Random walk theory in the case of generalized Totally Asymmetric Simple Exclusion Process

Теория случайных блужданий в случае обобщенного Полностью Асимметрического Процесса с Простым Исключением

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We are inspired to summarize some of our new results, concerning a model of aggregation and fragmentation of clusters of particles, obeying a stochastic discrete-time discrete-space kinetics of the generalized TASEP (gTASEP). The phase structure (diagram) of the model system, depending on the rates of input and output of particles at the open ends of the chain, the gap distribution between neighboring clusters of jammed aggregates at large lengths L of the chains were investigated by using both theoretical and numerical methods. The special focus is on the use (application) of Random walk theory in our investigation.

Keywords: non-equilibrium phenomena, one-dimensional processes, generalized TASEP, Random walk theory, stationary states, phase transitions

Based on:

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Brankov J.G., Bunzarova N. Zh., Pesheva N. C., Priezzhev V. B.. (2018) *A model of irreversible jam formation in dense traffic*. **Physica A: Statistical Mechanics and its Applications**

N. Zh, Bunzarova, N. C. Pesheva, V.B. Priezzhev, and J.G. Brankov (2017), *A model of jam formation in congested traffic*, **Journal of Physics: Conf. Series,** 012026, 936, IOP,

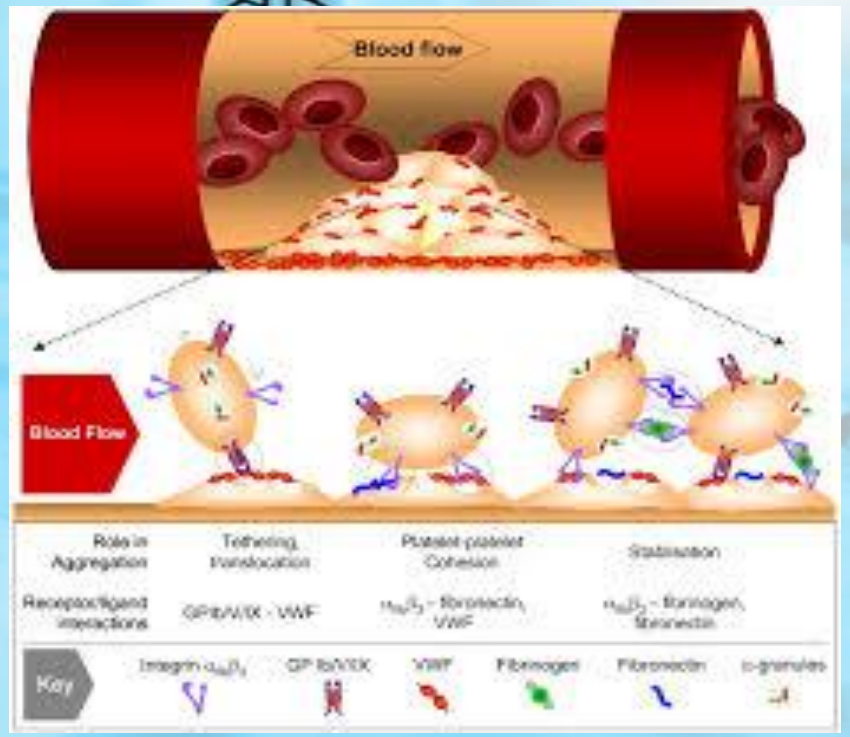
N. Zh. Bunzarova and N. C. Pesheva (2017) *One-dimensional irreversible aggregation with dynamics of a totally asymmetric simple exclusion process*, **PHYSICAL REVIEW E, 95, 052105, 2017**

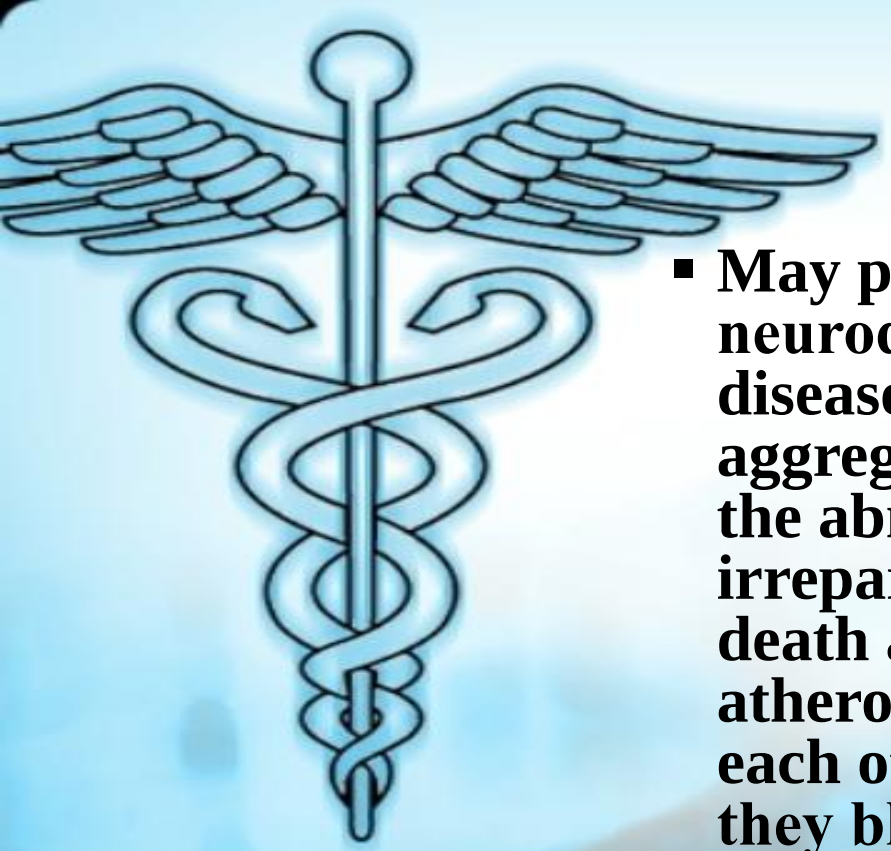
Motivation

Aggregation and fragmentation of clusters

of arbitrary size arises in many physical-chemical processes: aerosol physics, polymer growth, aggregation of platelets, protein aggregation and even in astrophysics.

- Aggregation of platelets is an important mechanism of clumping together of blood cells, possibly forming a clot. Platelets, also called thrombocytes, have no cell. In the circulating blood the platelets are normally carried along separately from each other. When the wall of a blood vessel is injured, it activates platelets to adhere to it immediately and to each other to form aggregates on the damaged area. In the first stage, the platelets aggregation is reversible, but later the process may become irreversible.



