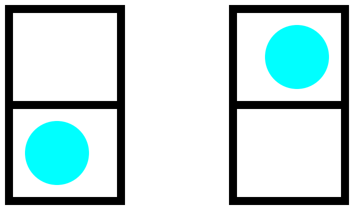
In the system 2 types of vertical clusters: P_{11} and P_{10}, P_{01}

P_{11} – new "effective" particles

P_{10}, P_{01}-new "effective" holes



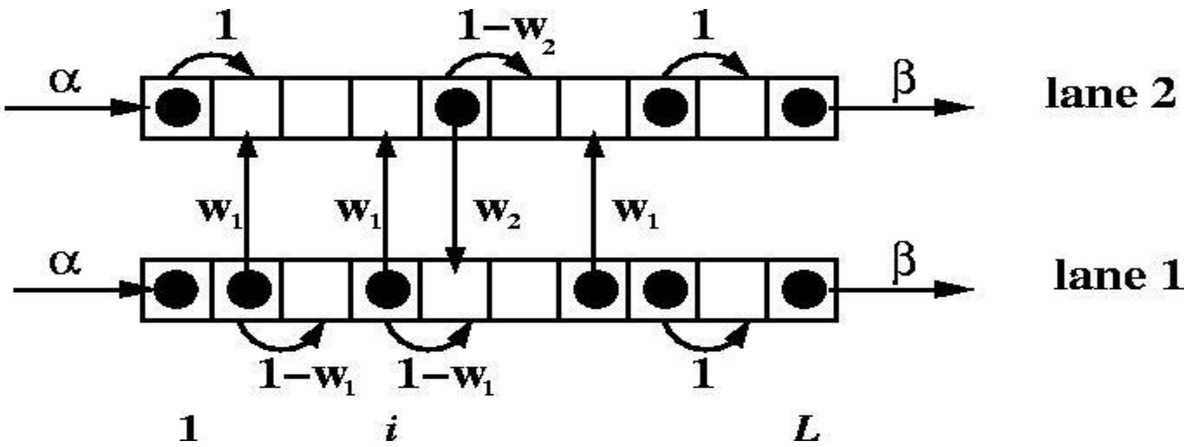
or



2-channel TASEP with strong coupling is mapped into 1-channel TASEP with $\alpha_{eff}=\alpha$, $\beta_{eff}=2\beta$

Simple Mean-Field Approach

Probability of occupancy of any state is independent of occupancies of other sites

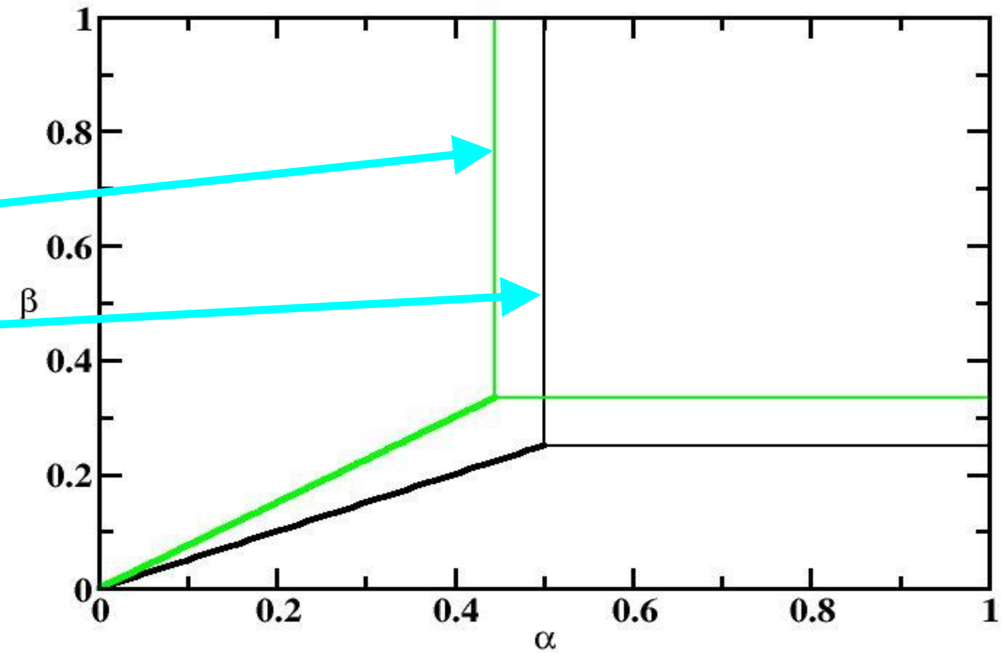


Phase diagram for strong coupling:

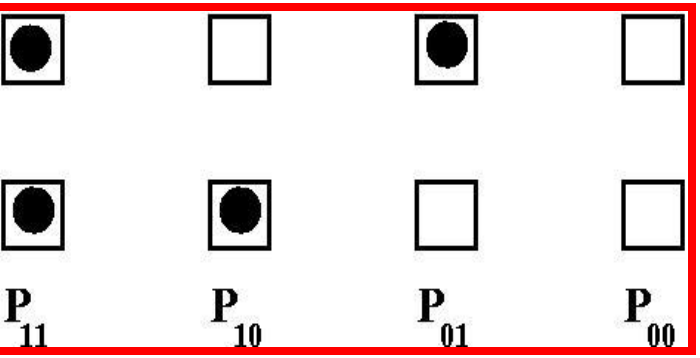
simple mean-field

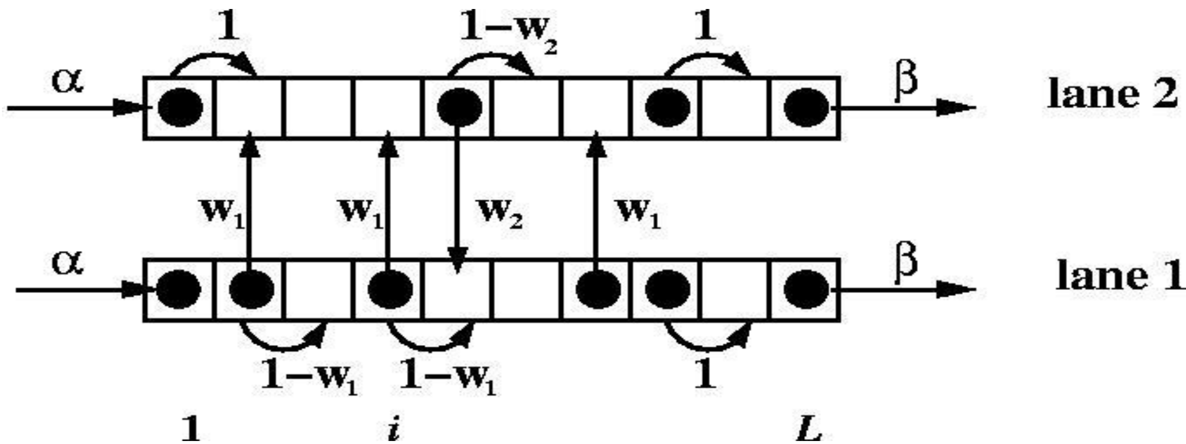
exact

Simple mean-field – crude approximation



Our Approach: Vertical Cluster Mean Field





Correlations inside of the vertical cluster are treated **exactly**

Correlations between different vertical clusters – in mean field

Assume in the bulk: $P^i_{00} = P_{00}, P^i_{11} = P_{11}, P^i_{10} = P^i_{01} = P_{10}$

Master equation for vertical cluster dynamics:

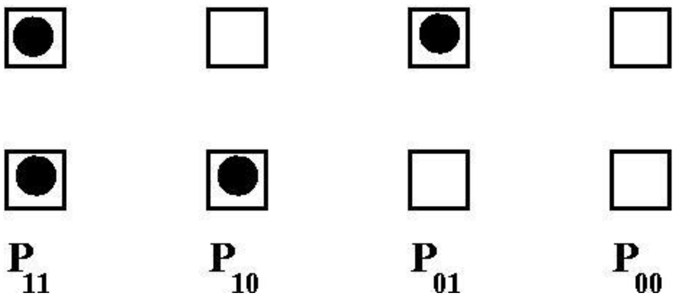
$$\frac{dP_{11}}{dt} = P_{11}P_{10} + P_{11}P_{01} + (1-\omega)P_{10}P_{01} + (1-\omega)P_{01}P_{10} - 2P_{11}P_{00} - P_{11}P_{10} - P_{10}P_{01}$$

MONTE CARLO SIMULATIONS

- BKL algorithm: event-driven Monte Carlo simulations to accelerate computations
- 10^7-10^{10} Monte Carlo steps per site;
- lattice size L=100-10000
- Typically first 3-5% of steps have been omitted to insure that the system reached stationary state

TWO-CHANNEL TASEP: RESULTS

Densities:



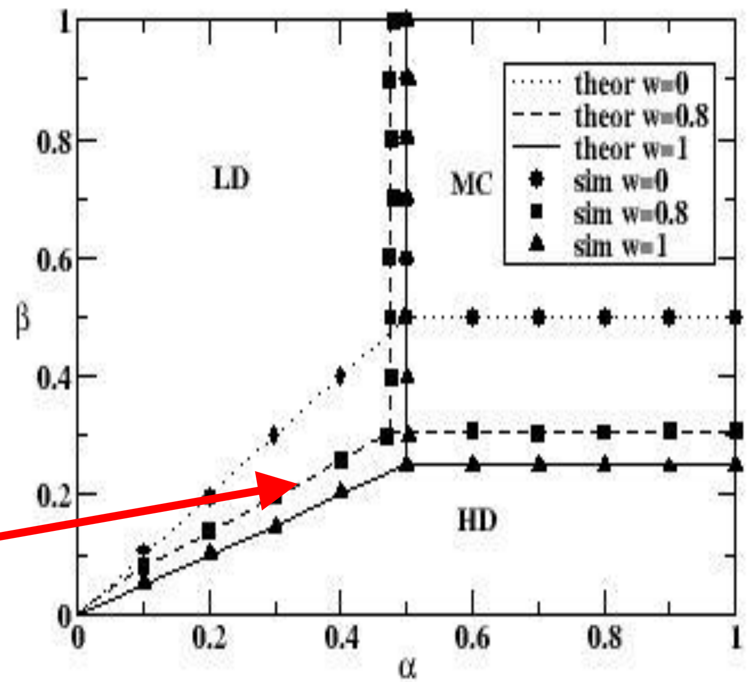
Lane 1 $$\rho_1 = P_{11} + P_{10}$$

Lane 2 $$\rho_2 = P_{11} + P_{01}$$

Not a straight line!

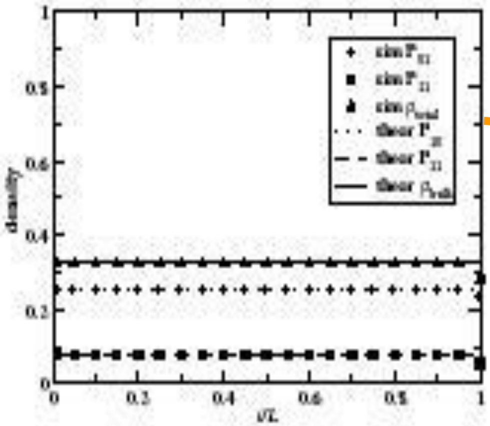
Phase diagrams for $0<w<1$

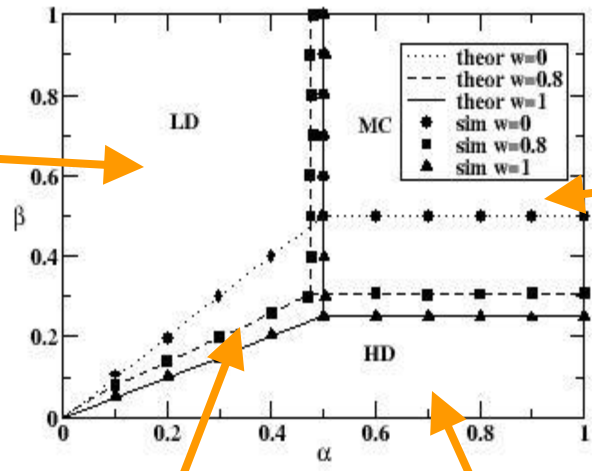
3 phases: high-density, low-density and maximal current



