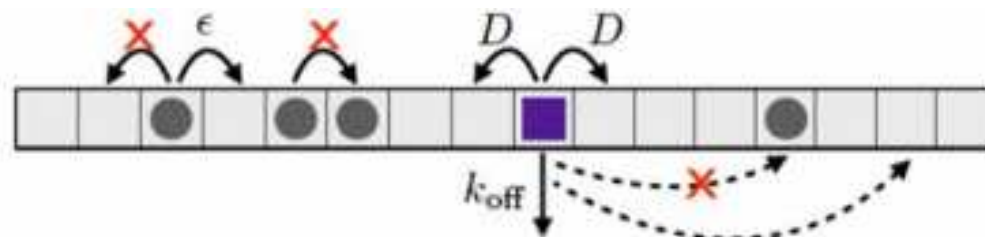


Dynamic roadblock particle in an exclusion process



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Thiruvananthapuram

Exclusion Process

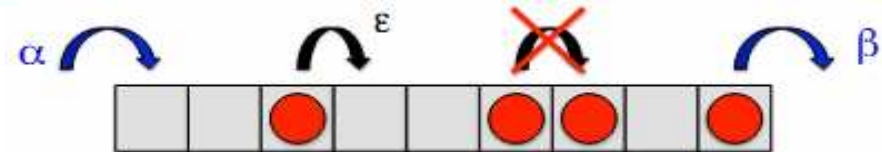
- ▶ Simple exclusion process: Nonequilibrium driven diffusive system of particles $\rightarrow$ exclusion interaction.
 - ▶ No multiple occupancy in one site



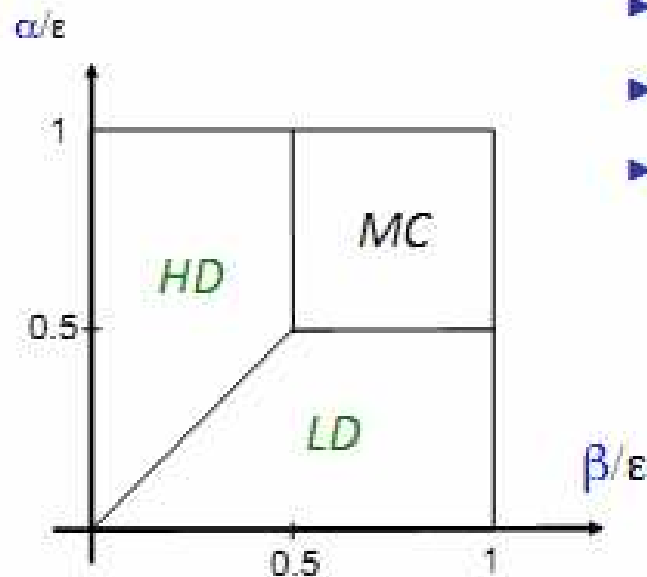
- ▶ Asymmetric Simple Exclusion Process (ASEP): Particles may hop to the right or left with a bias to one direction.
- ▶ Symmetric simple exclusion process (SSEP): Equilibrium process where the particles hop in both the directions with equal rates.
- ▶ Totally asymmetric simple exclusion process (TASEP): Particles hopping to the nearest-neighbor sites in one direction.

Models for dense traffic: TASEP etc.

Totally Asymmetric Exclusion Process



- ▶ Periodic Boundary Condition $\rightarrow$ Trivial steady state
 - ▶ Particle flux, $J = \epsilon \rho(1 - \rho)$
- ▶ Open Boundary Condition $\rightarrow$ Boundary-induced phase transition



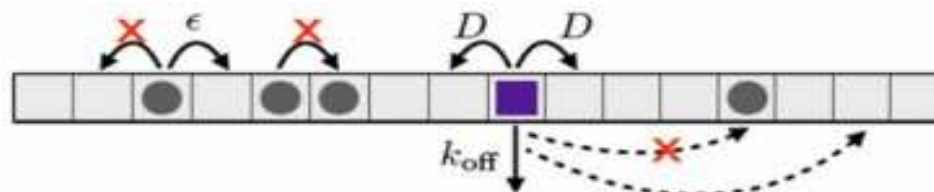
- ▶ LD $\rightarrow J = \alpha(1 - \alpha/\epsilon)$.
- ▶ HD $\rightarrow J = \beta(1 - \beta/\epsilon)$
- ▶ MC $\rightarrow J = \epsilon/4$

MacDonald et al. 1968,
Spitzer 1970, Krug 1991
exact solution: Derrida et al. 1993,
Schütz & Domany 1993