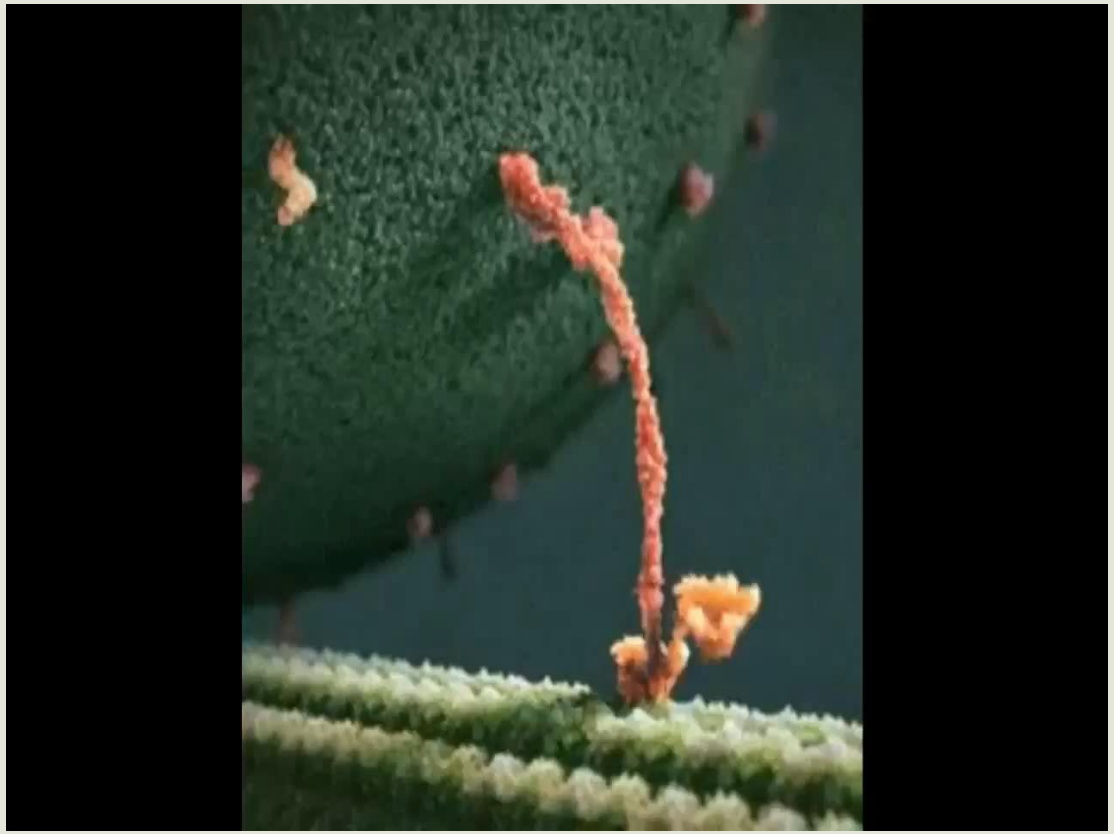


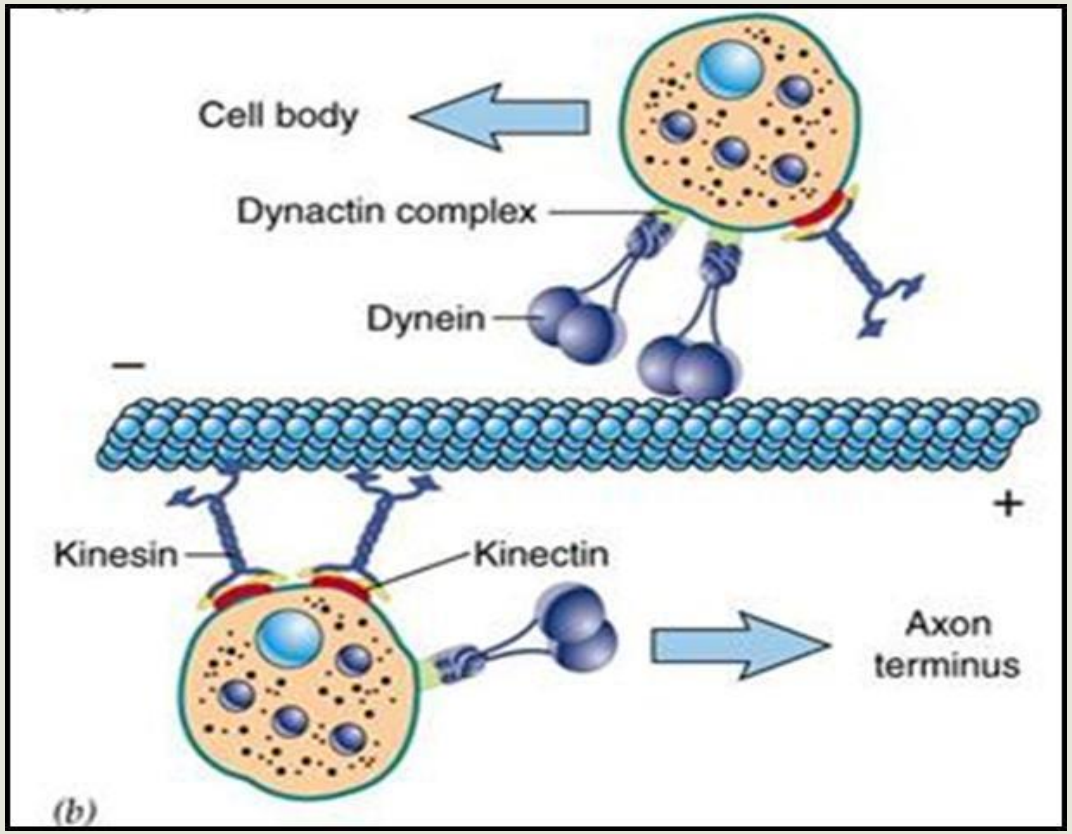
- **Irreversible aggregation**

  - **May play a destructive role in biochemistry. Many neurodegenerative disease (Alzheimer's disease, Parkinson's disease, and prion diseases) are characterized by intracellular aggregation and deposition of pathogenic proteins. Moreover, the abnormal irreversible aggregation of ribosomes leads to irreparable damage of protein synthesis and results in neuronal death after focal brain ischemia. When diseases, for example, atherosclerosis, damage the intima platelets adhere to it and to each other. The aggregates so formed may increase in size until they block the flow of blood. That's why the aggregation of platelets is one of the direct reasons of thrombosis.**
  - **The ability to control protein aggregation could be an important tool in the drug development**

The model we study here is designed to be simple rather than realistic, but we believe that it can be helpful in understanding various types of systems in Nature and in particular in biophysics.

TASEP has been used since **1968** to model different biochemical processes: kinetics of protein synthesis, molecular motors traffic, collective effects of genetic transcription.