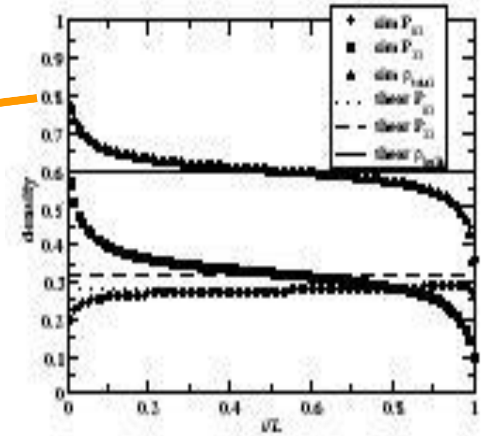
TWO-CHANNEL TASEP: RESULTS

low-density

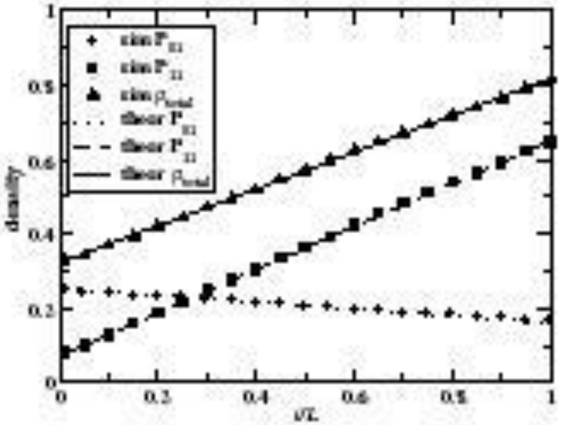




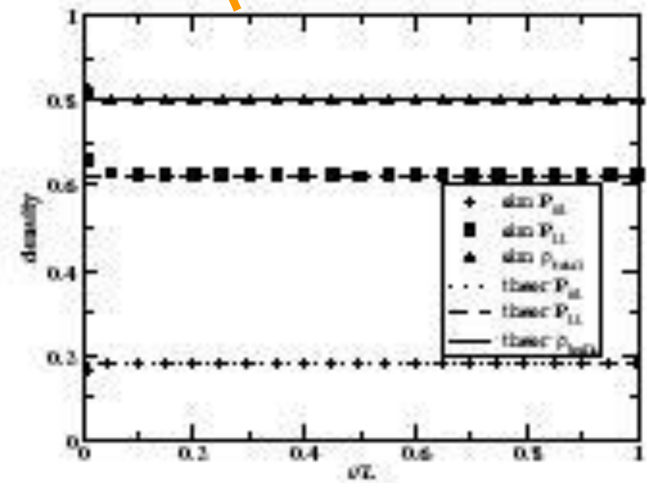
maximal current



Phase transition line between HD and LD

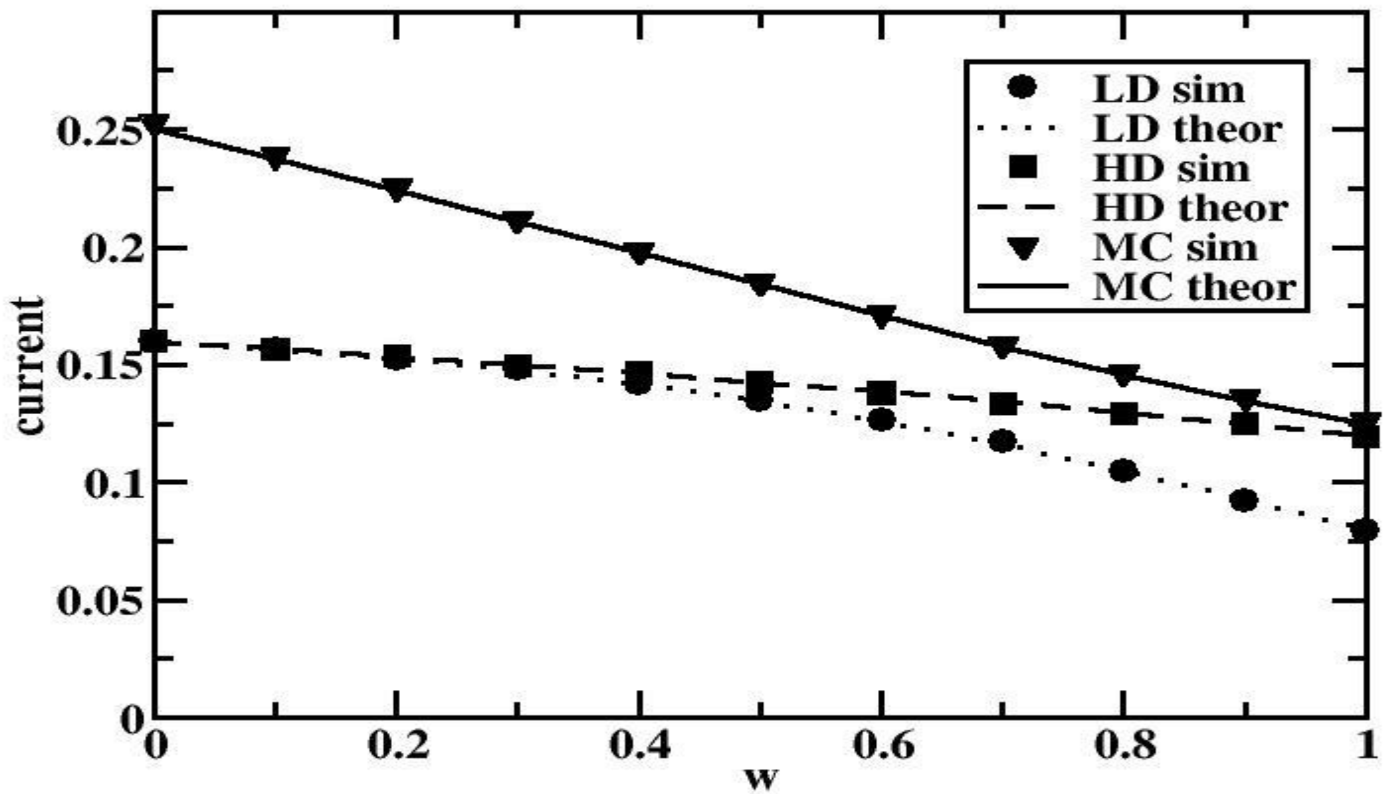


high-density



TWO-CHANNEL TASEP: EFFECT OF COUPLING

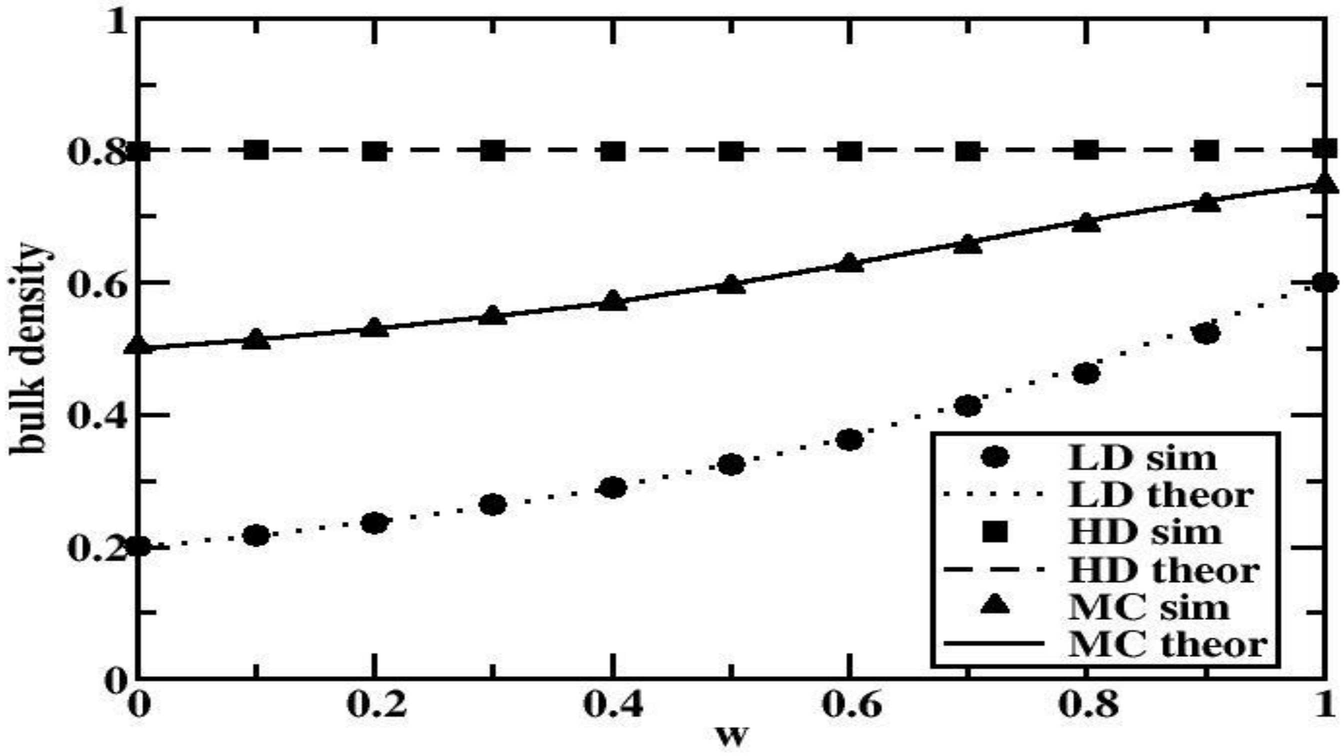
current per channel



The increase in the coupling lowers the current per channel

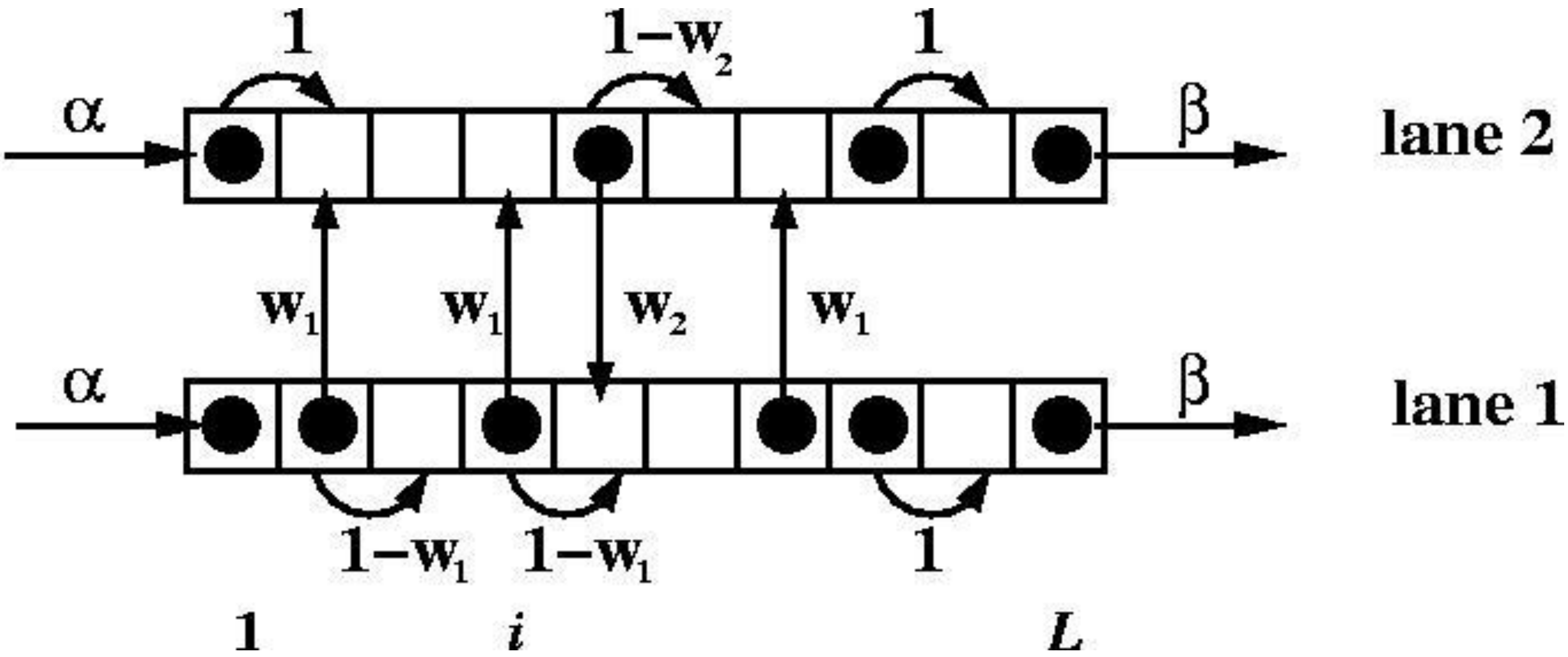
TWO-CHANNEL TASEP: EFFECT OF COUPLING

bulk density per channel



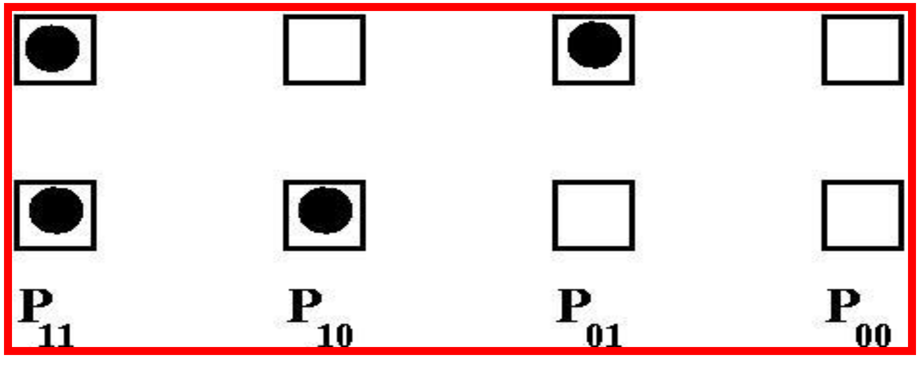
The increase in the coupling increases the bulk densities

