Complexity and Criticality of Nonequilibrium Systems

(Overview and recent developments w/ 1D model studies in diffusive flow)



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Outline

Overview

- Nonequilibrium Systems?
- Asymmetric Simple Exclusion Process (ASEP) What is it? Why do we need it? How to study it?

Recent Developments with ASEP

From Traffic to Intracellular Transport problems

Instability transitions and ensemble equivalence in diffusive flow

Take-home message

Nonequilibrium Systems?





- The systems driven by the net external force reach a steady state with non-vanishing current, which does not satisfy the detailed balance condition of equilibrium.
- In contrast to equilibrium case, several 1D driven systems with local dynamics exhibit long range order and spontaneous symmetry breaking, which cannot occur in equilibrium when the interactions are short-ranged.

Detailed balance condition of equilibrium

From the master equation of motion,

$$\frac{\partial}{\partial t}P(C,t) = \sum_{C'} \{W[C' \to C]P(C',t) - W[C \to C']P(C,t)\}$$

for equilibrium systems $P^*(C) \equiv P(C, t \to \infty) = P_{eq}(C)$

the detailed balance condition

$$\frac{W[C' \to C]}{W[C \to C']} = \frac{P_{eq}(C)}{P_{eq}(C')} = \exp\left(-\frac{\Delta H}{k_B T}\right)$$

Nonequilibrium steady state

There is currently *no* established systematic and analytic *procedure/formalism for predicting stationary-state ensembles* because physics far from equilibrium cannot be described by Gibbs-like ensembles (detailed balance) with a well-defined global Hamiltonian.

Then, what can we do?

Based on the microscopic level of a *master equation* and/or the mesoscopic continuum level of a *Langevin-type equation of motion*, *study its analytic solvability and dynamic mean-field theory if possible; otherwise (most cases), rely on simulation results and arguments.*

so what we will do?

• Find universal robust behaviors

in nonequilibrium driven stochastic processes, e.g., kinetic roughening, phase transitions, self-organized criticality, etc.

Identify universality classes

not only to determine their physical properties and critical exponents numerically but to gain fundamental and analytic insight.

Universal scaling properties near criticality

Near criticality (continuous phase transition point), major physical quantities exhibit power-law behaviors with universal critical exponents.

Therefore, the following three things are important:

- 1. To model physical systems with the most relevant control parameters.
- 2. To find out what a good order parameter is in the system.
- 3. Based on how the determined order parameter behaves, to indicate the existence and nature of phase transitions, e.g., 1st order (discontinuous) vs. 2nd order (continuous).

Kinetic roughening (experiment I):

Kardar-Parisi-Zhang (KPZ) universaility

Propagating flux fronts in high Tc superconductor (Wijngaarden's group in Netherlands, PRL 1999)

- (a) Magneto-optical image taken at 11 mT after zero-field cooling to 4.2 K of a 80 nm thick YBCO film on NdGaO₃ (sample No.2). Total length of the sample is 8.1 mm.
- (b) Flux fronts observed in sample No.2. The applied external field is increased by 1 mT from bottom (1 mT) to top (17 mT).



Kinetic roughening (experiment II):

Kardar-Parisi-Zhang (KPZ) universaility



• • •

Jussi Timonen's group in Finland, PRL & PRE + Ph.D thesis 2000~3

Slow combustion fronts of paper (Timonen's group in Finland, PRL 2000; PRE 2001)

Typical Digitized Fronts

The time step (bottom to top) between successive fronts is 10 s, and the width of the digitized area is 310 mm.

For a uniform propagation of slow combustion fronts, potassium nitrate (KNO₃) was added as an oxygen source to all grades of paper.



KPZ-type kinetic roughening





Surface Roughness

The surface width, *W*(*L*,*t*):

$$W(L,t) \equiv \sqrt{\frac{1}{L} \sum_{i=1}^{L} [h(i,t) - \bar{h}(t)]^2},$$

where h(t) is the average height at time t.

The general finite-size scaling form of W(L,t) is

$$W(L,t) = b^{\chi}W(b^{-1}L,b^{-z}t) = L^{\chi}f(t/L^{z}).$$

Data Collapse via Dynamic Scaling



KPZ-type kinetic roughening (Theory)

Kardar, Parisi, and Zhang, PRL 1986

$$\frac{\partial}{\partial t}h(x,t) = \nu(\nabla^2 h) + \frac{\lambda}{2} |\nabla h|^2 + \eta(x,t)$$

where
$$\langle \eta(x,t) \rangle = 0$$
, $\langle \eta(x,t)\eta(x',t') \rangle = 2D\delta(x-x')\delta(t-t')$.