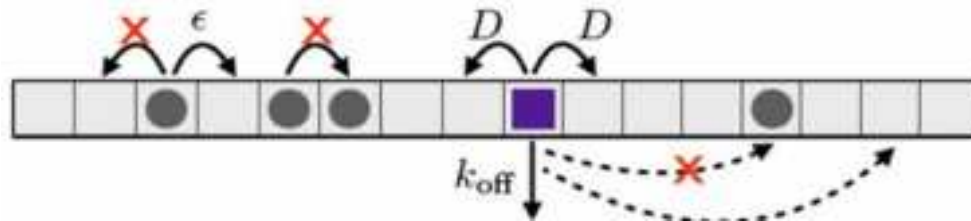
...
many TASEP variants

Exclusion processes with roadblock

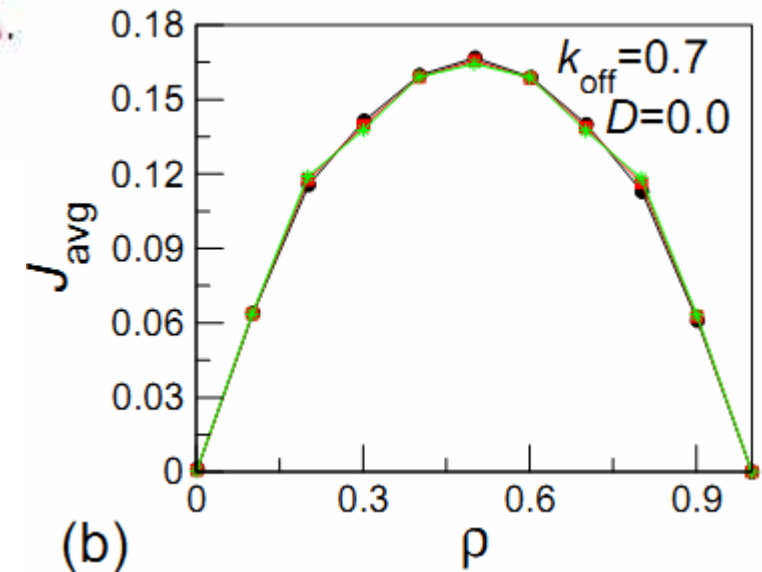
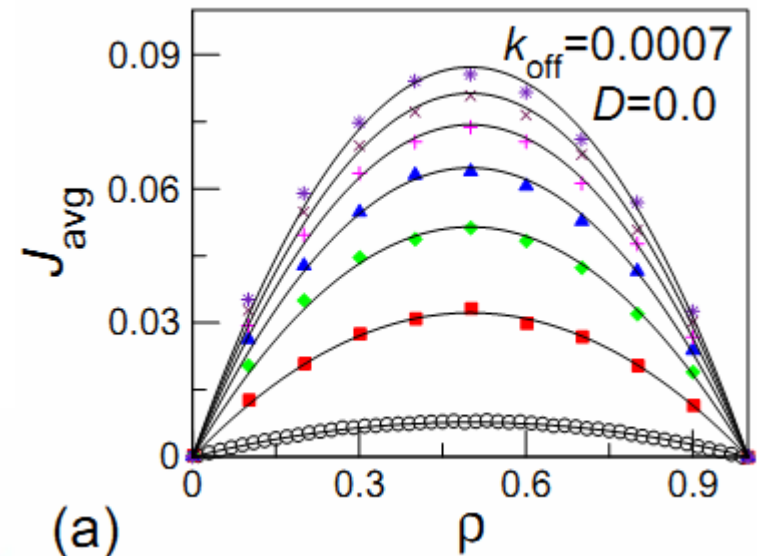
- ▶ Static Roadblock $\rightarrow$ No transport
- ▶ Dynamic roadblocks
 - ▶ open/close
 - ▶ on/off
 - ▶ diffusing ($\rightarrow$ ratchet)
 - ▶ hopping $\rightarrow$ reduced hopping at defect site
 - ▶ paused particle



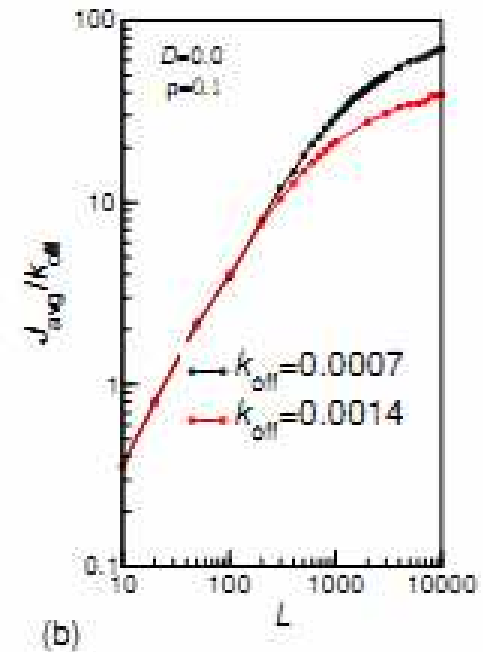
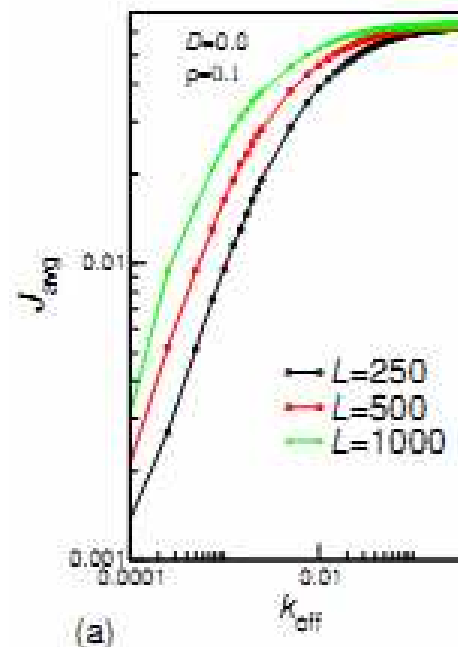
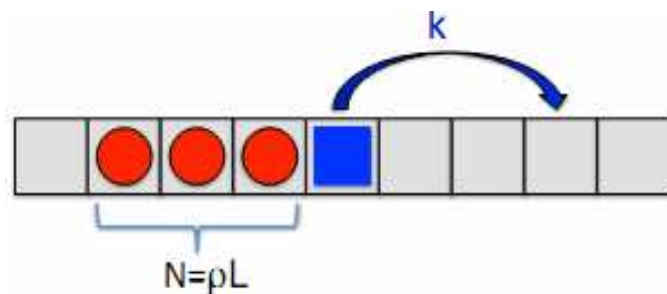
TASEP with a jumping roadblock