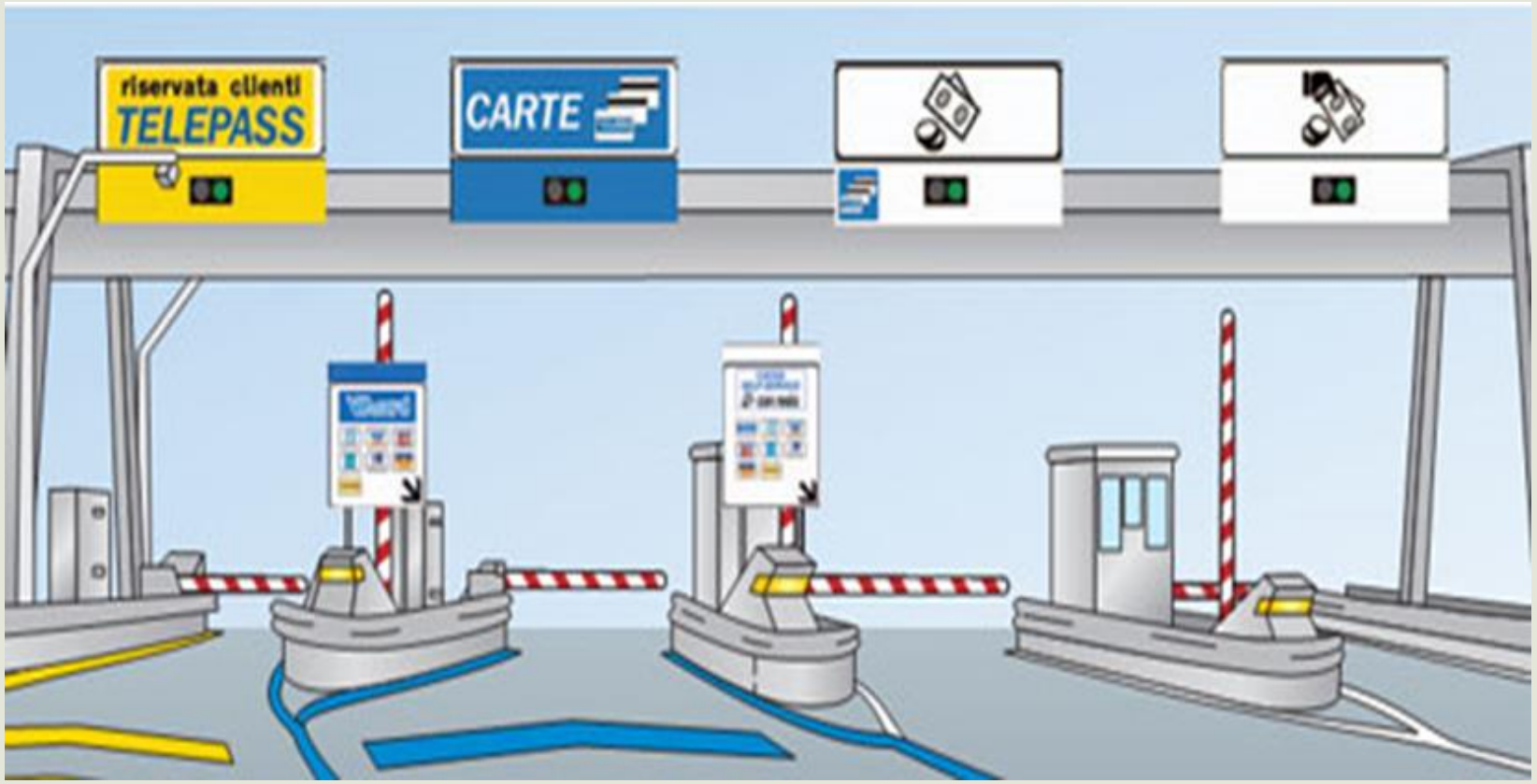


TASEP is one of the simplest exactly solved models of driven many-particle systems, with bulk particle conserving stochastic dynamics. Presently it found a number of applications in biological transport, vehicular traffic flow, forced motion of colloids in narrow channels, transport of data packets in internet, etc.

- We studied a new discrete-time stochastic model of aggregation and fragmentation of a clusters of hard-core particles on open chains using **gTASEP,** which is the ordinary **TASEP** with backward-ordered sequential dynamics (**BSU),** equipped with two hopping probabilities: p and p_m. The second modified probability p_m models a special kinematic interaction between the particles of a cluster in addition to the simple hard-core exclusion interaction.

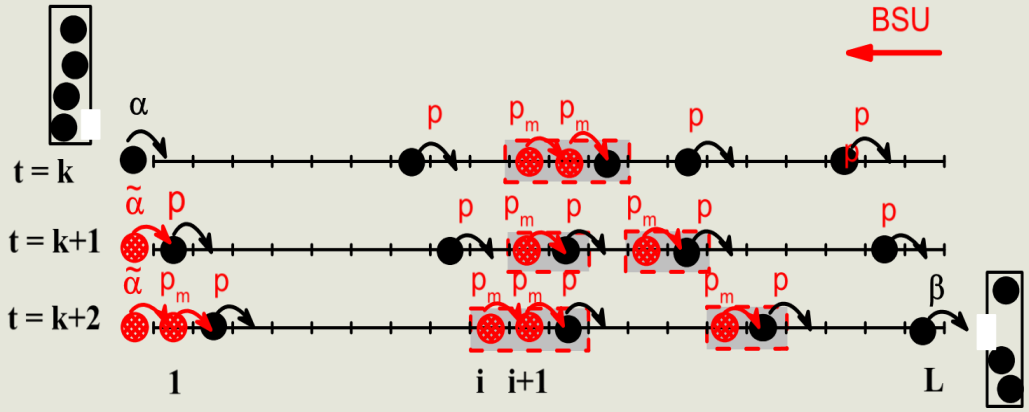
The case of attraction $(p < p_m)$ reflects the natural tendency of the driver to catch up with the car ahead. Thus, clusters of synchronously moving cars of particles appear, leading to higher current in the system. The limiting case of irreversible aggregation corresponds to the particular case $p_m = 1$. The case $p_m = 0$ corresponds to TASEP with parallel update, and $p_m = p$ to the backward ordered sequential one.

We can interpret the open boundary conditions at the ends of a finite segment of the road: one can consider the endpoints of a portion of a single-lane road as toll pay points, operating independently with different efficiency, say, proportional to $\hat{\alpha}$ at the entrance, and to β at the exit of the considered road segment.



The dynamics of our model - generalized TASEP is shown schematically in three consecutive time steps in the figure below.
The sites can be empty or occupied just by one particle. During each moment of discrete time t an update of the configuration of the whole chain with L sites takes place in L + 1 consecutive steps in a backward sequential order.