If *the local geometry of the interface* is the only relevant degree of freedom, then its scaling properties at large scale are governed by *Langevin-type KPZ equation*.

$$\chi + z = 2$$
 Galilean Invariance
 $\rightarrow \chi = \frac{1}{2}; z = \frac{3}{2}$ (1D).

Body-Centered Solid-On-Solid (BCSOS): KPZ-type Growth Model



Choose one of the columns at random.

If the chosen column is a local minimum (*maximum*), a 1X2 shaped particle deposits (*evaporates*) with probability p (*q*).

What for such a simple model?

•
$$s_i \equiv h_{i+1} - h_i = \pm 1$$
 only!

Its surfaces is fully characterized by spin-1/2-type spin variables and/or by lattice-gas-type representations:

e.g., XXZ quantum spin chain, six-vertex model, crystal faceting, etc.

• $\lambda \propto -(p-q)$ (local slopes are inactive!)

When $p \neq q$, it belongs to **the KPZ universality class.**

Lattice-gas representation

for KPZ-type BCSOS growth



ASEP? (p>q or q>p)

The simplest driven lattice-gas (Ising) model in many studies of <u>driven diffusive systems (DDS</u>)

No interaction between particles Only hard-core repulsions

Many Surprises!!!



First studies of **ASEP**



(Courtesy to G.M. Schuetz)

Physical Examples of DDS

- Biased diffusion of atoms on surfaces
- Steady sedimentation of colloidal crystal
- Transport in nanoscale systems
- Motion of flux lines in superconductors
- Slow combustion fronts of paper
- Motion of molecular motors
- Traffic

more examples in Schmittmann and Zia's "Statistical Mechanics of Driven Diffusive Systems: Phase Transitions and Critical Phenomena", edited by Domb and Lebowitz, volume 17 (1995)

Well-known exact results of ASEP w/o defect

Periodic case (Gwa and Spohn '92; Dhar '87)

Its time development is exactly soluble by Bethe ansatz. -Noisy Burgers (KPZ) equation: KPZ-type BCSOS growth

Open case (Krug '91; Derrida et al. '92; Schütz and Domany '93) Its steady state is only exactly soluble by matrix formalism. -Boundary/reservoir-induced phase transitions occur. **Open ASEP:** (CONTINUOUS time updating)





Update scheme in MC simulations

In which order are the sites or particles updated ?

random-sequential:

one of sites or particles is picked randomly at each step

- (= standard update for ASEP; continuous time dynamics)
- parallel (synchronous):

all particles or sites are updated at the same time

• ordered-sequential:

update in a fixed order (e.g. from left to right)

shuffled:

at each time step all particles are updated in random order

Phase Diagram for ASEP w/ OBC

Maximal current phase



Periodic ASEP with a slow (defect) bond



Known Results of ASEP with a defect bond

 Mean-field (MF) study (Wolf and Tang '90)
 The KPZ equation with a local inhomogeneity says infinitely long queue for r<1 & no queue (log depletion) for r>1.

Periodic case with a blockage (Janowsky and Lebowitz '92, '94)
 The finite-size scaling of shockwave fluctuations was studied with *MF phase diagram* (as if r_c=1 in the half-filled system).

r: hopping prob. at the defect bond

Applications of ASEP

ASEP = "Ising" model of nonequilibrium physics

since it is simple, exactly solvable, and has many applications as follows:

- Protein synthesis
- Surface growth
- Boundary induced phase transitions
- Real and/or Model Traffic
- Intracellular Transport
- Ant Trails



- macroscopic system of interacting particles
- Nonequilibrium physics:
 Driven systems far from equilibrium
- Various approaches: hydrodynamic gas-kinetic car-following cellular automata (discrete in space, time, state variables)



(Courtesy to A. Schadschneider)







Advantage: very efficient implementation for large-scale computer simulations

However, we need OFTEN stochastic dynamics to mimics real situations

(Courtesy to A. Schadschneider)

Spontaneous Jam Formation



Phantom jams, start-stop-waves interesting collective phenomena



Relation: current (flow) vs. density



(Courtesy to A. Schadschneider)

CA model for highway traffic

(Nagel, Schreckenberg 1992)

Update Rules:

- (1) Acceleration: $vj \rightarrow min(vj + 1, vmax)$
- (2) Braking: $v_j \rightarrow min(v_j, d_j)$
 - (dj = # empty cells in front of car j)

(3) Randomization: $vj \rightarrow vj - 1$ (with probability p)

(4) Motion: $xj \rightarrow xj + vj$

• • Interpretation of the Rules

Acceleration: Drivers want to move as fast as possible (or allowed)

Braking: no accidents

Randomization:

- a) overreactions at braking
- b) delayed acceleration
- c) psychological effects (fluctuations in driving)
- d) road conditions

Driving: Motion of cars

• • Experiments vs. Simulations

a) Empirical results

b) MC simulations



occupancy ρ [%]

(Courtesy to A. Schadschneider)

Analytical Methods for CA

- Mean-field: $P(\sigma_1,...,\sigma_L) = P(\sigma_1) \cdots P(\sigma_L)$
- Cluster approximation: $P(\sigma_1,...,\sigma_L) = P(\sigma_1,\sigma_2) P(\sigma_2,\sigma_3) \cdots P(\sigma_L) \bullet_1 \bullet_2 \bullet_3 \bullet_4$
- Car-oriented mean-field (COMF):
 P(d₁,...,d_L)=P(d₁)… P(d_L)
 with d_j = headway of car j (gap to car ahead)



Summary for Traffic

- Cellular automata are able to reproduce many aspects of highway traffic (despite their simplicity):

Spontaneous jam formation Metastability, Hysteresis Existence of 3 phases (novel correlations)

- Simulations of networks faster than real-time possible Online simulation; Forecasting
Transport in Cells



Microtubule



Mechanism of Motion



hand-over-hand: leading and trailing head change

ASEP-like Model of Molecular Motor-Traffic

(Lipowsky, Klumpp, Nieuwenhuizen, 2001; Parmeggiani, Franosch, Frey, 2003; Evans, Juhasz, Santen, 2003)



ASEP + Langmuir-like adsorption-desorption

Competition bulk – boundary dynamics

Ant trails

ants build "road" networks: trail system



Chemotaxis

- Ants can communicate on a chemical basis: Chemotaxis
- Ants create a chemical trace of pheromones trace can be "smell ed" by other ants follow trace to food source etc.



How to model ant trails

- Basic ant trail model: ASEP + pheromone dynamics
- hopping probability depends on density of pheromones
- distinguish only presence/absence of pheromones
- ants create pheromones
- 'free' pheromones evaporate

• • • Ant trail model 1. motion of ants

(Chowdhury, Guttal, Nishinari, Schadschneider, 2002)

Dynamics:

2. pheromone update (creation + evaporation)



parameters: q < Q, f

equivalent to bus-route model

(O'Loan, Evans, Cates 1998)

• • Limiting cases of ATM

f=0: pheromones never evaporate
 > hopping rate always Q in stationary state

o f=1: pheromone evaporates immediately
 => hopping rate always q in stationary state

o For f=0 and f=1: ant trail model = ASEP (with Q, q, resp.)

So far we found

 Various very different transport and traffic problems can be described by similar models

Variants of the Asymmetric Simple Exclusion Process

- Highway traffic: larger velocities
- Intracellular transport: adsorption + desorption
- Ant trails: state-dependent hopping rates
- Pedestrian dynamics: 2-dimensional motion

What can we do more?

Parking Garage Model

(HA and den Nijs, PRE 2002)



Queuing phenomena, such as traffic jams, exhibit a nonequilibrium phase transition from finite queue length to infinite one in the thermodynamic limit.

$$N_P(\alpha, N_c, N_s)$$

number of parked cars

Dynamic Analogue of Bose Condensation: macroscopic car condensation in parking garage





Finite-size scaling (FSS) analysis

Dynamic analogue of Bose condensation



Queuing in ASEP with a blockage

(HA, Timonen, and den Nijs, PRE 2003)



Whether do stochastic fluctuations destroy the queue at weak obstacle strengths $0 < r_c < 1$?

YES, they do!

Faceting induced by a columnar defect

(Timonen's group, HA, and M. den Nijs, PRE 2003)



Queuing transition

in ASEP with a defect bond at rc=0.80(2)<1



Relevant Physical Quantities?

density profile steady-state current



FSS Analysis

queuing transition in ASEP with a slow bond



Scaling Function

$$S(N_s^{\mathcal{Y}}\varepsilon) = N_s^{x_{\Delta}}\Delta_b(N_s,\varepsilon)$$



TASEP + nonlocal hopping: its mappings



Nonlocal hopping promotes clustering and coarsening towards a phase-ordering state, namely "Empty-Road" (ER) or "Fully-Condensed" (FC) phase.