- ▶ Periodic Boundary Condition
- ▶ Rate k_{off} $\rightarrow$ long-range jumps
- ▶ Small k ($k < \frac{\epsilon}{L}$) $\rightarrow$ Flux depends on system size, L .
- ▶ Large k $\rightarrow$ TASEP



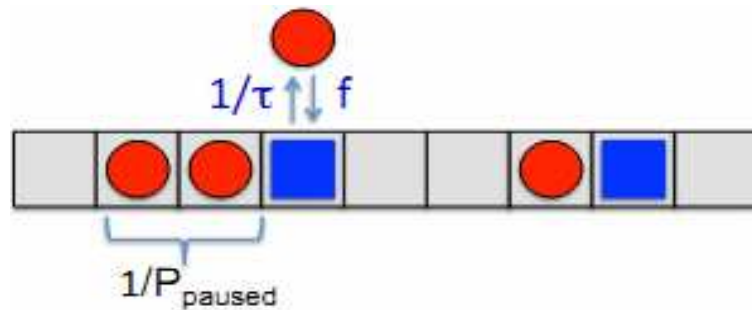
TASEP with a jumping roadblock



Sahoo, Dong, Klumpp, J Phys A 2015

- ▶ Jump over $\frac{L(1-\rho)}{2} \rightarrow$ All the particles follow
- ▶ Flux, $J_{avg} = v\rho = k_{off} \frac{N}{L} \left(\frac{L-N}{2} \right)$
- ▶ $= \frac{k_{off}L}{2} \rho(1-\rho) = \frac{k_{off}L}{2\epsilon} J_{TASEP}.$
- ▶ Crossover to TASEP behaviour $\Rightarrow \frac{k_{off}L}{2\epsilon} = 1.$