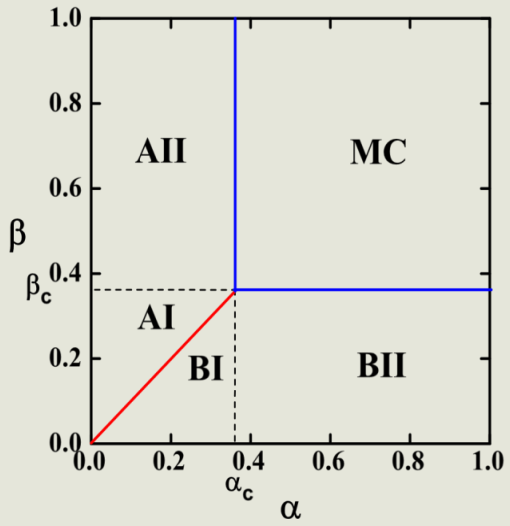
In gTASEP there are two hopping probabilities p and p_m. Each integer time moment t (or else configuration update) starts with the update of the last site of the chain: if site i = L is occupied, the particle at it leaves the system with probability β and stays in place with probability $1-\beta$. Isolated particles and the first particle of a cluster on the right may move one site to the right with probability p (or to stay at place with 1-p). Particles, which belong to a cluster (except the head particle), may move one site to the right (provided the particle in front of them has moved at the same time step) with a modified probability p_m (or to stay at place with 1- p_m). When $p_m > p$ ("attraction" interaction) the particles have higher probability to stay in clusters than to split. The left boundary condition is also modified accordingly to ensure consistency with the update rules. If site $i = 1$ was empty at the beginning of the current update, a particle enters the system with probability α, or site $i = 1$ remains empty with probability $1-\alpha$. If site $i = 1$ was occupied at the beginning of the current moment of time, but became empty under its current update, then $\tilde{\alpha} = \min\{\alpha\, \hat{p}\, /p, 1\}$

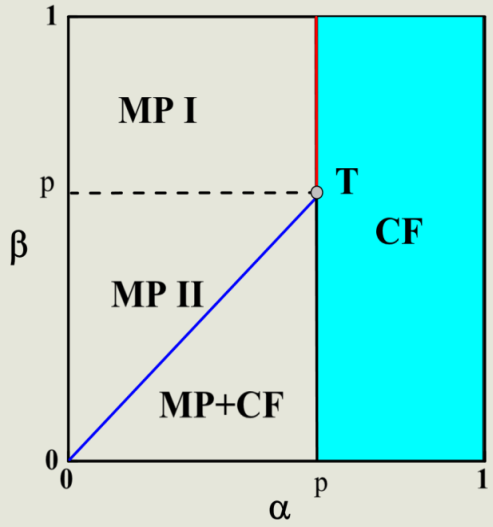


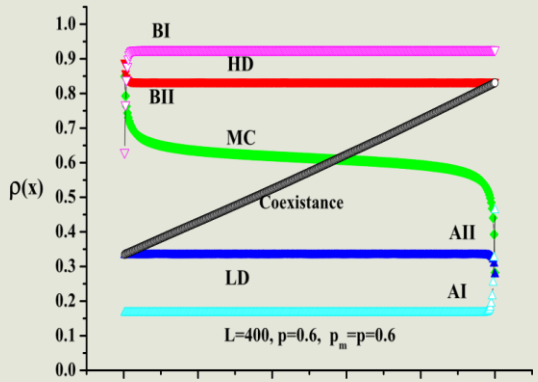
Known results in particular cases

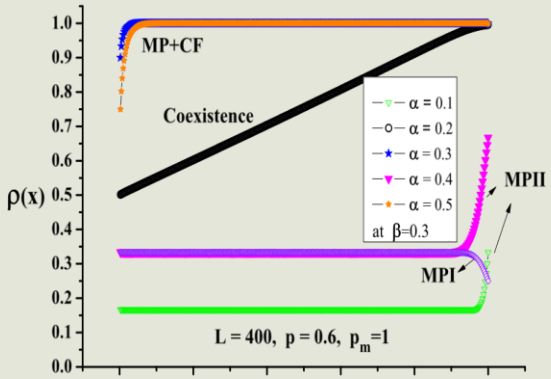
Phase diagrams of gTASEP in the particular cases of $p_m = p$ (the ordinary TASEP with BSU) and $p_m = 1$ (irreversible aggregation). Density profiles are shown at representative points of the different phases of the respective phase diagrams.

L = 400, p = 0.6









Ordinary TASEP with BSU ($p_m = p$): two points in the LD phase, $\alpha = 0.2$, $\beta = 0.6$ (AII) (blue), $\alpha = 0.2$, $\beta = 0.1$ (AI) – (cyan); coexistance $\alpha = 0.2$, $\beta = 0.2$ – (black); MC phase $\alpha = 0.6$,$\beta = 0.8$ – (green), and two points in HD phase, $\alpha = 0.2$,$\beta = 0.1$ (BI)– (magenta), $\alpha = 0.6$,$\beta = 0.2$ (BII)– (red).

gTASEP in the limit case of irreversible aggregation ($p_m = 1$) at fixed ejection probability $\beta = 0.3$: two values of α from phase MPII: $\alpha = 0.1$ – (green), and $\alpha = 0.2$ – (magenta), the coexistence line of phases MPII and MP+CF, appearing when $\alpha = \beta = 0.3$ – (black), and phase MP+CF at $\alpha = 0.4$ –(orange) and $\alpha = 0.5$ – (blue). A point form MPI phase is shown, appearing when $\alpha = 0.2$ and $\beta = 0.8$ – (purple). The density profiles in the CF phase are not shown to avoid overcrowding the figure.

RANDOM WALK THEORY FOR THE GAP EVOLUTION
Irreversible aggregation $p_m = 1$

One often uses the dual representation of configurations in terms of empty sites positions, instead of particle coordinates. In our case, such a representation leads to a peculiar dynamics of the inter-cluster gaps: **(1)** gaps may appear only at the first site of the chain; **(2)** gaps disappear when two consecutive clusters merge or when the rightmost cluster leaves the system and the one following it reaches the last site of the chain; **(3)** as long as two consecutive gaps exist, the distance between them remains constant (because of particle conservation in the bulk, the number of particles in a cluster between two gaps remains fixed). The width of each gap performs a random walk, with an initial state having one or several neighboring empty sites, and ends up when the random walk reaches to the origin.

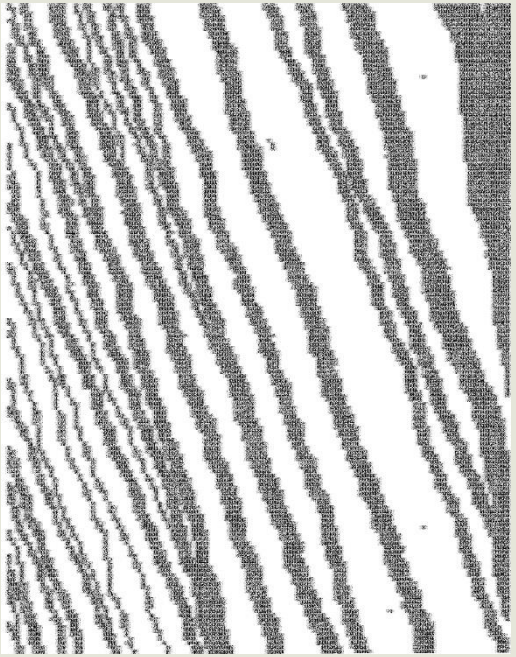
When $\beta \neq p$, the size of the rightmost gap performs an **asymmetric random walk**: its right edge belongs to the cluster which moves to the right with the ejection probability β and its left edge moves to the right with probability p. Therefore, after each update, the gap width **increases** by one site with probability $p_g = \beta(1 - p)$, **decreases** by one site with probability $q_g = p(1 - \beta)$, and **remains the same** with probability $r = 1 - p_g - q_g = 1 - \beta - p + 2\beta p$.