"Instability Transitions & Ensemble Equivalence" studies

(1) Dynamic instability transitions in 1D driven diffusive flow with nonlocal hopping (HA, Park, and den Nijs, PRE 2007)

(2) Boundary-induced abrupt transitions in symmetric simple exclusion process (SSEP) (Nagar, HA, and Park, arXiv:0804.4214)

Model (1): Set-up & Dynamics

Consider TASEP with local (1-p) and nonlocal (p) hopping events on a open chain, in contact with two reservoirs.

Nonlocal hopping events from the entry side reservoir are not allowed.



The nonlocal skids promote strong clustering in the stationary populated phase.

p=0 case: ordinary Totally Asymmetric Simple Exclusion Process

Potential Applications

Our process mimics viscous and/or dissipative stick-slip type phenomena caused by gravity & inertia effects.





Inertia effects on avalanche dynamics





Phase Diagram $(p vs. \alpha)$



Model (1)

Dynamic Instability transitions



We have found for steady states:

- **1.** Instability threshold exists at finite value of p.
- The transition into FC from N/MC is 1st order, while from Condensed (low density) it is 2nd order.

(a) MC-ER Transition (1st order)



Model (1)

(b) C-ER Transition (2nd order)



Model (1)









Mean-Field Analysis for steady-state current

Using the fact that in the steady-state limit

 $J = J_{0,1} = J_{1,2} = \dots = J_{N_s - 1, N_s}$:

$$J_{0,1} = \tilde{\alpha}(1-\rho_1), \quad J_{1,2} = \langle n_1(1-n_2) \rangle,$$

$$J_{i,i+1} = \langle n_i(1-n_{i+1}) \rangle + P \sum_{j=1}^{i-1} \langle [n_j \prod_{k=j+1}^{i} (1-n_k)](1-n_{i+1}) \rangle,$$

$$J_{N_s-1,N_s} = \rho_{N_s-1} + P \sum_{j=1}^{N_s-2} \langle [n_j \prod_{k=j+1}^{N_s-1} (1-n_k)] \rangle.$$

For simplicity, site-MF approximations are considered as

$$J_{i,i+1} = ilde{
ho}_i (1 -
ho_{i+1}),$$

where $ilde{
ho}_i \equiv
ho_i + P \sum_{j=1}^{i-1} [
ho_j \prod_{k=j+1}^{i} (1 -
ho_k)].$



 $ho_i \equiv \langle n_i
angle \ L \equiv N_s$

Mother Cluster Analysis & States

Mother cluster self consistency equations

$$J = \alpha v_1 = (1 - rv_c)v_c = p + \rho_c u_F \quad , \qquad u_F = r - \frac{p}{\rho_F}$$
$$v_{x+1} = \frac{J}{1 - rv_x - pP_x} \quad , \quad P_{x+1} = v_x P_x$$

$$P_x = probability$$
 for entire road between $x = 0$ and x to be empty

F_{up}

Fd

۱D

MC

р

1/3-

p-

 $\overset{\widetilde{\omega}}{=} \overset{\widetilde{\omega}}{=} \overset{\widetilde{\omega}}{=$

R

R_d

1/2 α

R_{up}



Good

The F and MC mother cluster states are similar to the free cluster states, which explains why J becomes independent of the input parameter in the MC phase

The locations of the critical line and endpoint are reproduced accurately. The R state is identical to the global MF solution with uniform density (clustering unstable), acting like a finite open system.

Bad



Summary for model (1) study

The conventional TASEP uniform stationary state is unstable towards clustering and queuing. Such clustered states, even when involving only mesoscopic clusters, communicate badly with each other and have a hard time developing novel type fluctuations (typically rather simple scaling properties, like at the C-ER & MC-ER phase boundaries).

How the inclusion of stick/slip-type nonlocal hopping events affects the open TASEP stationary states:

- Clusters develop, only mesoscopic one (no macroscopic queuing transitions).
- Dynamic instability transitions occur towards an ER phase, which are 1st order* from the MC phase & 2nd order** from the C phase.
- Clusters behaves as independent objects.
 - * the reversal of the drift velocity of free cluster
 - ** simple critical exponents; all current fluctuations are generated and limited to the "mother clustering" near the entry reservoir.