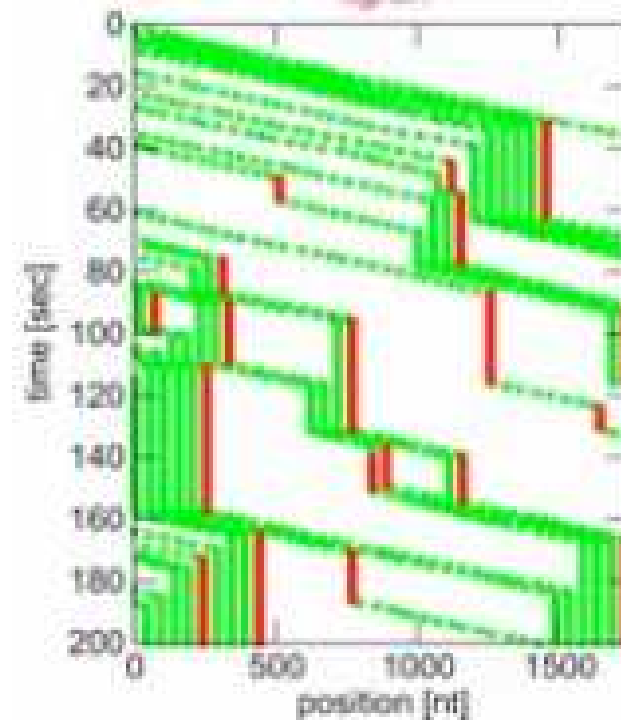
TASEP with pausing



- Pausing in transcription
 - Klumpp & Hwa 2008
 - Yuzenkova et al 2015

$$J = \frac{1}{\tau}(1 - \rho) \times \frac{1}{P_{\text{paused}}}$$

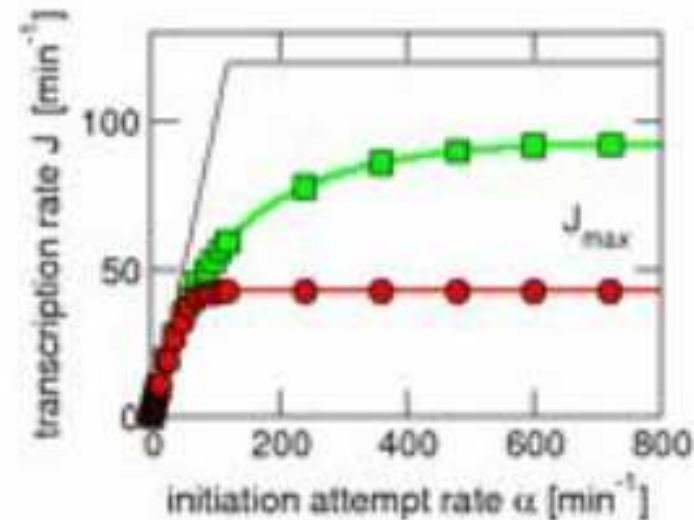
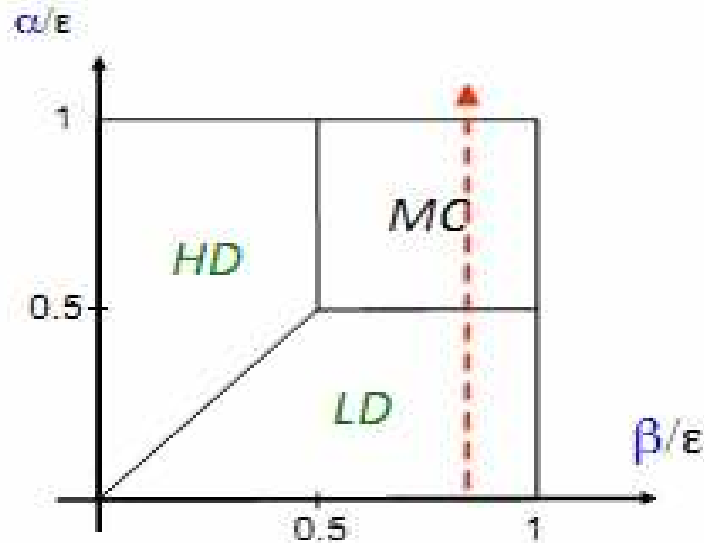
$$= \frac{1}{\tau}(1 - \rho) \times \frac{1 + f\tau}{f\tau}$$



also: Wang et al.
PRE 2014
3-state model

for tsx: generaliz.
to particle size > 1

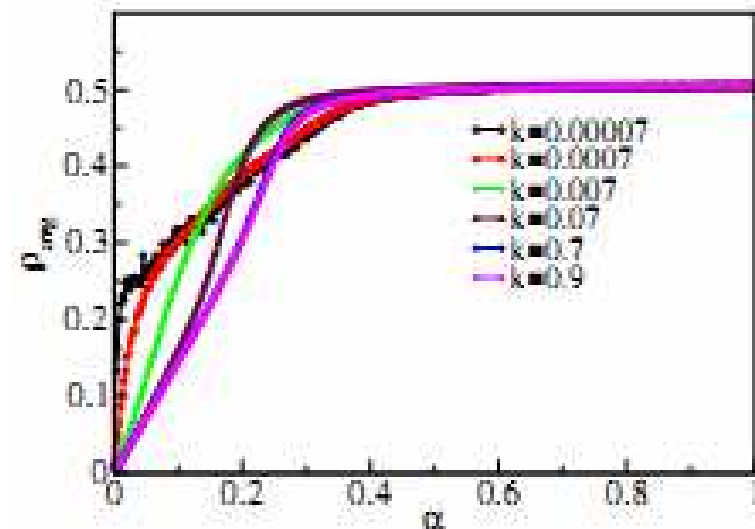
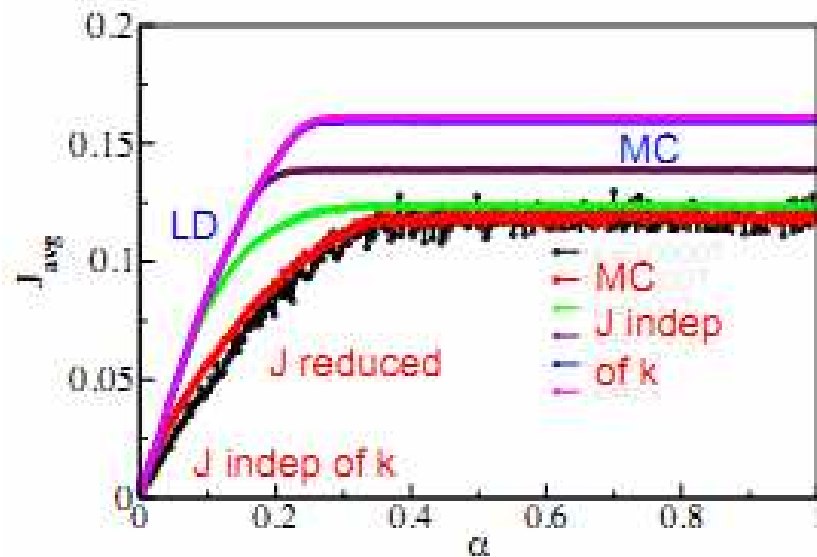
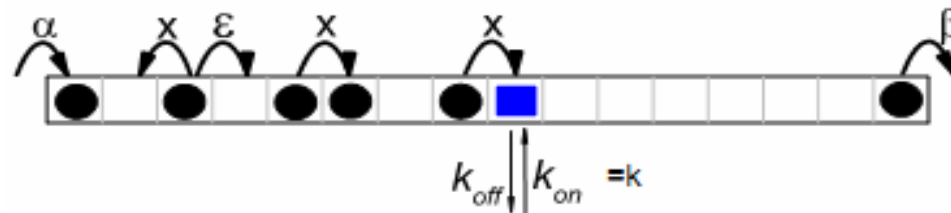
Open Systems