In general, when $\beta \neq p$, the size of the rightmost gap performs an asymmetric random walk. We have found three regimes of the gap width evolution:

1. Growing rightmost gap

This case takes place in the domain MP I, when $\beta > p$, hence, for the rightmost gap $p_g > q_g$. All the gaps on the left of it perform symmetric random walks.

2. Short-living rightmost gap

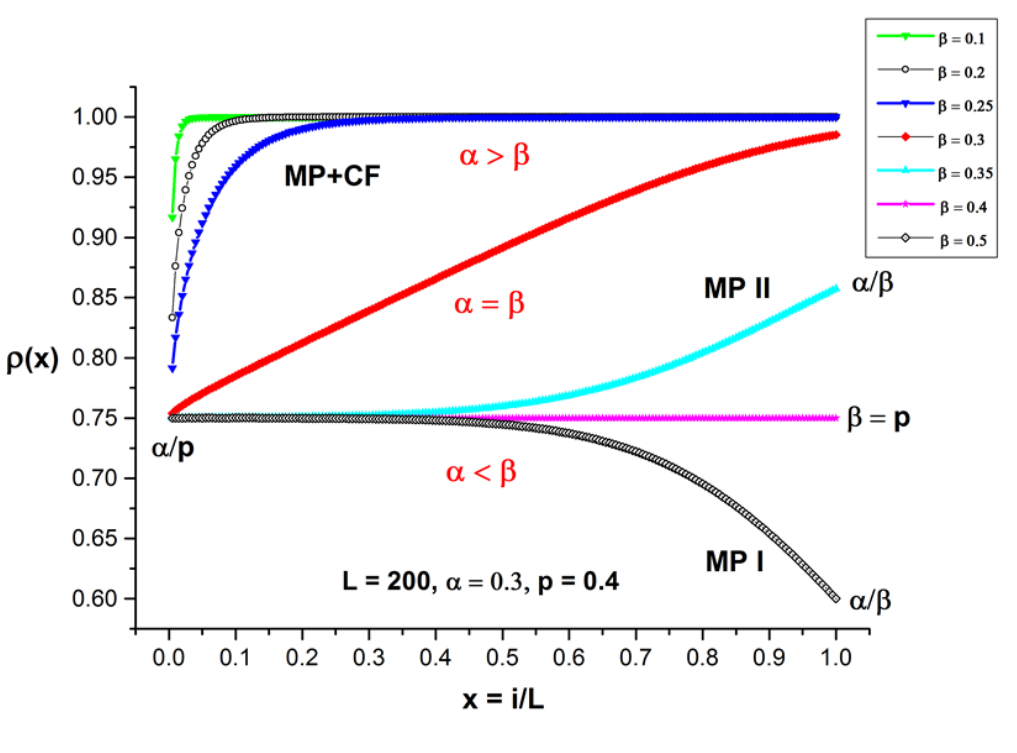


In the domain MP II, where $\beta < p$, the random walk of the rightmost gap is performed with $p_g < q_g$. All the gaps on the left of it perform symmetric random walks.

3. Critical gaps

When $\beta = p$, the widths of all the existing gaps perform symmetric random walks, starting from the corresponding initial conditions.

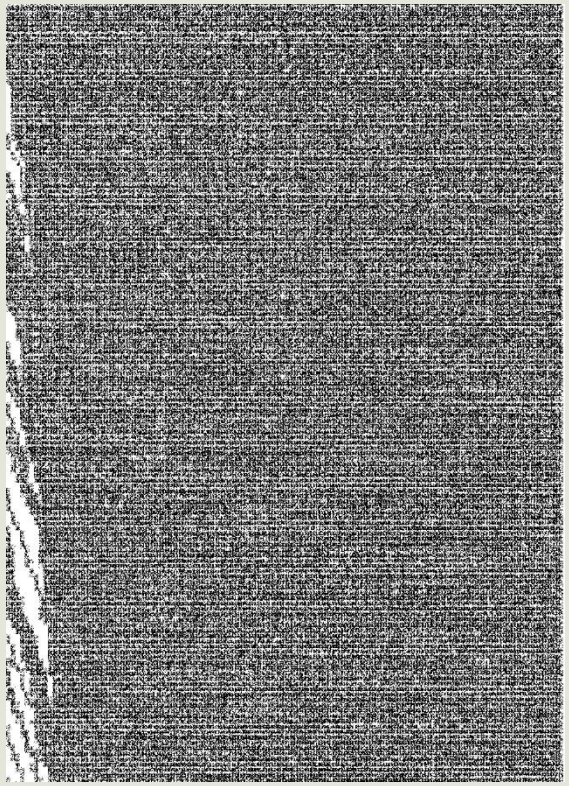
The time evolution of the rightmost gap affects the behavior of the local density profile near the chain end.



In regions MPI and MPII ($\alpha < p$ and $\beta > \alpha$) the bulk particle density is $\rho_b = \alpha/p$, and at the last site $\rho_L = \alpha/\beta$.

In the phase MP+CF ($\beta < \alpha < p$) the road is completely jammed from the bulk up to the last site. We have proved the result $\rho_1^{MP+CF} = 1-(1/\alpha-1/p)\beta$

The nature of the boundary perturbed MP+CF phase



A distinguishing feature of the boundary perturbed phase MP+CF is the appearance of inter-cluster gaps only at finite distance from the left end of the chain. At that, the time evolution of the gap configurations dramatically varies with time from situations shown on the left-hand side space-time plot, where one sees completely filled configurations, to the one shown on the right-hand side.

Evolution of single-gapped configurations

We can estimate analytically the probability P(1) (of completely jammed configuration) in the case when the appearance of a vacancy at the first site of a CF configuration is a rare event. That event happens when: (i) a particle of the completely filling cluster leaves the system from its right end, which takes place with probability β, and leads to the deterministic translation of all the remaining $L-1$ particles by one sight to the right; (ii) the resulting vacancy of the first site is not immediately filled by a particle from the left reservoir, which takes place with probability $(1-\hat{\alpha}) \ll 1$. Thus, the appearance of a vacancy at the first site of a CF configuration will take, on the average $\bar{N} = [(1-\hat{\alpha})\beta] - 1 \gg 1$ updates.