TWO-CHANNEL TASEP: ASYMMETRIC COUPLING

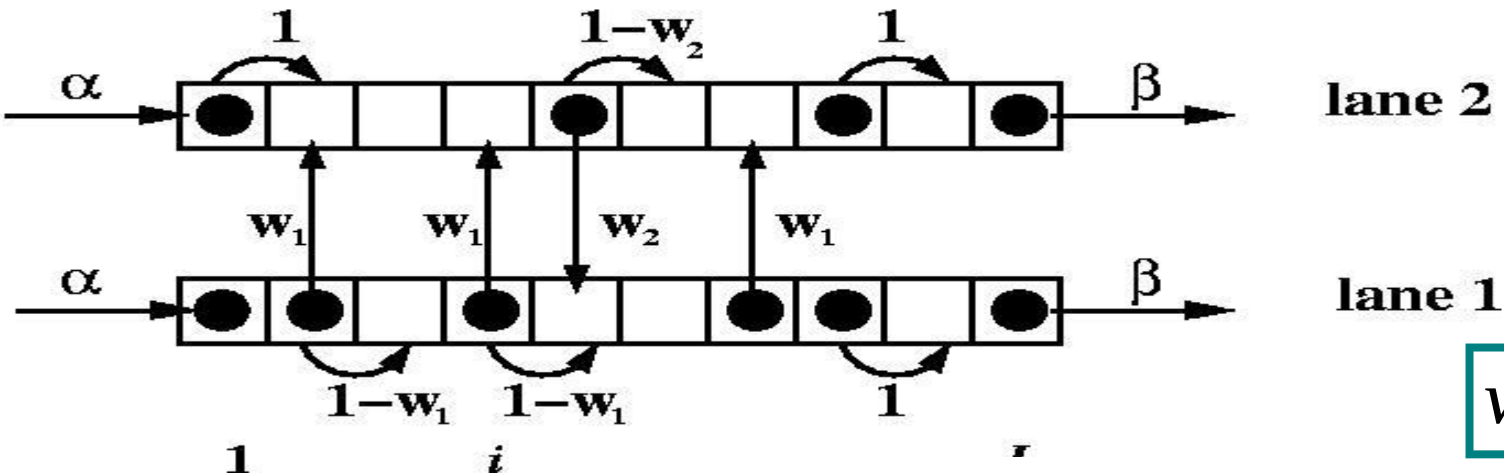


Vector cluster mean-field approach

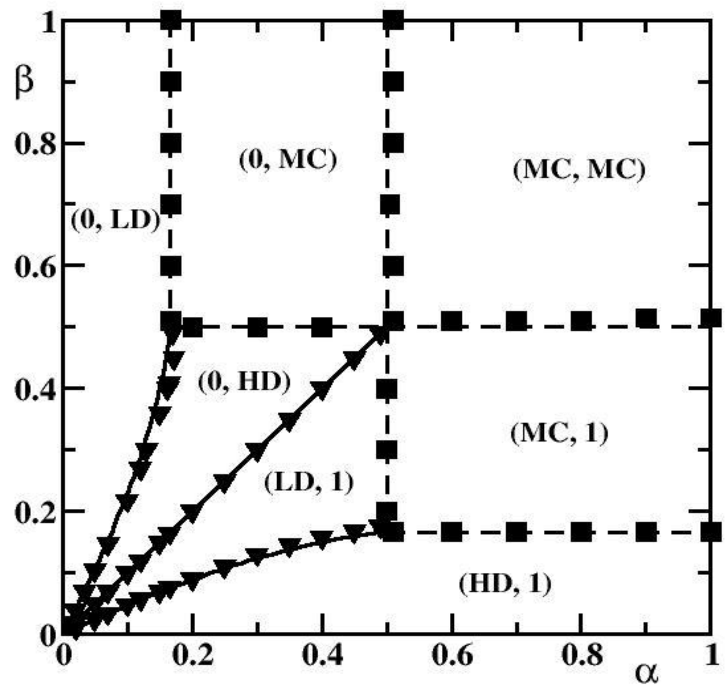
$$w_1 \neq w_2$$



TWO-CHANNEL TASEP: ASYMMETRIC COUPLING



$w_1 = 1, w_2 = 0$



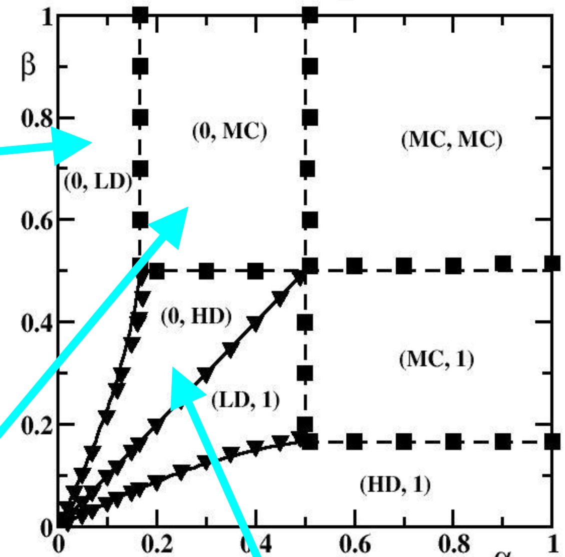
Phase diagram using vector cluster mean-field approach

7 phases!

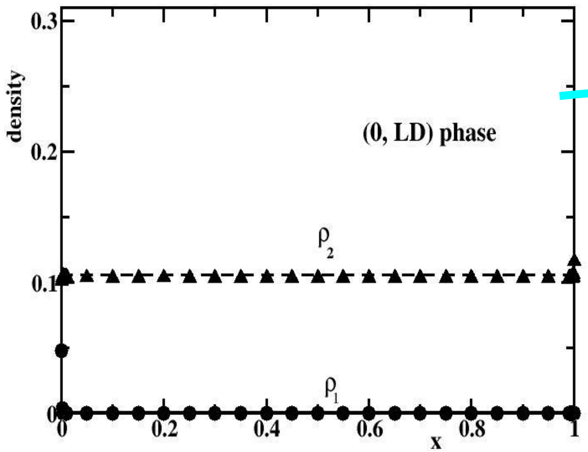
channel 1 and 2 are different

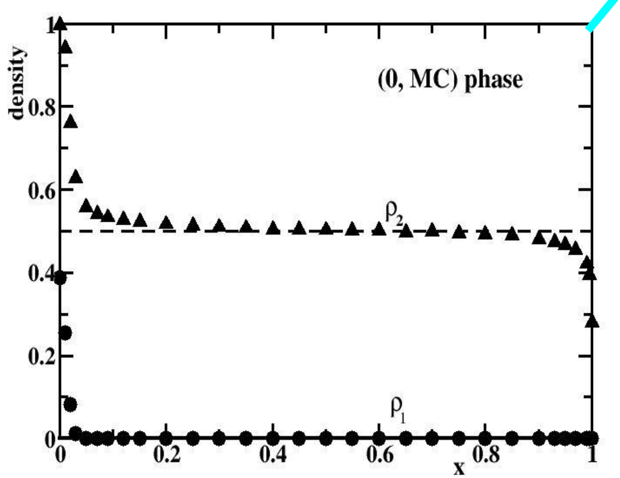
TWO-CHANNEL TASEP: ASYMMETRIC COUPLING

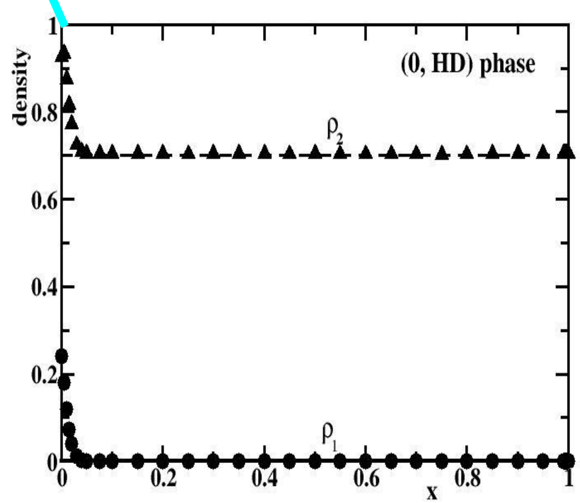
phase diagram



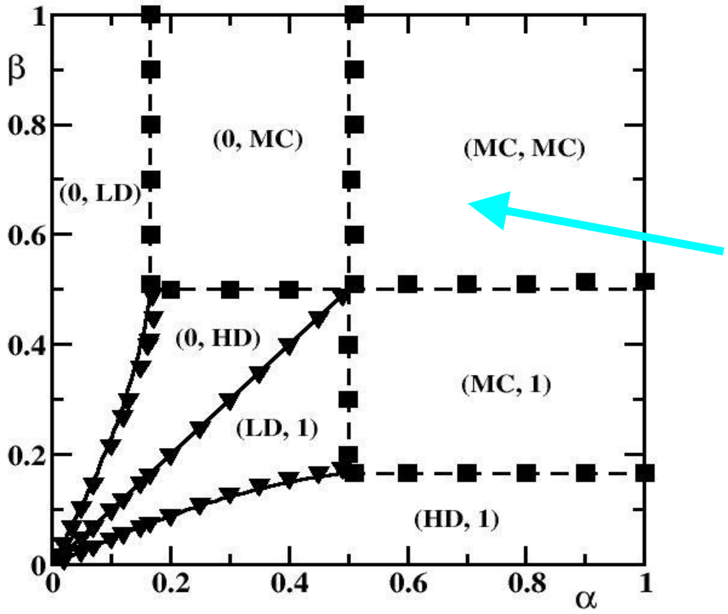
Density profiles:

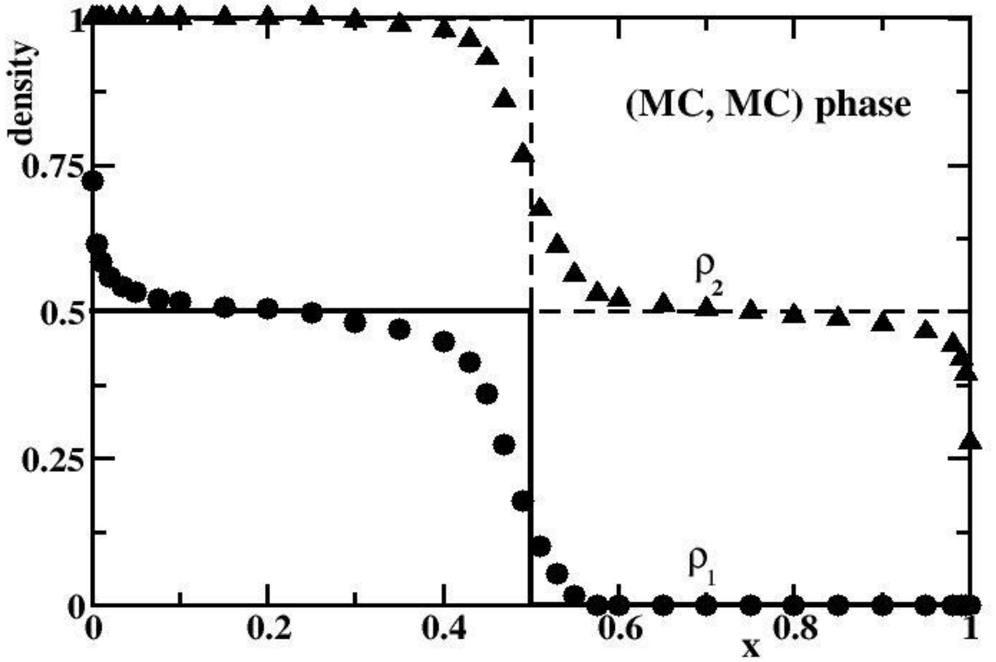






TWO-CHANNEL TASEP: ASYMMETRIC COUPLING





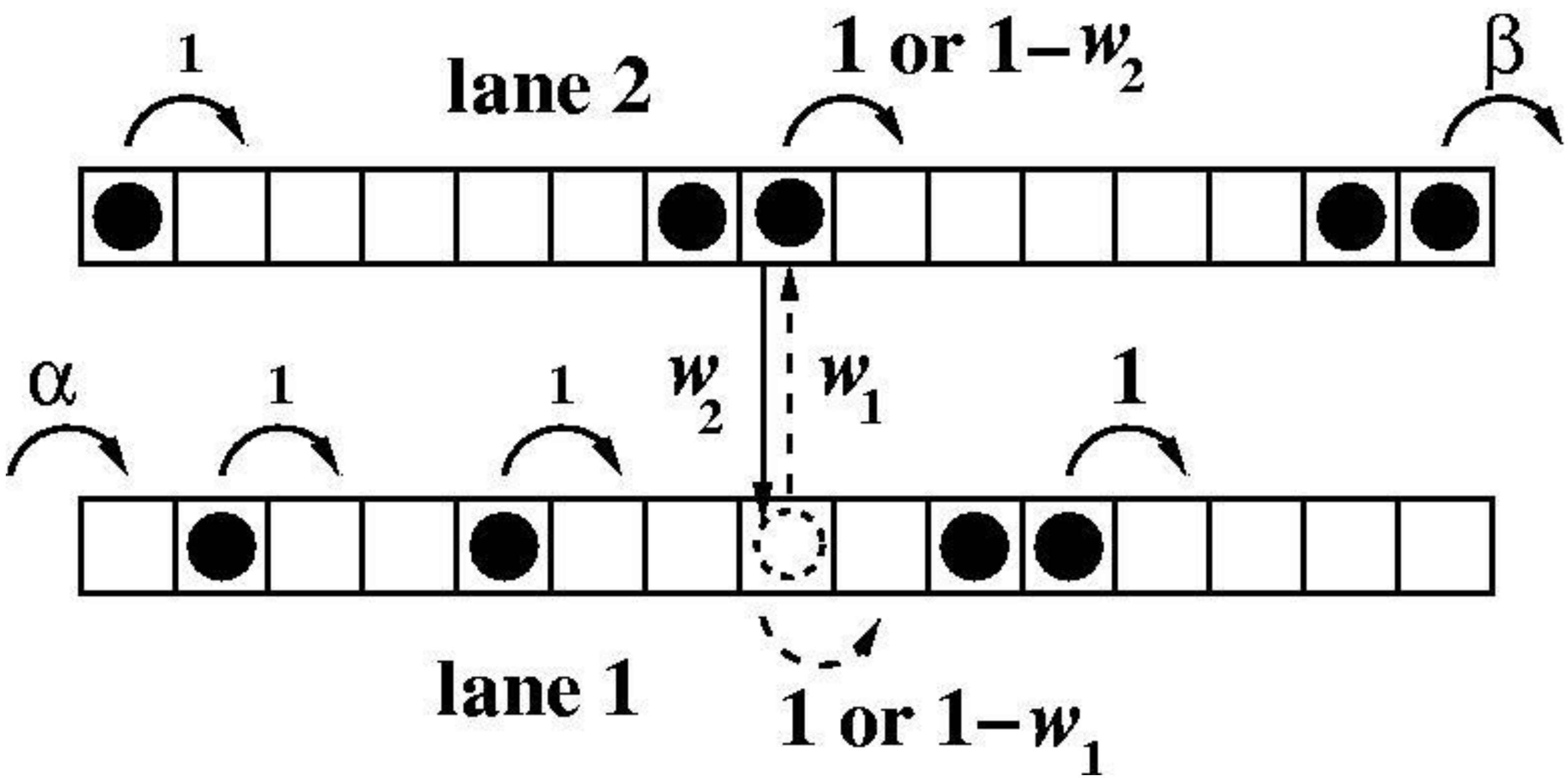
$\alpha=\beta=0.9$

Nature of this phase – unclear!

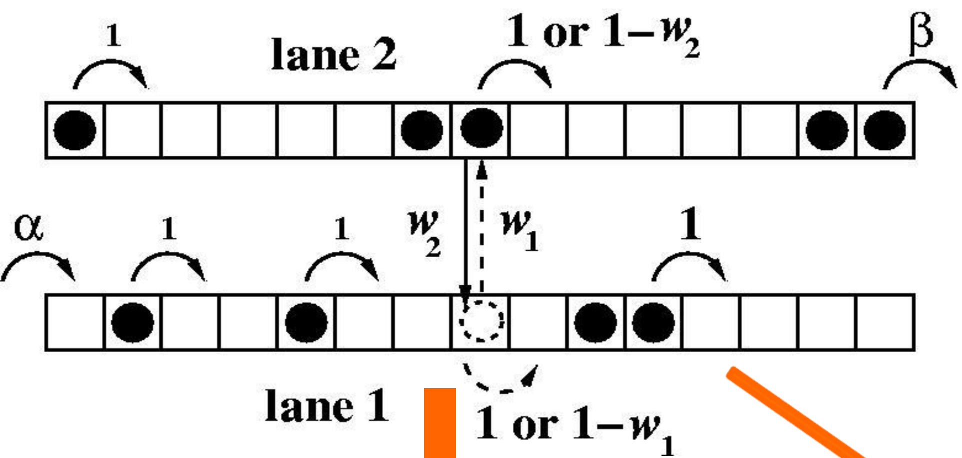
Coexistence of (0,MC) and (MC,1) phases?

TWO-CHANNEL TASEP: INHOMOGENEOUS COUPLING

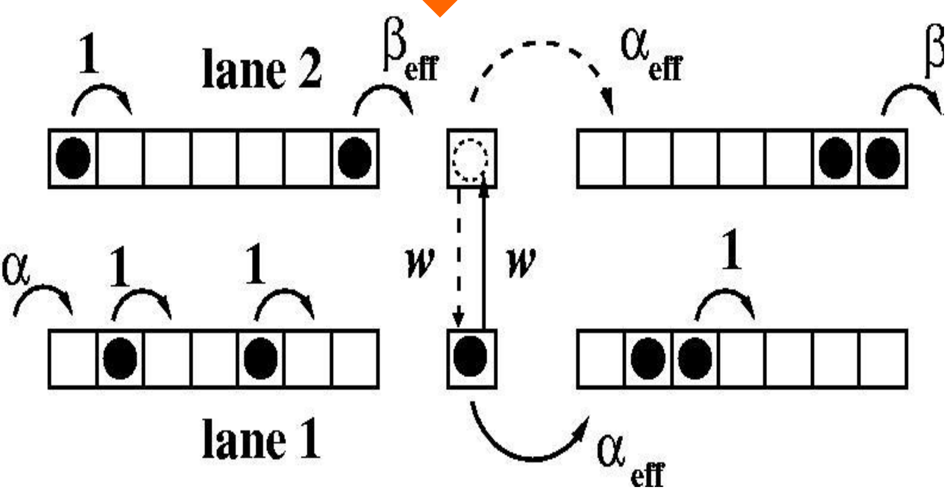
Simplest inhomogeneous coupling problem - stimulated, e.g., by slow codons in protein synthesis and motor proteins transport (in the presence of defects or roadblocks)



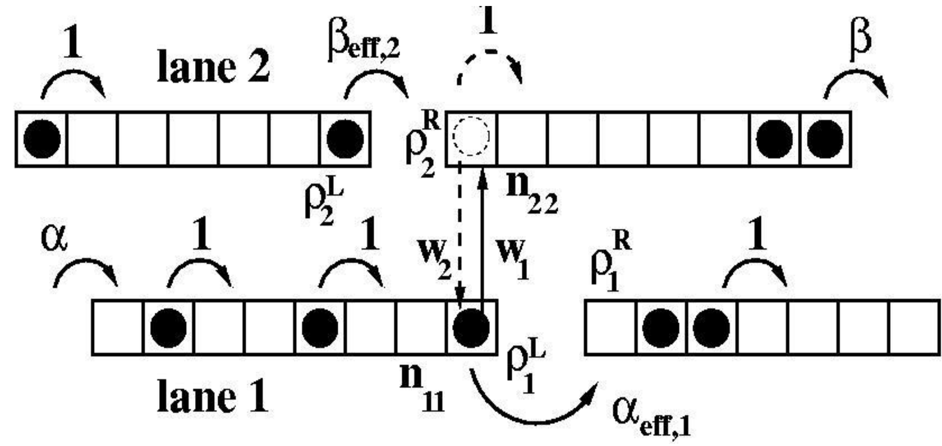
TWO-CHANNEL TASEP: INHOMOGENEOUS COUPLING



Our approach: treat exactly the vertical transitions, and view 4 other segments as coupled single-chain TASEP, correlations near the vertical cluster are neglected



symmetric



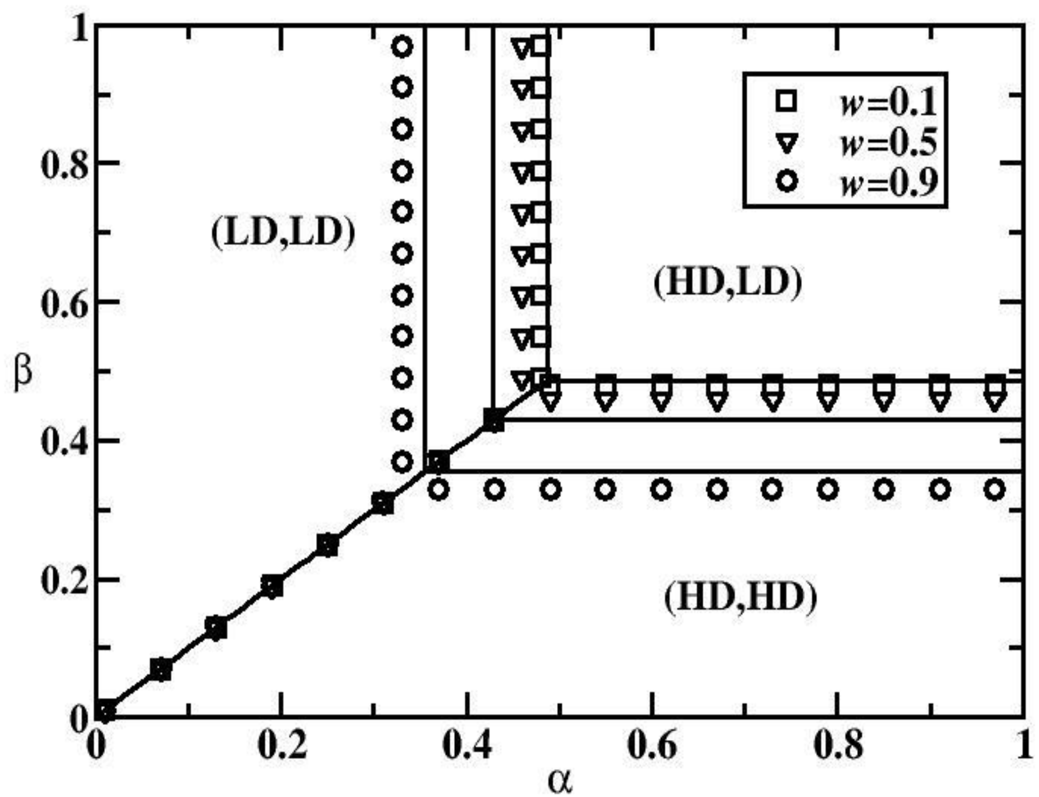
asymmetric

TWO-CHANNEL TASEP: INHOMOGENEOUS COUPLING

Phase diagram for symmetric inhomogeneous coupling of two channels

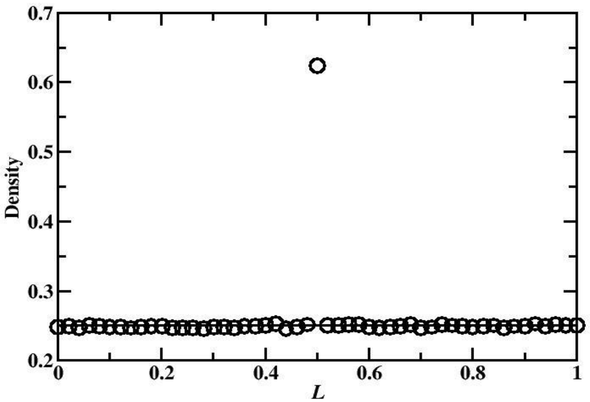
3 stationary phases

Our approximate theory works excellently for weak couplings, and qualitatively good for stronger couplings

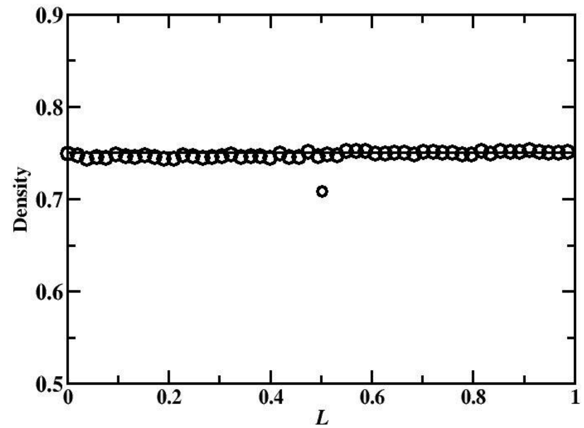


TWO-CHANNEL TASEP: INHOMOGENEOUS COUPLING

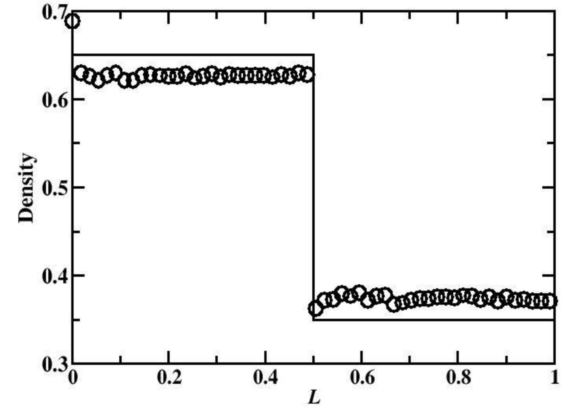
Density profiles for 3 phases for symmetric case:



LD/LD



HD/HD

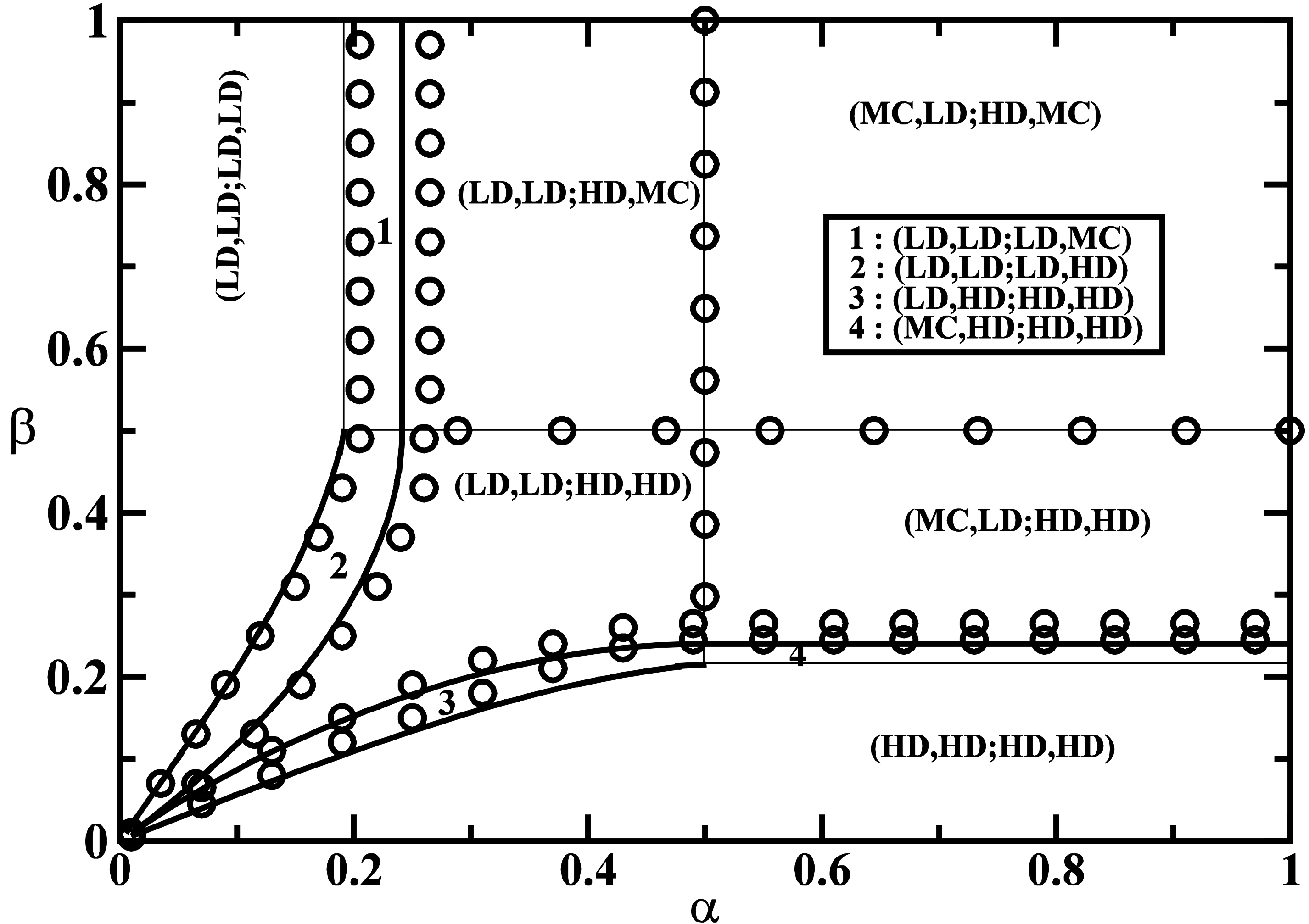


HD/LD

Agreement between our approximate theory and simulations is excellent at entrance/exit dominated phases, but for HD/LD phase – only qualitative agreement due to the neglect of correlations near the vertical junction

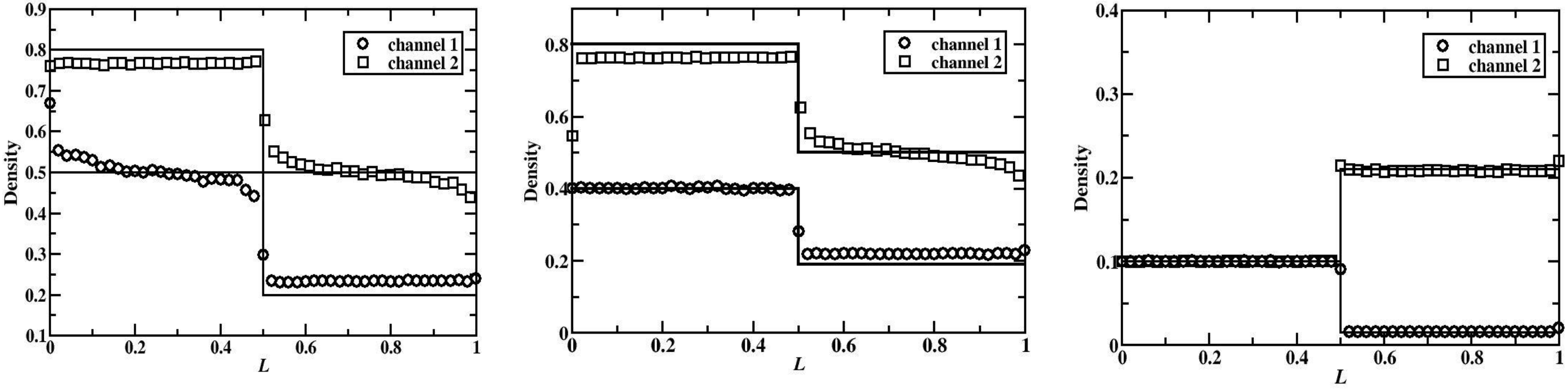
TWO-CHANNEL TASEP: INHOMOGENEOUS COUPLING

Phase diagram for asymmetric inhomogeneous coupling of two channels: complex -10 phases!



TWO-CHANNEL TASEP: INHOMOGENEOUS COUPLING

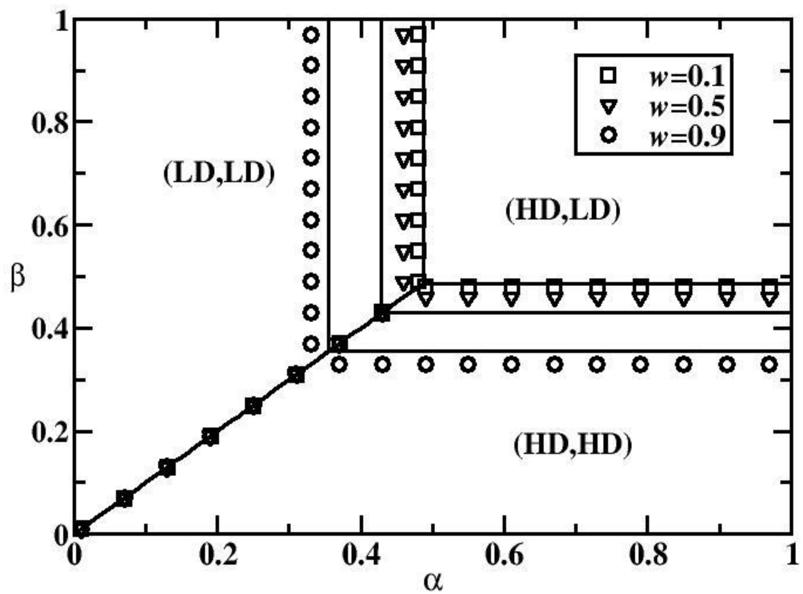
Density profiles for several phases for the asymmetric case:

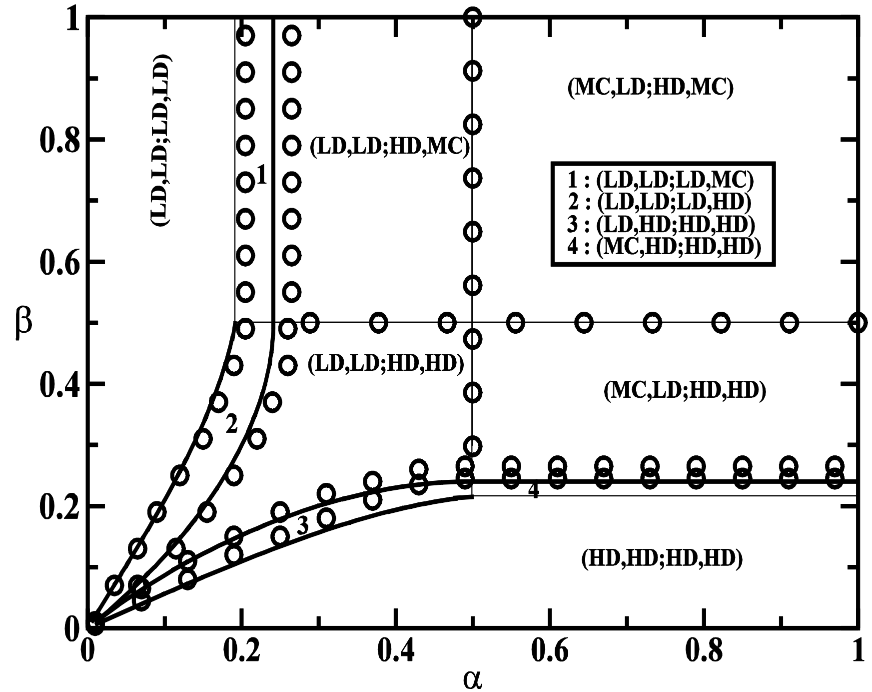


Again, our approximate theory is almost perfect for phases where entrance and/or exit are rate-limiting steps, and it is only qualitative for phases controlled by the processes near the vertical junction

TWO-CHANNEL TASEP: INHOMOGENEOUS COUPLING

Why phase diagrams are so different in symmetric and asymmetric cases?



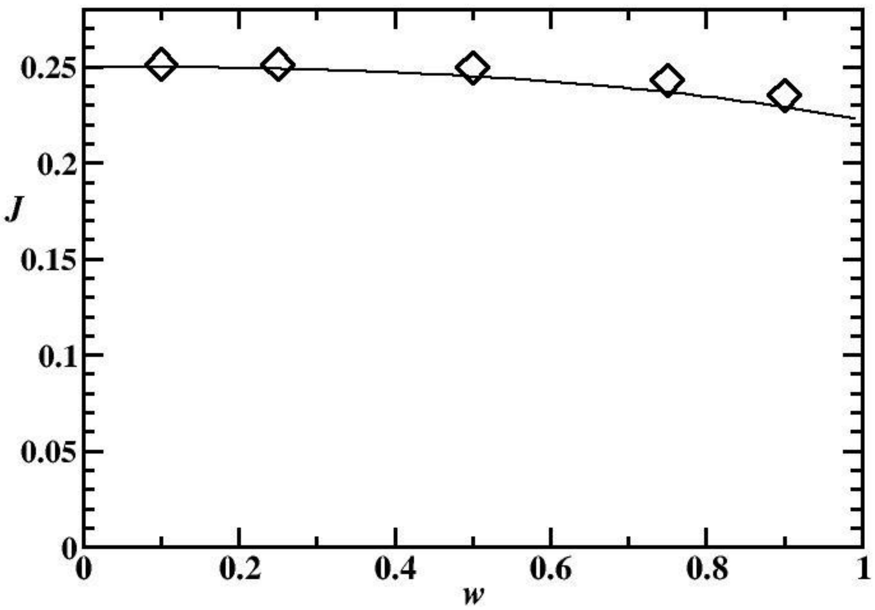


1) By symmetry currents in all segments are the same;
2) Maximal-current phase does not exist

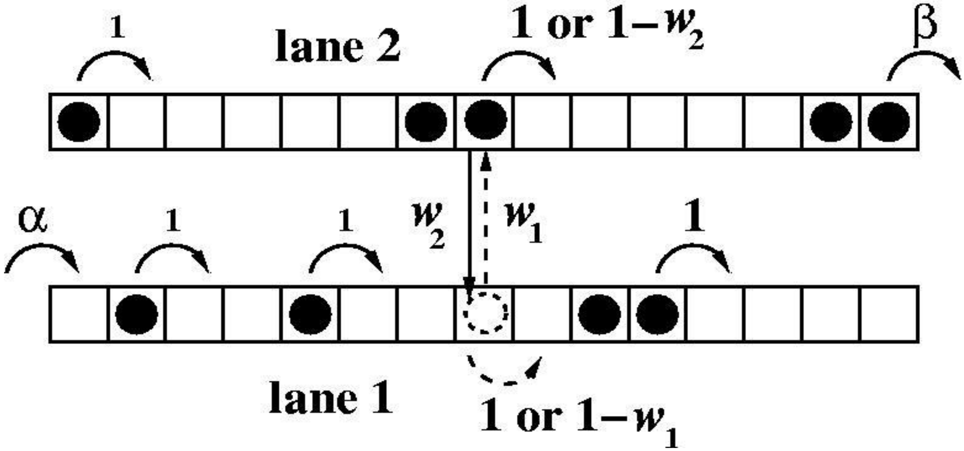
1) Current through segments are not the same
2) MC might exist at some conditions

TWO-CHANNEL TASEP: INHOMOGENEOUS COUPLING

Inter-channel coupling lowers the current per channel



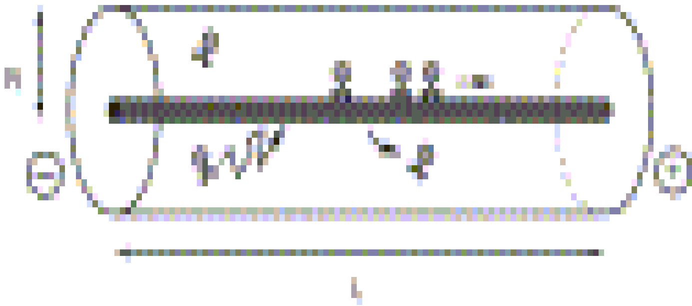
Increasing the inter-channel coupling lowers the effective entrance and exit rates in the segments



COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES

Stimulated by motor protein transport:

proteins bound to microtubules move in the biased fashion, the unbound motor proteins undergo the unbiased diffusion

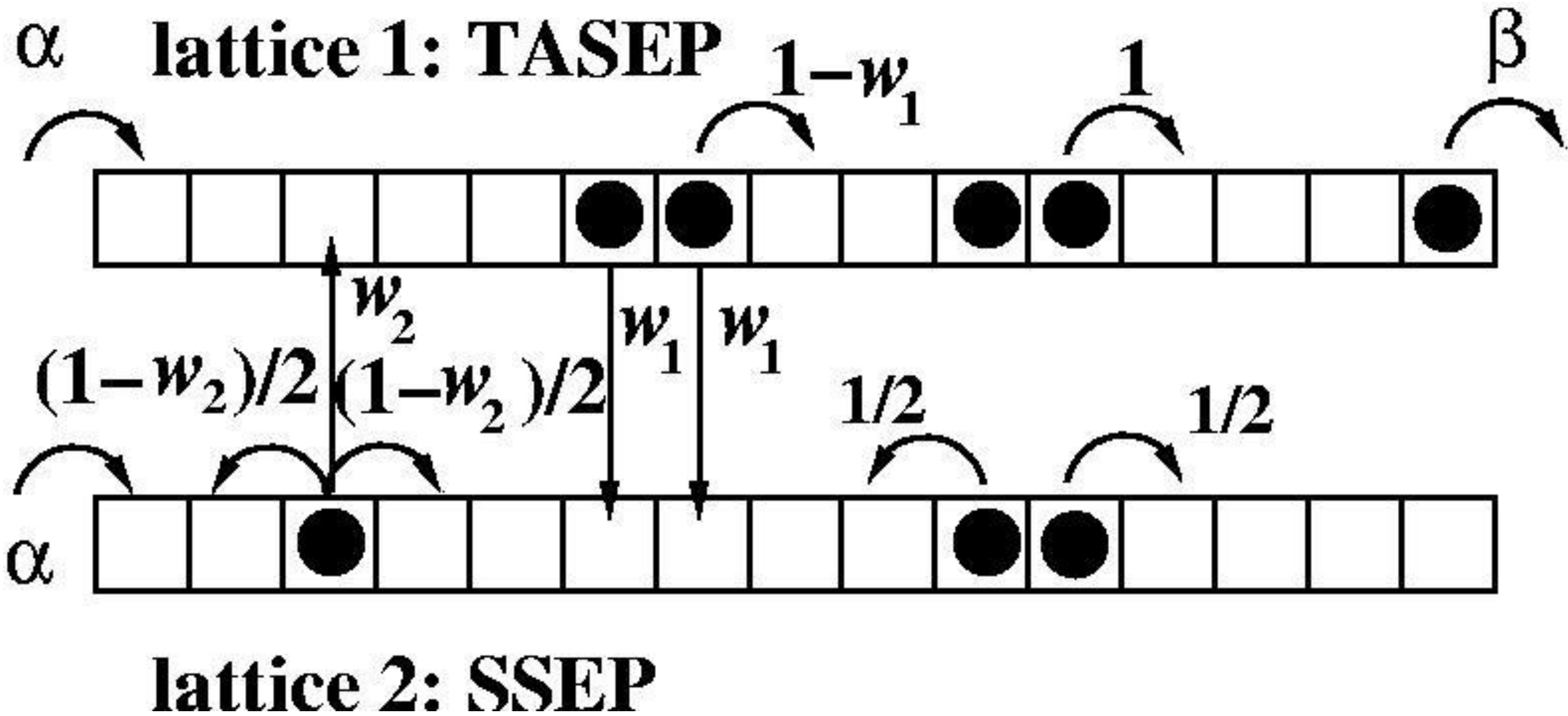


R. Lipowsky and S. Klumpp, *Physica A* **352** (2005) 53-112

Single-lane TASEP – 3 phases

Single-lane SSEP – 1 phase

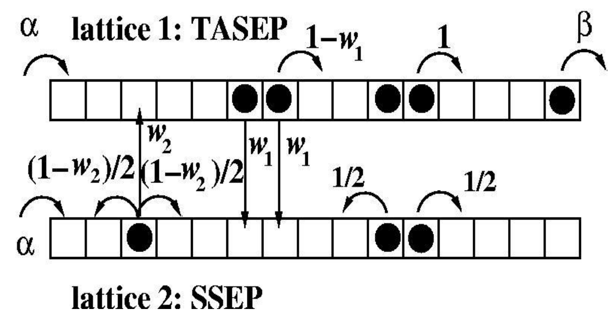
COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES



Exact solutions can be obtained in the strong coupling limits:

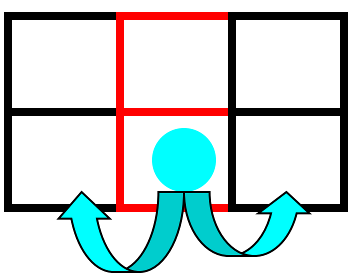
1) symmetric- $w_1 = w_2 = 1$; 2) asymmetric- $w_1 = 1$, $w_2 = 0$

COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES

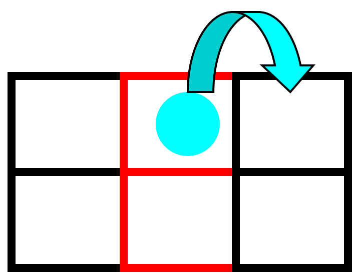


strong symmetric coupling $w_1=w_2=1$

How to get P_{00}?



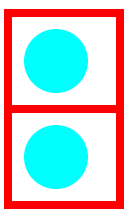
$(1-w_2)/2=0$



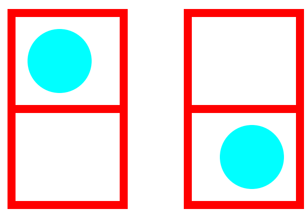
$1-w_1=0$

$P_{00}=0$

$P_{10}=P_{01}$ – by symmetry



"particle"

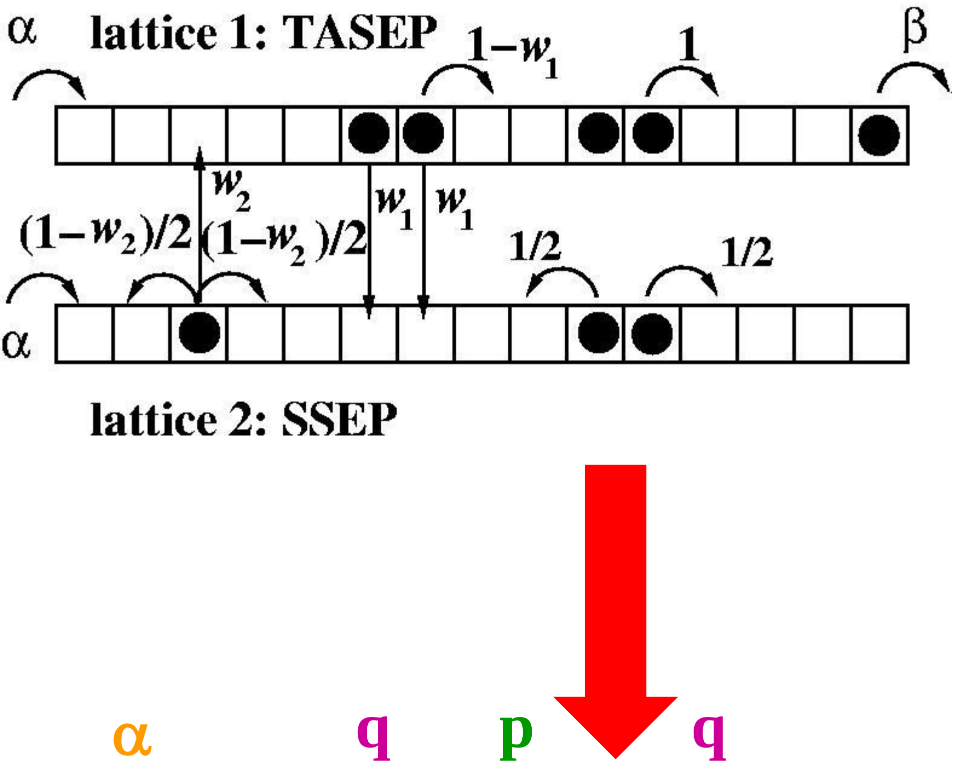


"hole"

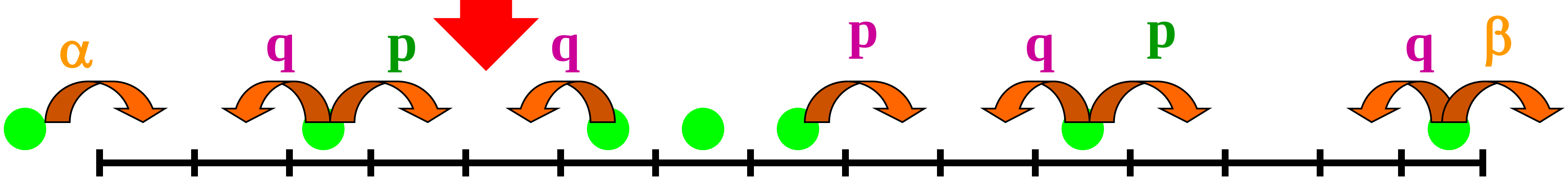
q=1/4 p=3/4

Partially asymmetric exclusion process (PASEP)

COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES

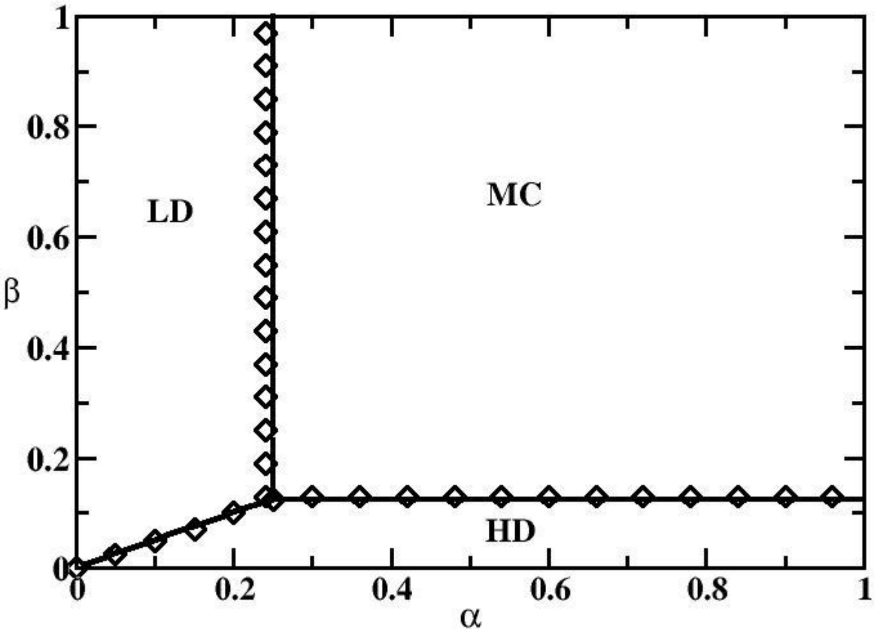


Symmetric coupling of TASEP and SSEP leads to an effective partially asymmetric exclusion process (PASEP) with known exact solutions

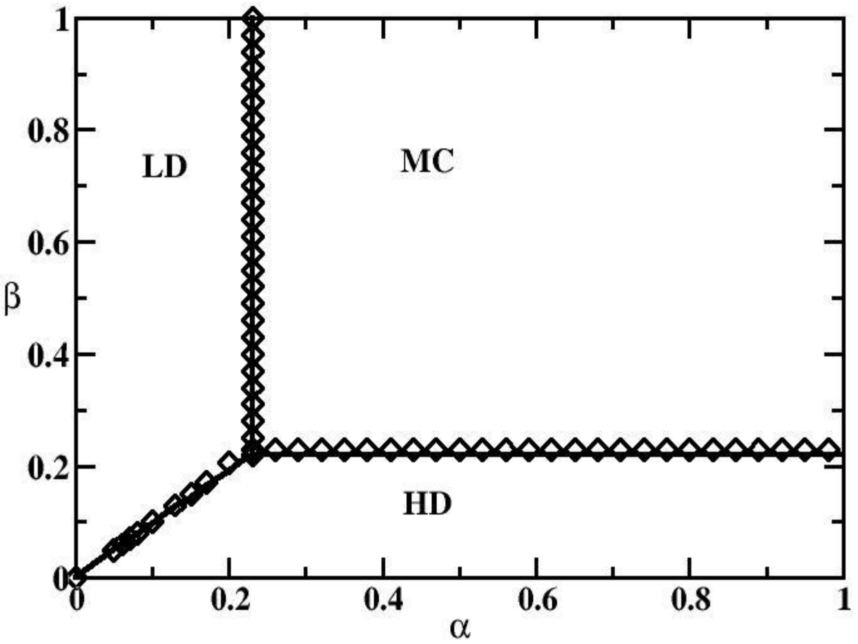


COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES

Phase diagrams for symmetric coupling:



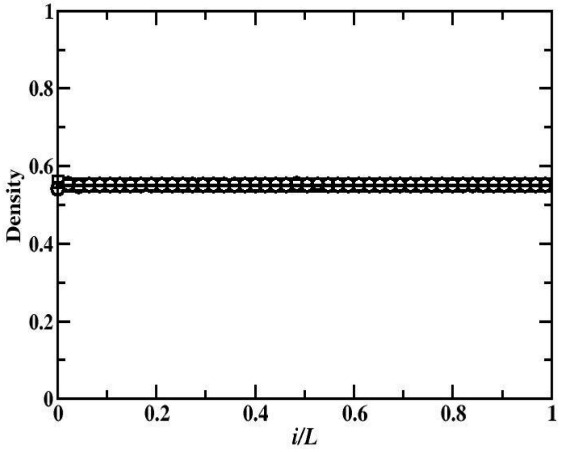
strong coupling $w_1=w_2=1$



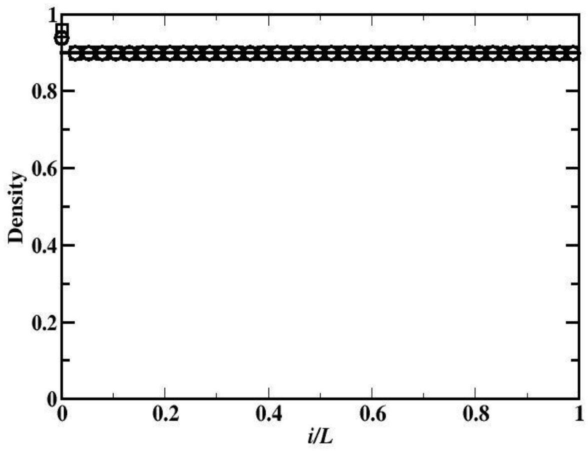
weak coupling $w_1=w_2=1/3$

COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES

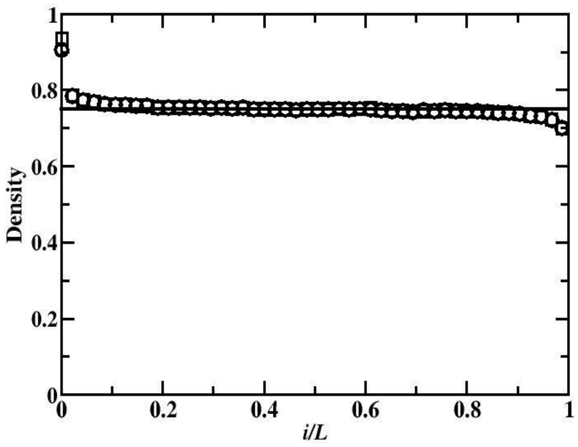
Density profiles for symmetric strong coupling $w_1 = w_2 = 1$



LD



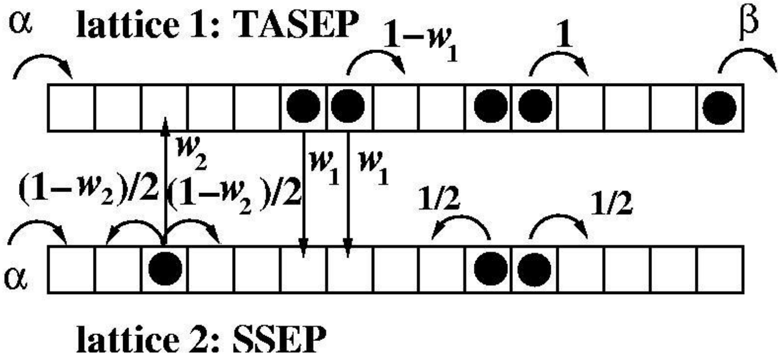
HD



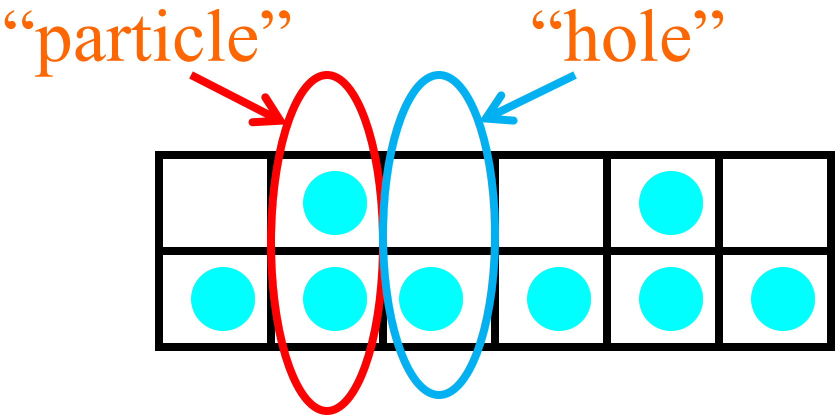
MC

Density profiles and particle currents are almost identical in both channels

COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES



strong asymmetric coupling $w_1=1$, $w_2=0$

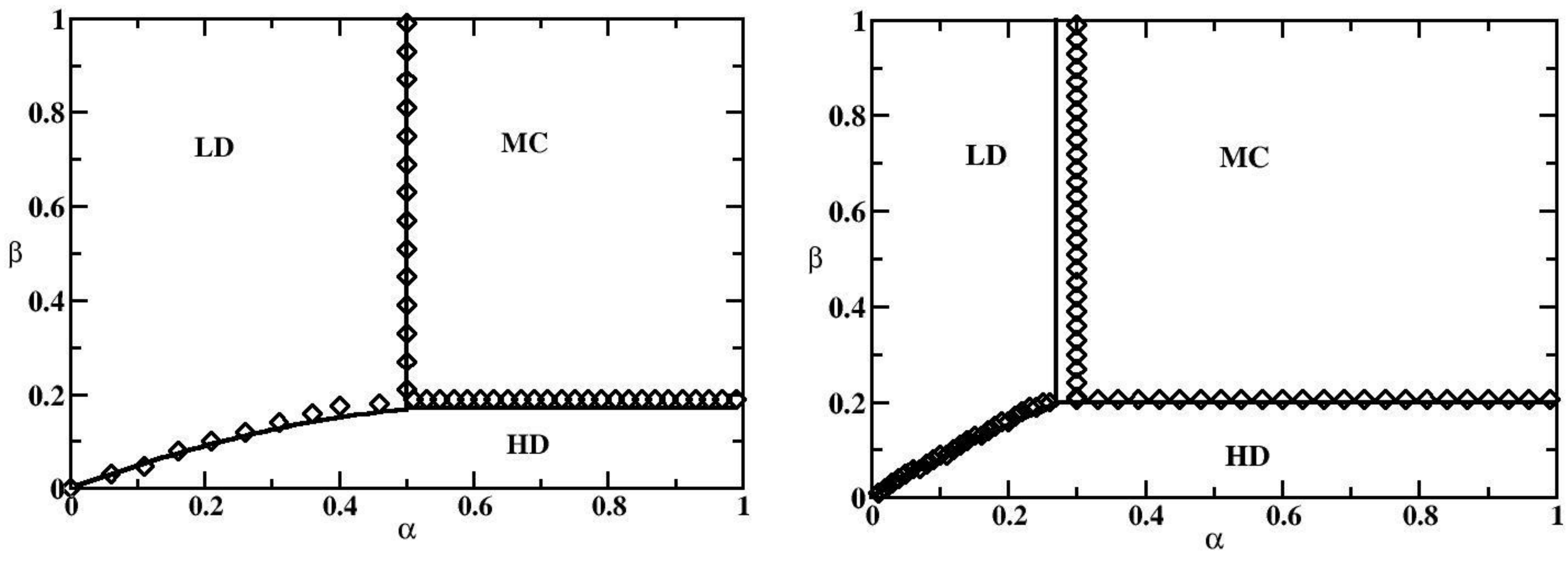


Asymmetric coupling of SSEP and TASEP leads to an effective TASEP

Channel 1 has a non-zero particle current
Channel 2 is fully occupied, flux is zero

COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES

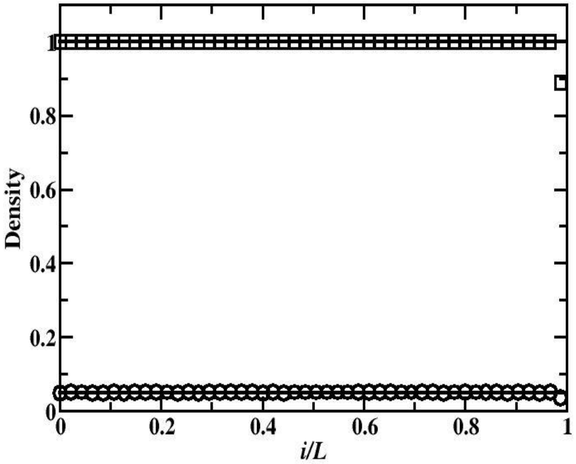
Phase diagrams for asymmetric coupling:



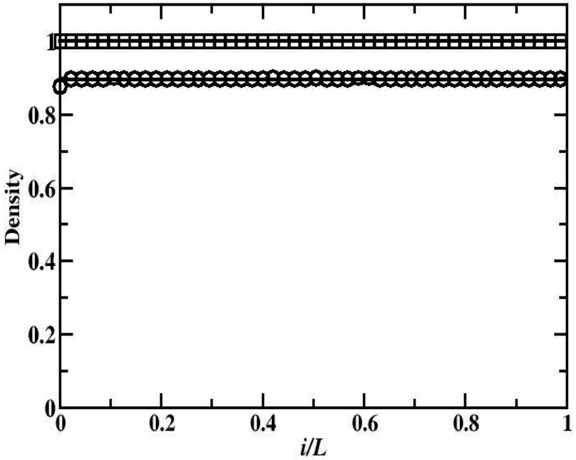
strong coupling w_1=1, w_2=0 weak coupling w_1=0.4, w_2=1/4

COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES

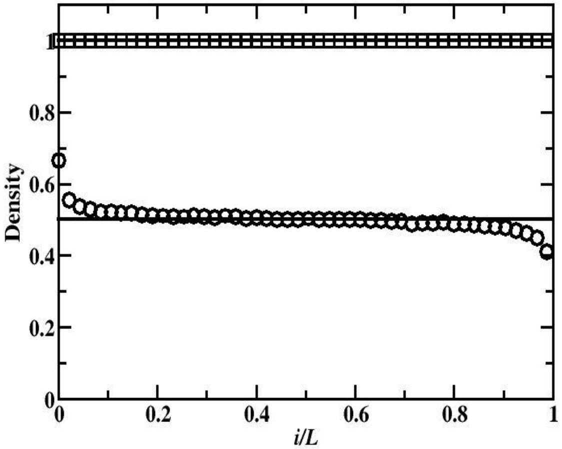
Density profiles for asymmetric coupling:



LD



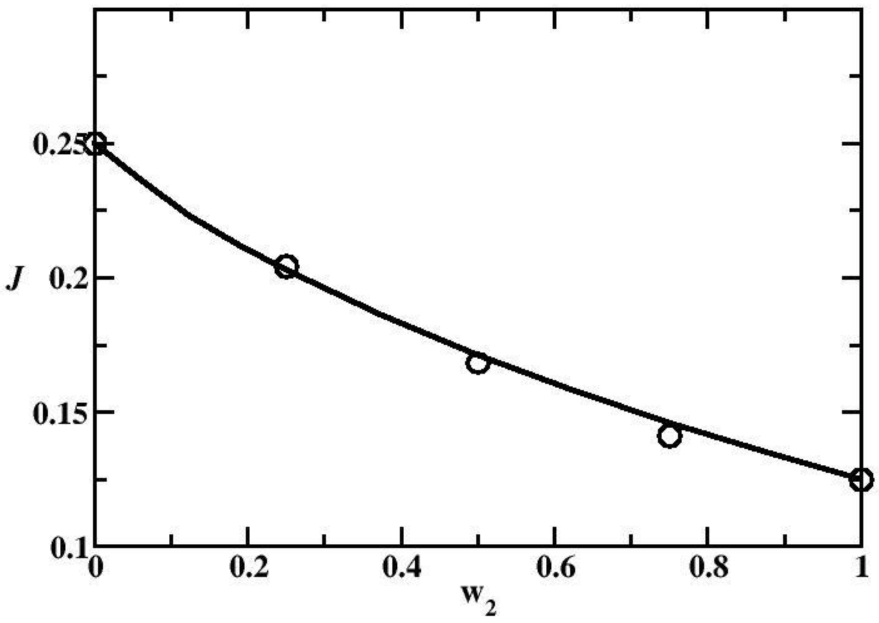
HD

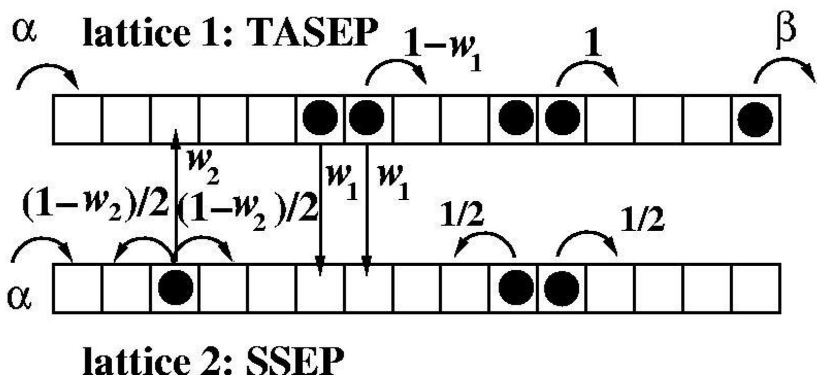


MC

strong coupling $w_1=1$, $w_2=0$

COUPLING OF SYMMETRIC AND ASYMMETRIC EXCLUSION PROCESSES





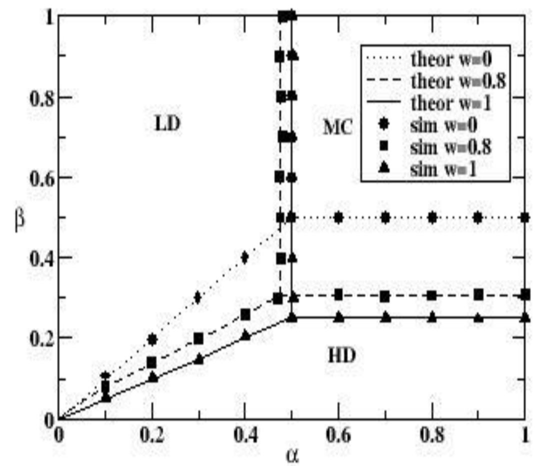
$\alpha=\beta=0.75,\ w_1=1$

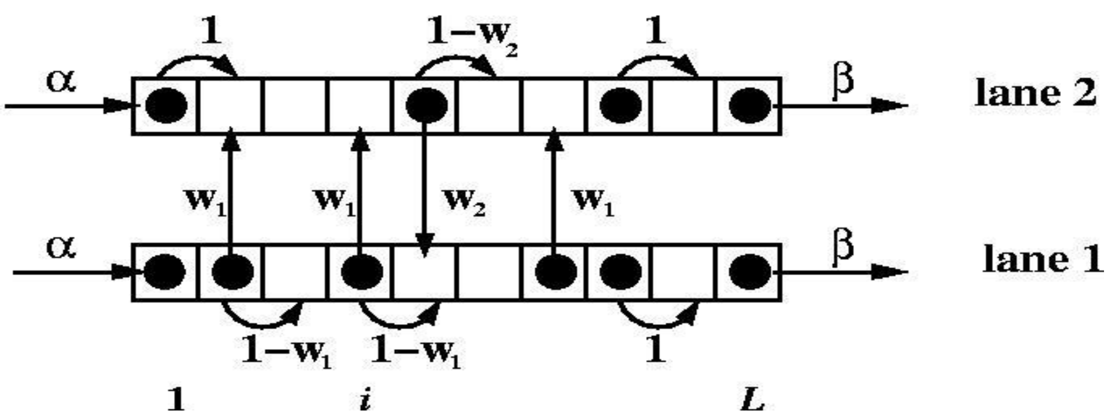
Breaking the symmetry in the coupling leads to the increase in the particle current through the system!

It might be important for motor proteins transport or other systems

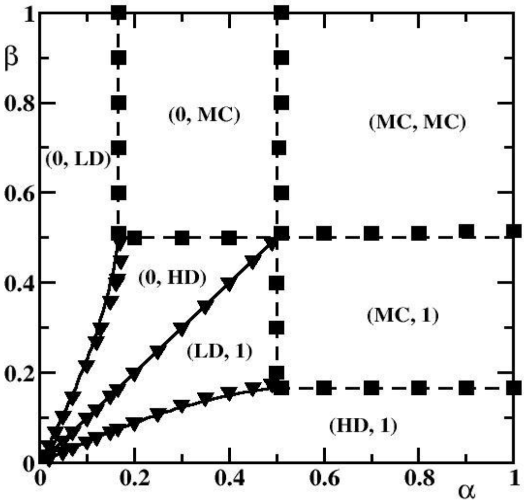
Results: Homogeneous Coupling

Symmetric coupling of 2 TASEP leads to an effective single-lane TASEP



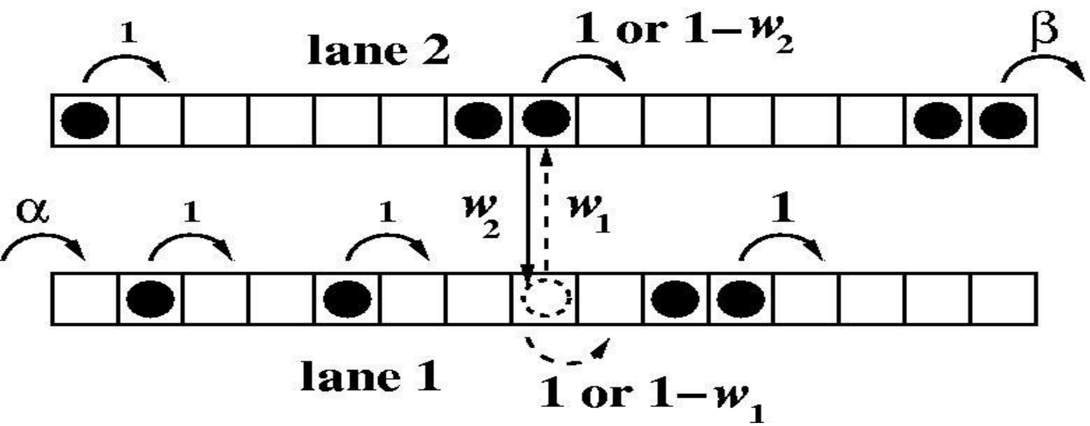


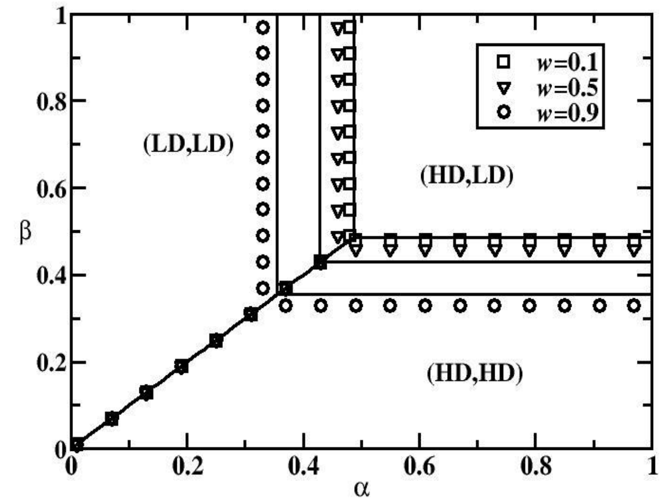
Asymmetric coupling between 2 TASEP produces complex stationary behavior



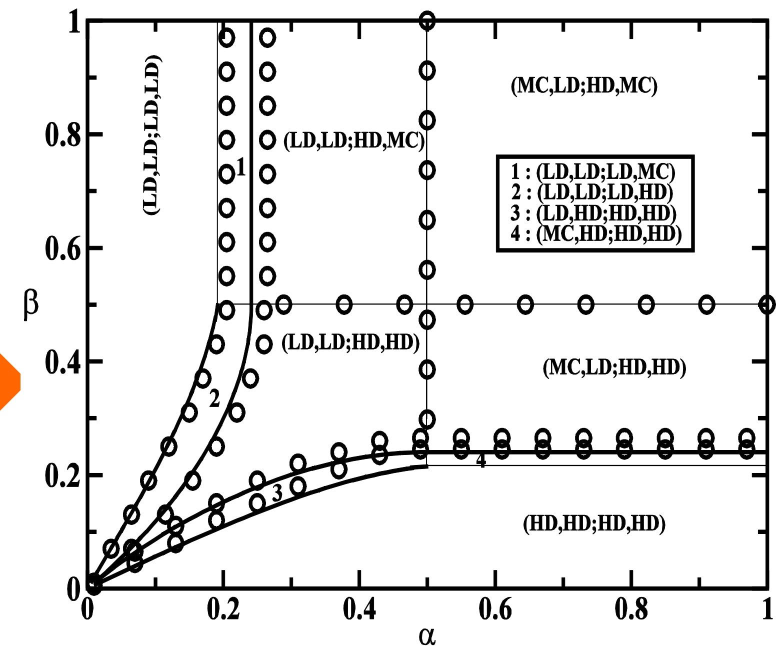
Results: Inhomogeneous Coupling

Symmetric inhomogeneous coupling of 2 TASEP can be viewed as TASEP with local defect



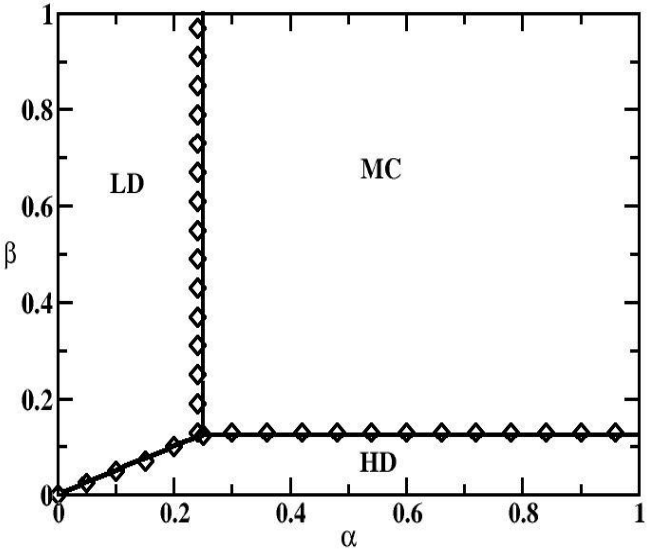


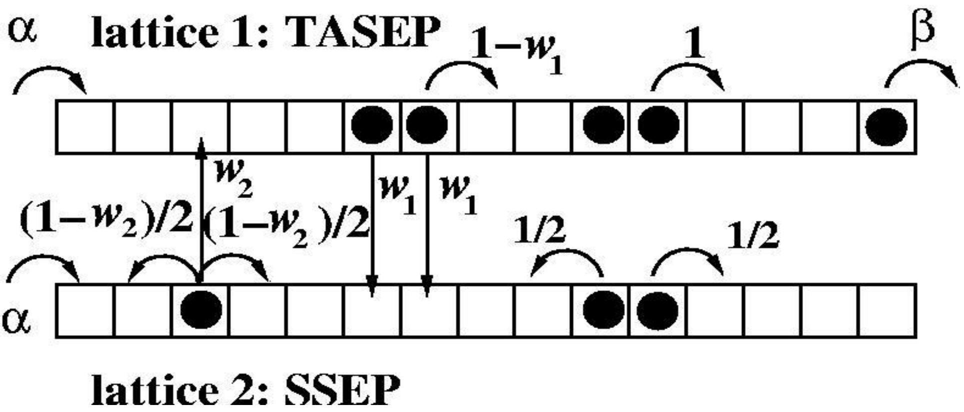
Asymmetric inhomogeneous coupling again leads to a complex dynamics



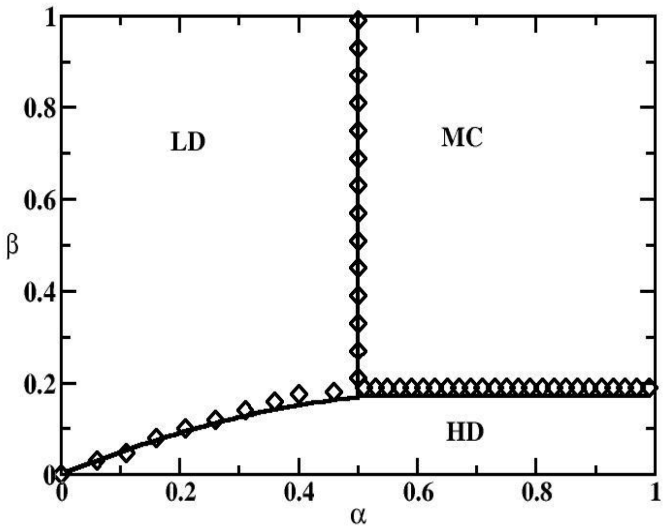
Results:TASEP+SSEP

Symmetric coupling TASEP and SSEP leads to an effective single-lane PASEP (partially assymetric)





Asymmetric coupling, in contrast, produces an effective single-lane TASEP



CONCLUSIONS:

- Coupled parallel exclusion processes are investigated using exact solutions, smart mean-field methods and Monte Carlo simulations
- Correlations in the vertical cluster are important
- Coupling decreases the current per channel and increases the bulk density
- Asymmetry in the coupling strongly effects the phase diagram: 3 phases for symmetric cases, and many more phases for the asymmetric cases
- Inhomogeneity in the coupling affects the overall dynamics of the system
- Coupling of SSEP and TASEP strongly depends on the symmetry in the vertical transitions

Acknowledgements:

Work: former graduate students E. Pronina and K. Tsekouras

Funding: National Science Foundation, The Welch Foundation

Publications:

1) J. Phys. A: Math. Gen. **37** (2004) 9907-9918;

2) *J. Stat. Mech*. (2005) P07010;

3) *J. Phys. A: Math Theor.* **41** (2008) 095002;

4) *J. Phys. A: Math Theor.* **41** (2008) 465001;