- ▶ No effect of the roadblock/defect/pausing on *LD* and *HD* phase.
- ▶ *MC* phase $\rightarrow$ Reduced flux $\rightarrow$ limited by the roadblock/pause/defects.

Janowsky & Lebowitz 1992,
Kolomeisky 1998,

Open System with on/off roadblock

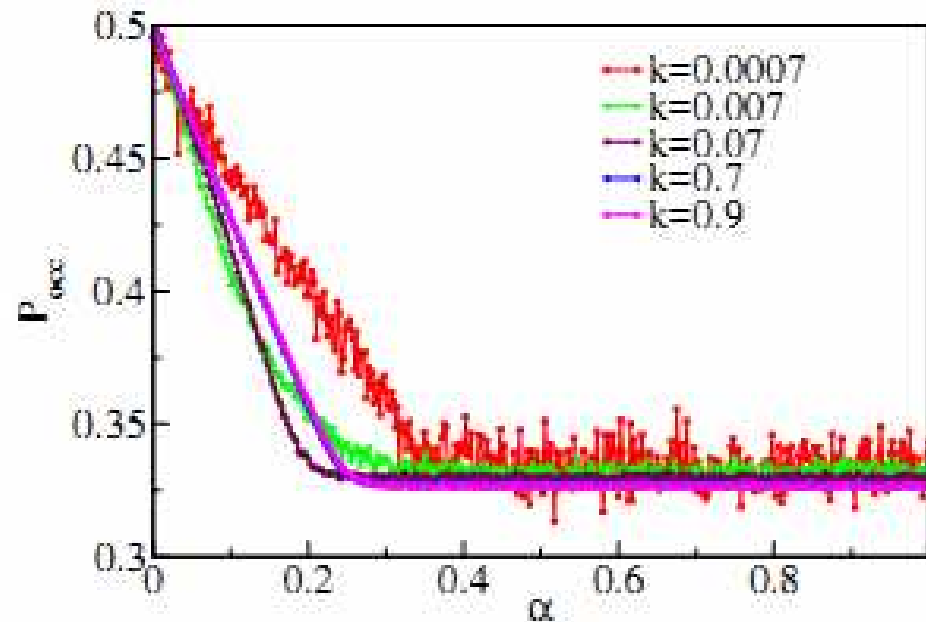


Sahoo & Klumpp, J Phys A 2016

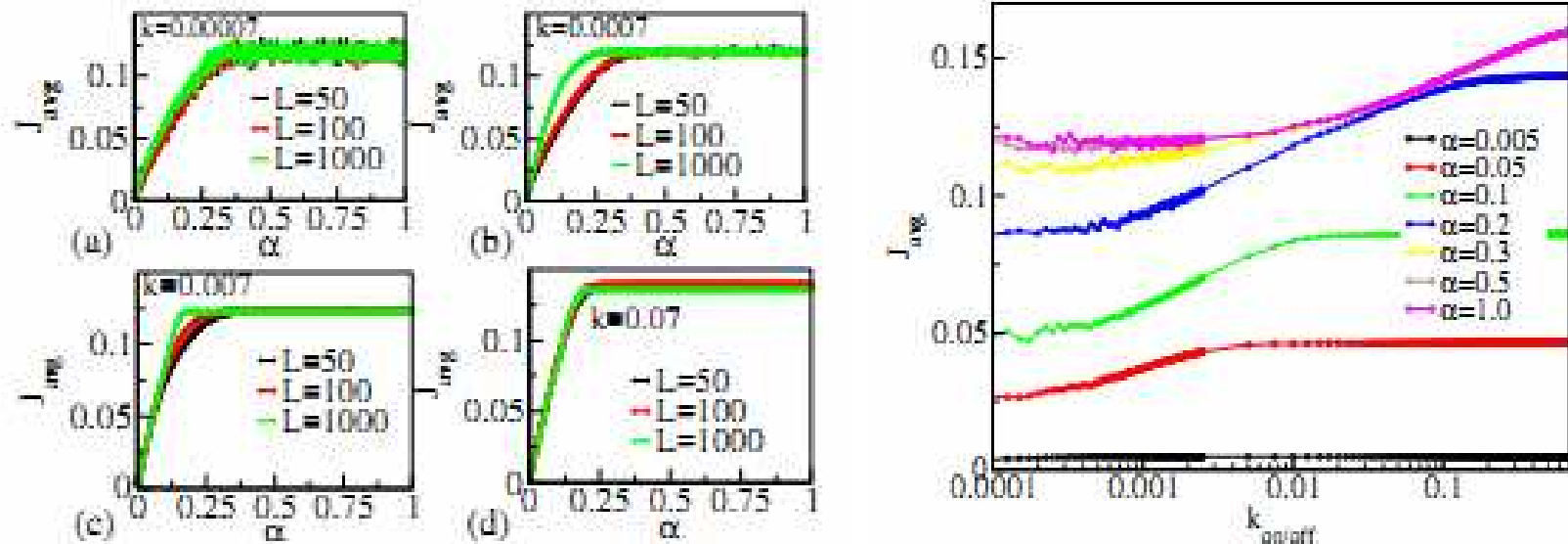
- ▶ Large $k \rightarrow$ Only MC affected $\rightarrow$ MC(d)
- ▶ Rapid roadblock ($k \geq \epsilon$) Slow site scenario
- ▶ small $k \rightarrow$ 3 regimes
- ▶ how small ? $k \leq \epsilon/L$ and $k \leq \alpha/L$