We have to evaluate the average lifetime (in number of updates) $\bar{n}$ of the gap in the different asymptotic regimes. If $\bar{n} < \bar{N}$, an estimate of the probability P(1) is given by the ratio

$$P(1) \simeq \frac{\bar{N} - \bar{n}}{\bar{N}}$$

Growing gap

Consider the case when the boundary $\alpha = p$ of the CF phase is approached from region MPI, i.e., at $\beta > p$. In this case $p_g > q_g$ and the gap asymptotically grows with the number n updates. It will exist until its edges reach the end of the chain, that is $\bar{n} \sim L$. Such a long gap, propagating through the whole chain, appears on the average after $\bar{N} \sim \frac{1}{\beta(p-\alpha)}$ updates. The crucial assumption is that $\bar{n} \ll \bar{N}$, and no other long-living gaps appear during the considered time interval. In such a case we obtain, $P(1) \simeq 1 - \alpha_1 L(p - \alpha)$. The important result here is the appearance of the finite-size scaling variable $L(p - \alpha)$. This result was confirmed by the data collapse method for different chain lengths L.

Short-living gap

When the boundary of the CF phase is approached from the boundary perturbed MP+CF phase, i.e., at $\beta < p$, one has $p_g < q_g$ and the gap between the newly growing cluster and the cluster which is leaving the system from its right boundary closes in a finite number of time steps. An upper estimate can be given by the result for a random walk on an infinite chain with initial state at site $i = 1$ and one absorbing state at the origin $i = 0$:

$$\bar{n} < q_g \frac{1}{p_g - q_g} = \frac{1}{p - \beta}.$$

Obviously, in this case $P(1) \approx 1 - \bar{n}/\bar{N} \to 1$, as $\alpha \to p$, at $\beta < p$.

Critical Gap

When the boundary $\alpha = p$ of the CF phase is approached along the line $\beta = p$, the gap width performs a symmetric random walk with $p_g = q_g = p(1-p)$, $r = 1-2p(1-p)$. The calculation of the average lifetime $\bar{n}$ in this case is involved, because the average length of a symmetric random walk on the infinite chain, with initial state at $i = 1$ and one absorbing state at $i = 0$, diverges. That is why, we have to take into account that the lifetime of the symmetric random walk on the finite chain of length L is limited, on the average, by L/p. Let us introduce the average lifetime $\bar{n}_M$ of the gap during M updates, $\bar{n}_M = \sum_{m=1}^{M} m f_{1,0}^{(m)}$, where $f_{1,0}^{(m)}$ is the probability that the initial gap of unit width will vanish at update m. By using the known generating function of $f_{1,0}^{(m)}$, we obtain the following exact expression:

RW

- $\overline{n_M} = \frac{p(1-p)}{r} \sum_{n=0}^{M/2} \left(\frac{p(1-p)}{r}\right)^{2n} \binom{2n+1}{n} \sum_{k=2n+1}^{M} r^k \binom{k}{2n+1}$.

To obtain a transparent expression for $M \gg 1$, we apply a chain of approximations, which finally lead to the estimate:

- $\overline{n_M} \cong \frac{1}{2\sqrt{\pi}\, p(1-p)} \int_0^{M/2} \frac{dx}{x} = \frac{\sqrt{M}}{\sqrt{2\pi}\, p(1-p)}$.

Hence, for $M = L/p$ we obtain:

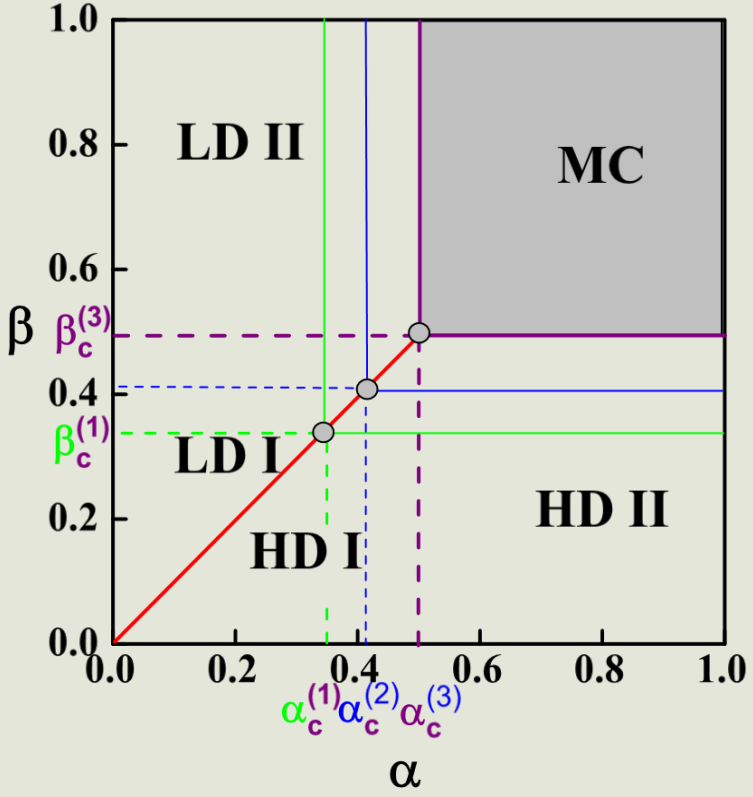
- $P(1) \approx 1 - b_1 L^{1/2}(p - \alpha)$.

This asymptotic result is supported by the data collapse method, applied to different chain lengths, as shown in the next figure.

THE GENERIC CASE OF ATTRACTION $p_m > p$

We analytically approach the question of how the completely filled phase (CF) at $p_m = 1$ is destroyed, when $0 < 1 - p_m \ll 1$, and transformed into new phases typical for $p_m < 1$. We used Random walk theory.

The topology of the modified phase diagram, the shift of the triple point ($\alpha_c(p, p_m)$, $\beta_c(p, p_m)$) under the change of $p_m \in [p, 1]$ at fixed p



We analyzed, within the Random walk theory, the evolution of a single gap between two large clusters of particles in different regions of CF phase.

With the aid of Random walk theory, supported by the Monte-Carlo simulations, the properties of the phase transitions between the three stationary phases are assessed.

RANDOM WALK THEORY FOR THE GAP EVOLUTION in the case of attraction $p_m > p$

Time evolution of configuration gaps

We find out the probability of a single gap appearance under boundary conditions corresponding to the CF phase and consider the first step in the time evolution of the gap width. The problem is rather complicated because the probability of appearance of a gap is position dependent in contrast to the case of $p_m = 1$, because when $\beta \neq p$, the gap width performs a special, position dependent random walk.

Here the gap appears at sites $2 \leq i \leq L$ (as the result of the left boundary condition) .