Model (2): Set-up & Dynamics

• Symmetric Simple Exclusion Process with nonlocal skids in an open chain



Usual mean-field treatment does not work!

- Clusters are stationary in average and stable only at the transition.
- Discontinuous phase transitions

from finite density (FD) into empty road (ER) as p increases.

- Internal structure is important (cluster analysis is needed).
- Relation to a mass-chipping & diffusion model (periodic version).
- Application to granular clustering, coarsening, and/or sudden collapse as shaking the container with several compartments.

Granular clustering & coarsening

D. van der Meer et al. (JSTAT 2004 & 07)





Sudden collapse

K. van der Weele et al. (EPL 2001); D. van der Meer et al. (PRL 2002)





Model (2)

Phase Diagram (cluster MF versus MC data)


Model (2)

Numerical Results

boundary-induced first order transition



$$\begin{array}{c} & \rho_r \simeq \left\{ \begin{array}{c} \rho_r^{\infty}(\alpha, p) + \tilde{B}L^{-1} + O(L^{-\kappa_b}) & \text{for } p < p_c, \\ \Delta \rho_r^{\infty}(p_c) + \tilde{C}x^{-\kappa} + O(L^{-1}) & \text{at } p = p_c, \\ \tilde{A}L^{-1} & \text{for } p > p_c. \end{array} \right\} \xrightarrow{\beta} \\ & \gamma \swarrow_{x=1} & (1-p)/2 & (1-p)/2 & x=L \longrightarrow \beta \end{array} \xrightarrow{\beta} \\ \end{array} \xrightarrow{\beta} \begin{array}{c} & \beta \\ & \gamma \swarrow_{x=1} & (1-p)/2 & (1-p)/2 & x=L \longrightarrow \beta \end{array} \xrightarrow{\beta} \\ & \beta \end{array} \xrightarrow{\beta} \begin{array}{c} & \rho_r^{\infty}(\alpha, p) + Bx^{-\kappa_b} & \text{for } p < p_c, \\ \Delta \rho_r^{\infty}(p_c) + Cx^{-\kappa} & \text{at } p = p_c, \\ \Delta \rho_r^{\infty}(p_c) + Cx^{-\kappa} & \text{at } p = p_c, \\ Ae^{-x/x^*}/\log(x) & \text{for } p > p_c. \end{array} \xrightarrow{\beta} \\ & = \frac{\rho_a(L+b}{L} \underset{\tau \simeq \tau}{\kappa_b} \underset{\sigma \rightarrow \tau}{\approx} \frac{3/2}{2}, \ \kappa \simeq 2/3 \end{array}$$

Cluster Mean-Field Analysis

critical density; $\rho_b(p, \alpha) = \rho^c = \sqrt{p}$ $(\rho_{\rm F} = \rho_{\rm S})$



Summary for model (2) study

Role of the boundary in SSEP with competing nonlocal and local hopping events? How the nonequilibrium system is affected by different boundary conditions?

We found the answers numerically and analytically using a cluster stability analysis:

"Nonlocal" hopping in open SSEP induces first order transition from finite density (FD) to empty road (ER) phase.

In periodic version, the transition is second order,

so NO Ensemble Equivalence exists at and above the transition.

Clusters are stationary in average and stable only at the transition.

This is quite different from those in the TASEP variant, where particle clusters are stable and moving with drift velocity depending on p in the most part of FD phase, and the first order transition is induced by the turnabout of drift velocity of free cluster.

Ongoing issues: Finite-Size effects; Ensemble Equivalence test in generalized SSEP and ASEP

e.g.) What if the left-right symmetry is broken? Any possibility w 2nd order transitions with other hopping rates, ZRP-type?

Take-home message

Simple variants of ASEP exhibit a rich variety of complex and surprising behavior with dynamic phase transitions.

- Macroscopic car condensation in a parking garage (ASEP + site defect)
- Queuing transition in the ASEP with a blockage

 (ASEP + bond defect)
 which is equivalent to faceting transition in KPZ-type
 slow paper-combustion experiment with a columnar defect*.
 *Related other problem: localization in directed polymer
- Instability Transitions in ASEP with nonlocal hopping (Lots of interesting things to be discovered and yet to be understood)

Many Possible Applications of ASEP JOIN PARTY of ASEP with a variety of methods !

Thank You~

Tack Kiitos Dhanyavaad

謝謝

감사합니다.