Open System with on/off roadblock

- ▶ Roadblock density $\rightarrow$ Prob. of roadblock occupying
- ▶ Decreases with increase in α



Open System with on/off roadblock



Sahoo & Klumpp, J Phys A 2016

- ▶ System size dependence
- ▶ Plateau at large $k \rightarrow$ LD phase
- ▶ Plateau at smaller $k \rightarrow$ Limiting cases

Concluding remarks & Outlook

- ▶ Dynamic roadblock particles/defects → Rich dynamic behavior
- ▶ System size effects seems typical
- ▶ Applications: Transcription and translation dynamics, regulatory mechanisms.

Acknowledgement

- ▶ Stefan Klumpp
(Institute for Nonlinear Dynamics, Göttingen University)



- ▶ J. J. Dong
(Bucknell University, USA)

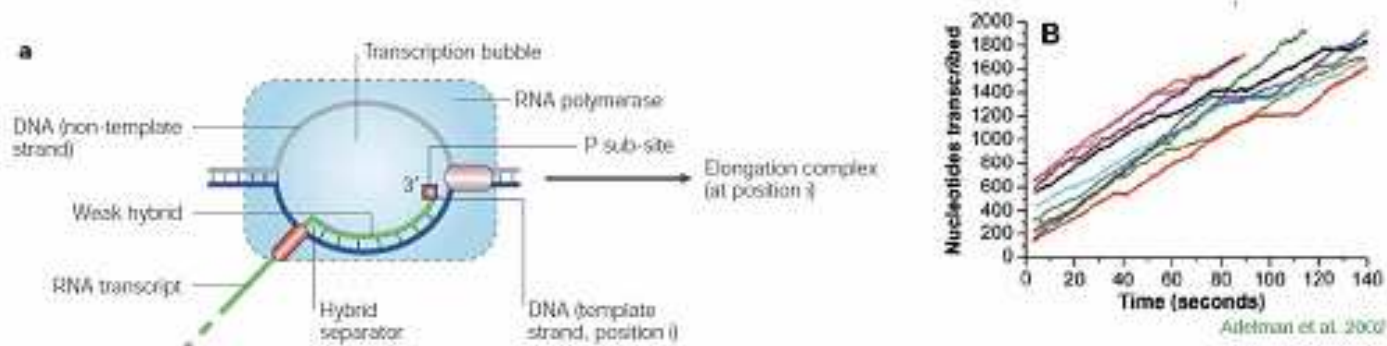


THANKS

??????????

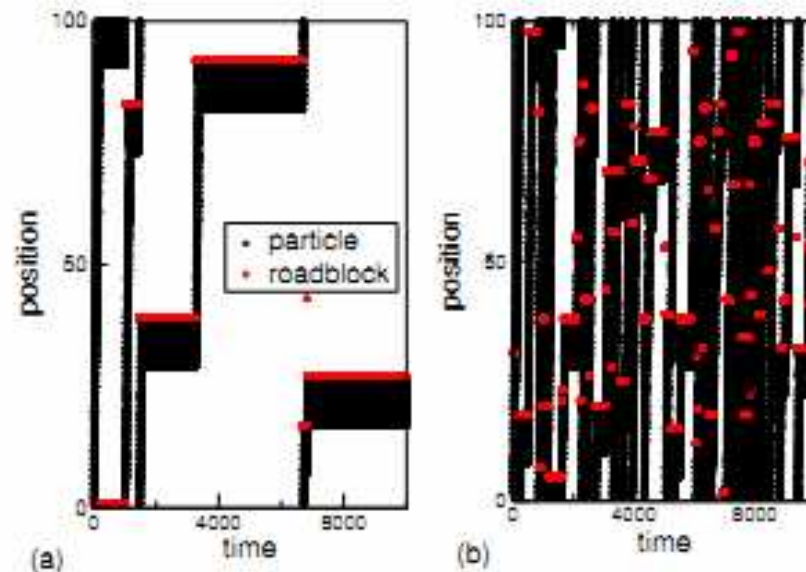
Transcription & Blockage in Transcription