The gap width increases by one site with probability

$$p_g(i) = (1-p)p_m^{L-i-1}\beta,$$

decreases by one site with probability

$$q_g(i) = [(1-\beta) + (1-p_m^{L-i-1})\beta]p = (1-p_m^{L-i-1}\beta)p,$$

and remains the same with probability

$$r_g(i) = 1 - p + p_m^{L-i-1}\beta(2p-1)$$

RW

We average the gap width evolution over the initial probabilities given by

$$P_{L-k}(p, p_m) = (1 - p_m)p_m^k\beta,\ k = 0, 1, \ldots L-2, \quad P_1(p, p_m) = (1 - \tilde{\alpha})p_m^{L-1}\beta.$$

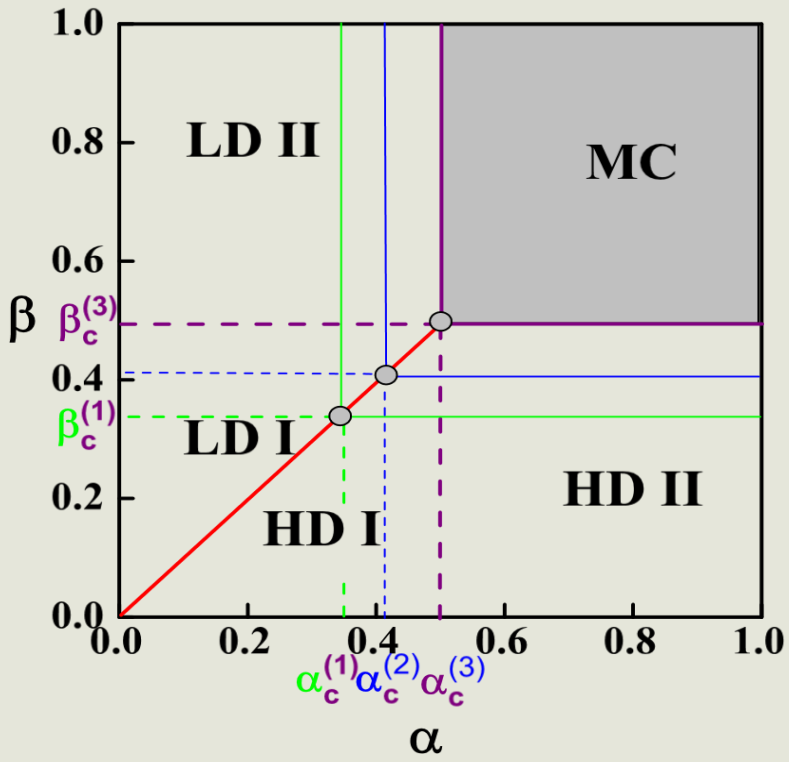
and conclude that on the average a single-site gap will grow after the first time step of its evolution when

$$\beta > p\frac{p_m(1 + p_m)}{(1 + p_m^{L-1})}$$

When $p_m \to 1$ and L is fixed, or $L \to \infty$ so that $p_m^L \to 1$ this condition simplifies to $\beta > p$. However, for fixed values of p_m close to 1, p_m^L will decrease to zero as $L \to \infty$.

On the ground of our Random walk theory and the computer simulations, we conjecture that the simple criteria $\beta > p$ for growing gaps, and $\beta < p$ for decreasing gaps, hold true.

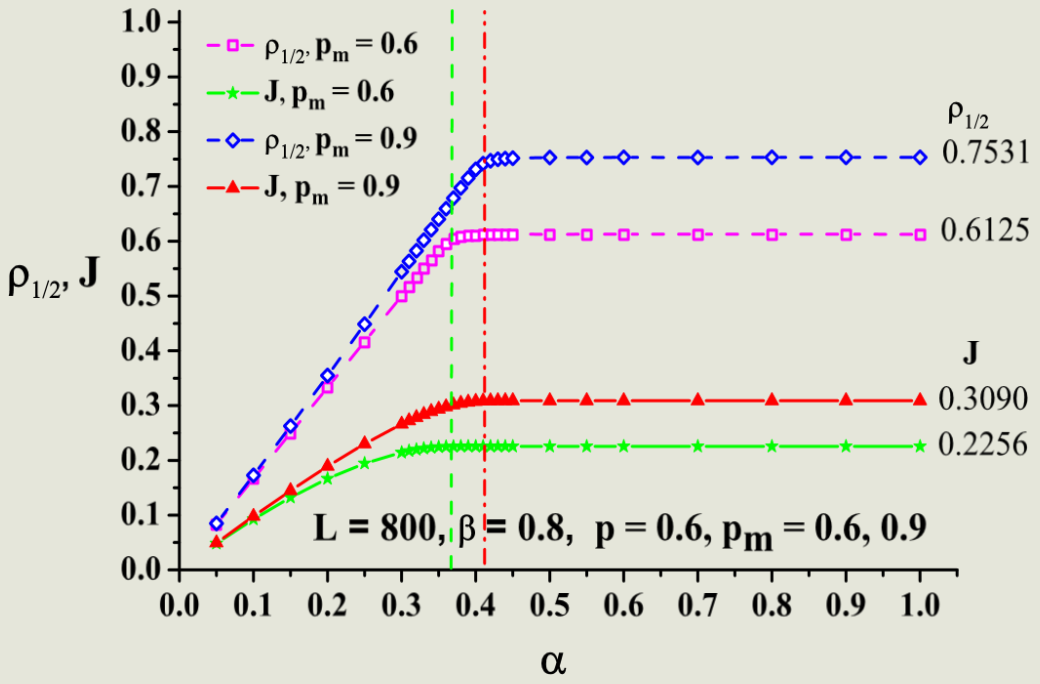
Thus, our expectation, confirmed by the computer simulations, is that in the upper region $(p < \alpha \leq 1] \times (p < \beta \leq 1]$ of the CF phase a maximum-current phase will appear. Its local density profile satisfies the inequalities $\rho_1 = 1 > \rho_{l/2} > \rho_L$, which follow from the conditions $\hat{\alpha} = 1$, and the larger probability of gap formation near the end of the chain. In the lower region $(p < \alpha \leq 1] \times (0 < \beta < p]$ of the CF phase the gaps are scarce, small and short-living, which is indicative of a high-density phase. Again, the left-hand side of the local density profile bends upward to $\rho_1 = 1$.



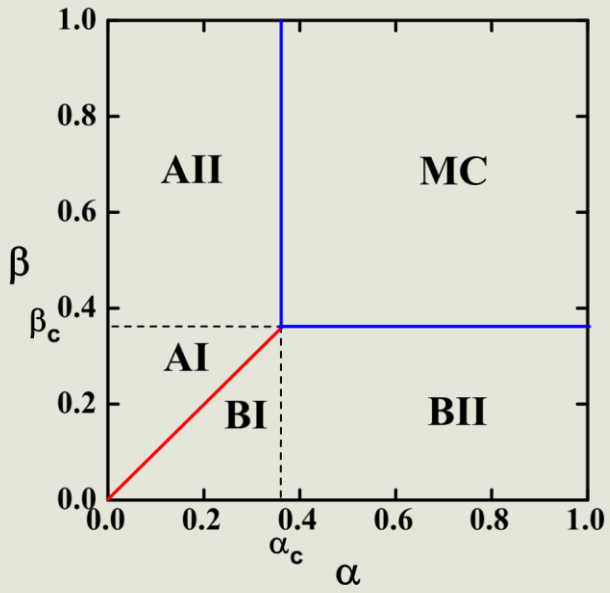
Phase diagram and phase transitions

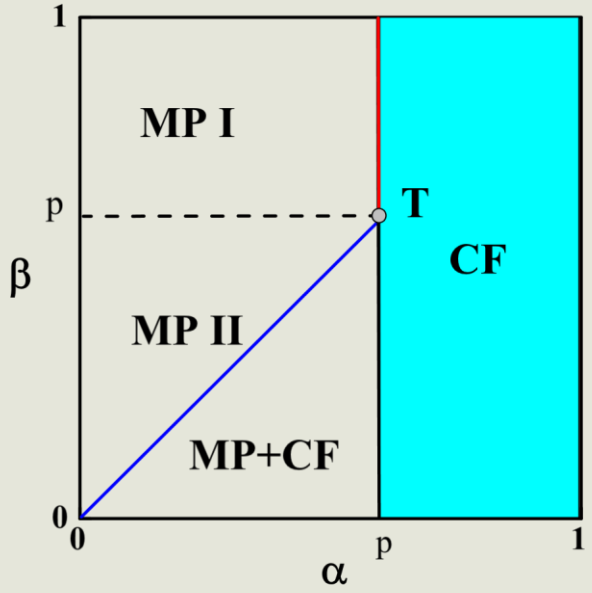
We performed Monte Carlo simulations of the gTASEP on open chains of mainly L = 800 and L = 1600 sites and compare the behavior of the current, J, and the local density at the midpoint of the chain, $p_{1/2}$, under two modified hopping probabilities $p_m = 0.6$ and $p_m = 0.9$ as a function of the input rate α, at chain length $L = 800$ sites, fixed $p = 0.6$ and output rate $\beta = 0.8$.

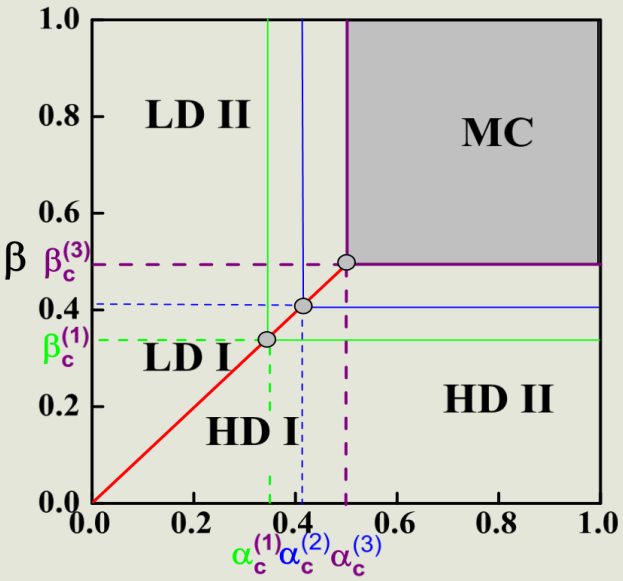
Our results indicate that the unusual phase transition, found in at $p_m = 1$ across the boundary $\alpha = p$ becomes a continuous one.



We summarize our results to conjecture a generic phase diagram of the gTASEP with $p_m < 1$ with the same topology as in the case of the TASEP with BSU, but with (p,p_m)-dependent triple point (α_c,β_c). with the increase of p_m at fixed $p = 0.6$.







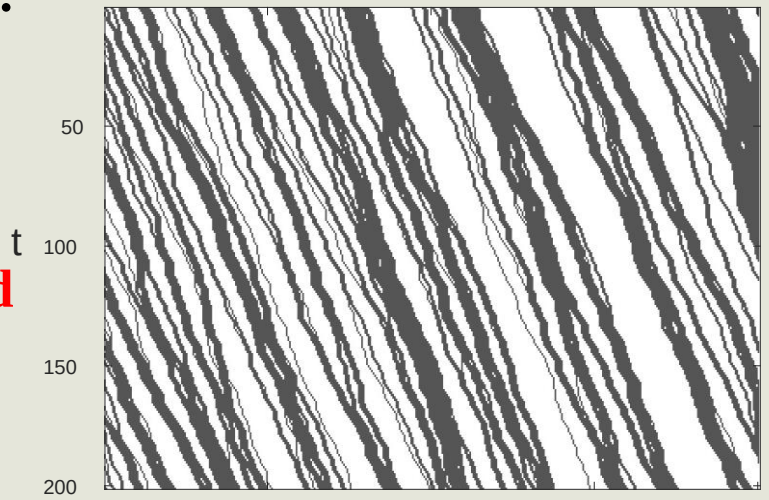
We exemplify the phase diagram of the gTASEP in the particular case of $p = 0.6$ and $p_m = 0.99$ and the shift of the triple point (α_c,β_c) with the increase of p_m at fixed $p = 0.6$.

The main difference between the phase diagrams for $p_m = 1$ and $p_m < 1$ turned out to be the dependence of the critical probabilities $\sigma_c(p,p_m)$ on p_m, at fixed p.

Additional information can be found in the different gaps evolution regimes in regions LDI and HDI:

In both cases $\alpha < p$, which implies $\hat{\alpha} < 1$, so that gaps can appear at the first site $i = 1$ and evolve throughout the chain; however, in LDI the gaps are wide and long living, while in HDI they are small, scarce and very short living, The typical gaps pattern in LDII (HDII) is similar to the one shown for LDI (HDI). These features may explain the large difference in the particle densities in the low-density and high-density phases.

We emphasize that the gTASEP does not satisfy the particle-hole symmetry inherent to the standard versions of TASEP.



Main results

1. We proposed and studied a new one-dimensional model of irreversible aggregation on finite open chains, based on a special discrete-time TASEP-like kinetics.
2. We have obtained a phase diagram with a novel topology in the case of irreversible aggregation.
3. We have analyzed, within the Random walk theory, the evolution of a single gap between two large clusters of vehicles. Three qualitatively different regimes were established when the injection rate approaches from the left the boundary $\alpha = p$ with the CF phase: (i) the lifetime of the rightmost gap in the jammed configuration is of size O(L) in the MP phase; (ii) macroscopic jams, separated by short-living gaps of length O(1), exist in the MP+CF phase; and (iii) there is a critical regime when the macroscopic jams are divided by gaps of intermediate lifetime of the order O(L 1/2) when the triple point $\alpha = \beta = p$ is approached.
4. We studied the generalized TASEP in the regime of particle attraction ($p_m > p$) when cluster aggregation and fragmentation is allowed in the system. and illustrated.
5. With the aid of Random walk theory we analytically approach the question of how the completely filled phase (CF) at $p_m = 1$ is destroyed, when $0 < 1 - p_m \ll 1$, and transformed into new phases typical for $p_m < 1$.
6. On the grounds of our RW theory and the computer simulations, we have conjectured that the

Thank You

For Your Attention

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