- ▶ Transcription → RNA polymerase moves along the length of a DNA template by a single base pair → creating a complementary RNA.
- ▶ One single nucleotide elongation step
 - ▶ appropriate binding of NTP
 - ▶ single step forward



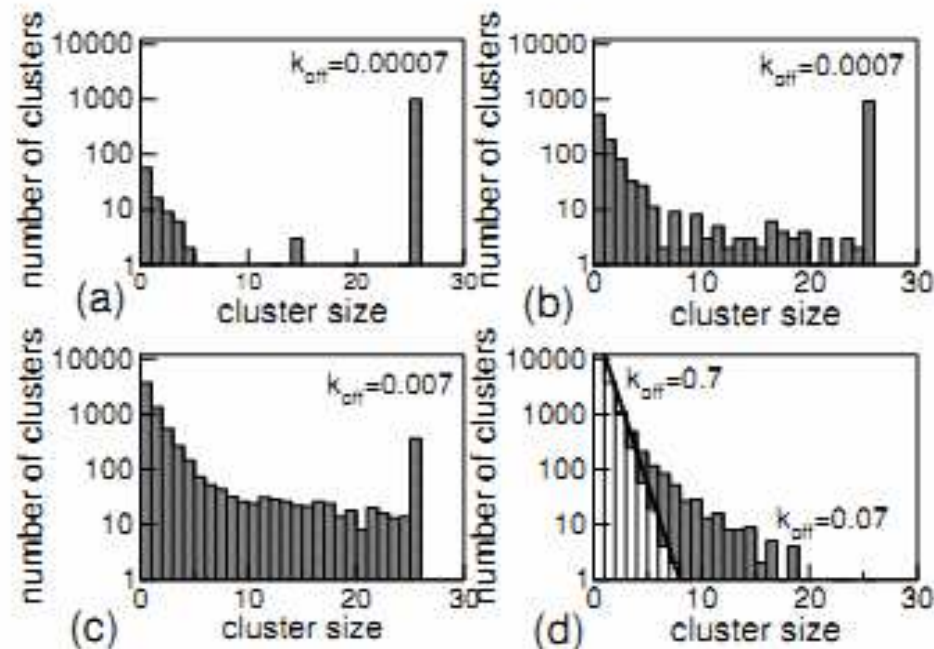
- ▶ Transcriptional elongation is interrupted with pauses/errors/blockages.
- ▶ Pauses are of stochastic in nature → different kinds → DNA binding proteins/transcription factors.

Space-time trajectory of the dynamics



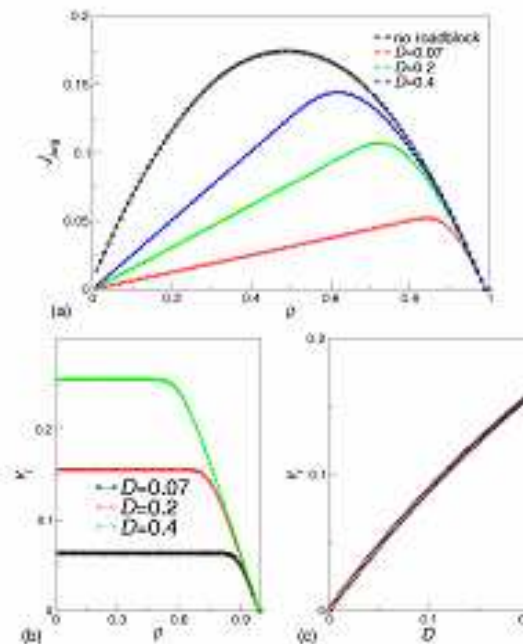
- ▶ For small k_{off} → Sudden (short-lived) burst of particle flow → until dense cluster of particles has formed again behind the roadblock.
- ▶ For large k_{off} , Flow of particles is more continuous.

Cluster size distributions



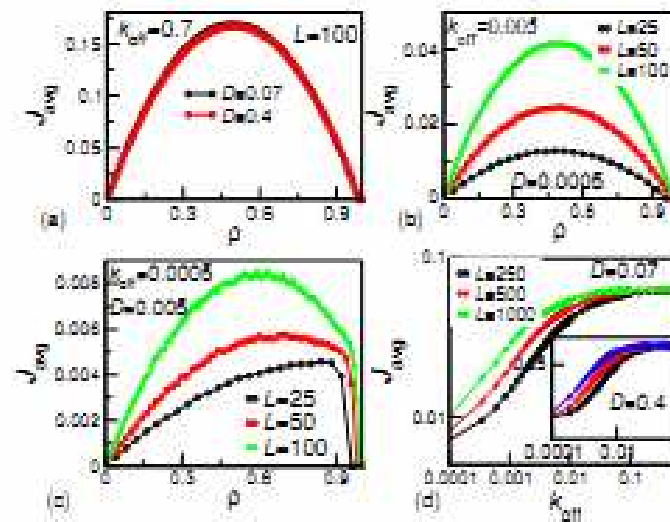
- ▶ For small k_{off}
 - ▶ Distributions $\rightarrow$ dominated by a peak cluster size, N .
 - ▶ A minor peak (smaller clusters) $\rightarrow$ Breaking up of clusters.
- ▶ For large k_{off} $\rightarrow$ The cluster size distribution is exponential $\rightarrow$ Conventional TASEP.

Diffusive dynamics of roadblock without unbinding



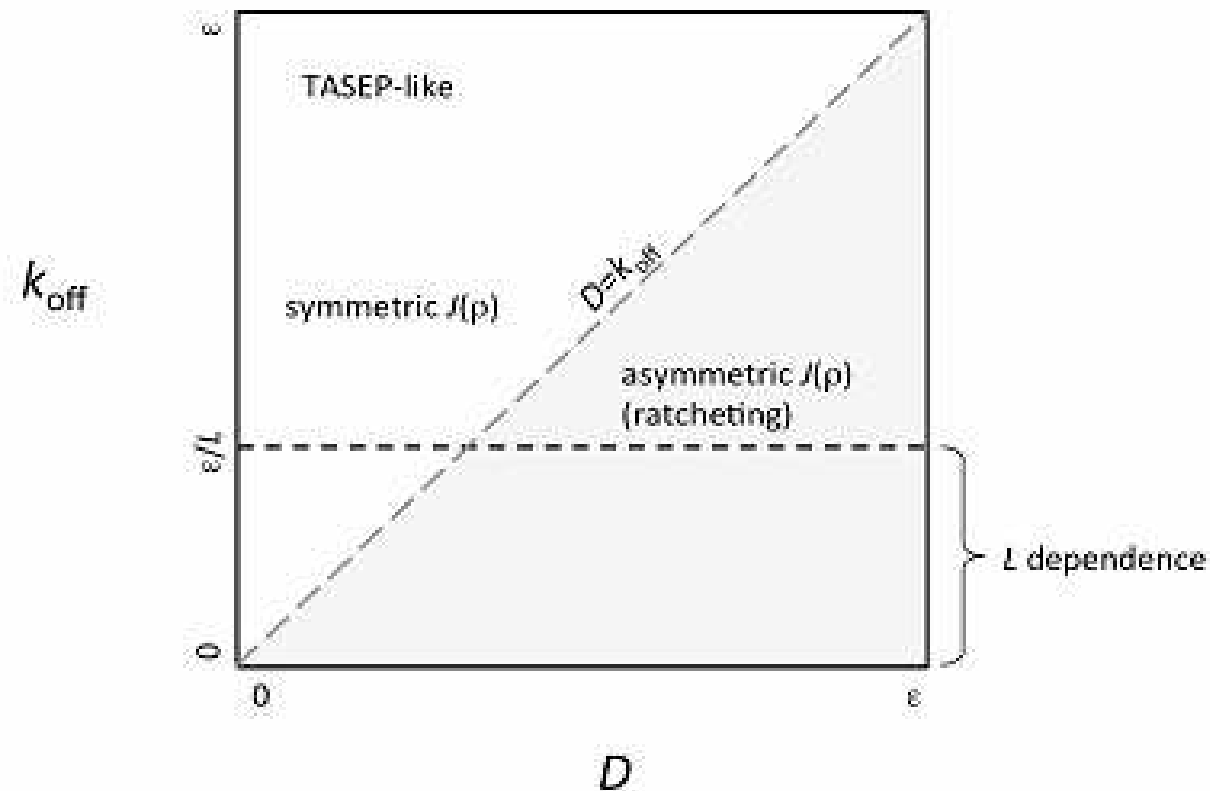
- Current-density relation $\Rightarrow$ Asymmetry with maximal current at $\rho > 0.5$.
- Roadblock velocity, $v_r \rightarrow$ constant over wide range of particle density $\rightarrow$ decreases at higher densities.
- Analytical estimate, $v_r = \frac{D\epsilon}{(D+\epsilon)}$ $\rightarrow$ Good agreement with simulation.

Combined effect of diffusive dynamics and unbinding



- ▶ Large k_{off} ($k_{off} > \epsilon/L$) $\rightarrow$ TASEP like behavior $\rightarrow$ independent of D as well as system size, L .
- ▶ Small k_{off} ($k_{off} < \epsilon/L$) $\rightarrow$ System size dependence, independent of D .
- ▶ Both $k_{off}, D \ll \epsilon/L$,
 - ▶ $k_{off} < D \rightarrow$ Ratchet like behavior
 - ▶ $k_{off} < D \rightarrow$ Current density relation symmetric.

Schematic summary of different dynamic behavior



- Different dynamic behaviour $\rightarrow$ New phase diagram in (k_{off}, D) space.