Driven Diffusive Systems with Glassy Dynamics

Steady state and fluctuation properties

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Motivations

Understanding the interplay of driving and glassiness, in

- Non-monotonic (or negative differential) response to a driving force
  - Shear-thinning and shear-thickening (rheology)
  - Negative resistance (ion channels, homeostatic balance...)
  - Macromolecular crowding: anomalous diffusion
- Fluctuation relations
  - Approaching the large-deviation regime
  - Time-reversal symmetry of current fluctuations
  - Effective fluctuating hydrodynamics description

A double challenge

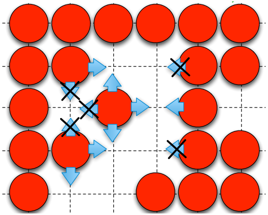
- No general Gibbs-Boltzmann framework in NESS
- We still do not know what an equilibrium glass is

The main ingredient

Cage effect in viscous liquids

Higher/Lower density regions prevent/facilitate particle rearrangements

- Ex.: a particle randomly jumps to a NN hole iff it has at least 2 NN holes before and after the move (detailed balance). No static interaction $\mathcal{H} = 0$

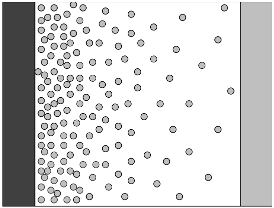


- At high density kinetic constraints are hardly satisfied, so dynamics is slow
- No particle is *permanently* blocked, (unless it was so in the initial state)
- Unlike *geometric* restrictions, where *states* (instead of *moves*) are forbidden, the *kinetic* restrictions imply a *trivial* thermodynamics

Plan of talk

1. Boundary-driven transport
   - Negative (differential) resistance and directed motion
   - Aging and steady state regime
2. Constrained exclusion processes
   - Transport and relaxation properties
   - Some features of the NESS measure
3. Fluctuation symmetry
   - Steady state fluctuation relation
   - Current fluctuations statistics

Boundary-driven transport



- boundary-induced dissipation
- density-dependent diffusion, $D(\rho)$
- vanishing diffusion at high density

$\rho(z,t)$ local density, $|z| \leq L$. Particle reservoirs at $\rho(\pm L, t) = \rho_\pm$.

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial z}\left[D(\rho)\,\frac{\partial \rho}{\partial z}\right]$$

An exactly solvable case is obtained for: $D(\rho) \sim (\rho_c - \rho)^\phi$

$\longrightarrow$ *Porous Medium Equation*

Non-equilibrium steady state

This is obtained by setting $\boxed{\partial_t \rho = 0}$ with $\boxed{\rho_- < \rho_+ < \rho_c}$

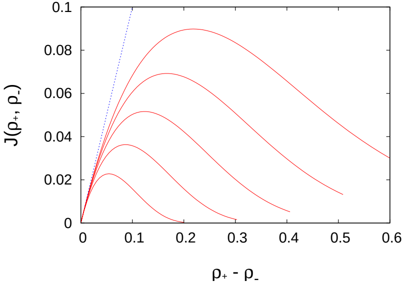
$$\begin{aligned} J(\rho_+, \rho_-) &\sim (\rho_c - \rho_-)^{1+\phi} - (\rho_c - \rho_+)^{1+\phi} \\ \rho_c - \rho(z) &= \left(a_+ - a_- \frac{z}{L} \right)^{1/(1+\phi)} \end{aligned}$$

with $a_\pm = \frac{1}{2} \left[(\rho_c - \rho_-)^{1+\phi} \pm (\rho_c - \rho_+)^{1+\phi} \right]$.

- density profile is nonlinear
- current depends on $\rho_c - \rho_\pm$, not simply $\rho_+ - \rho_-$

Negative differential resistance

To keep things simple, consider $\delta = \rho_- / \rho_+$ fixed.

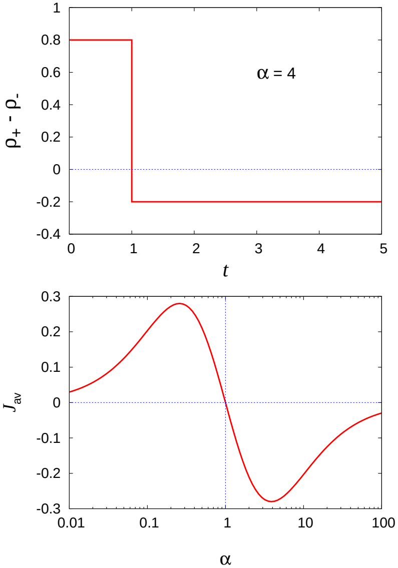


Current maximum and corresponding driving force can be computed by Lagrange multipliers method:

$$J^{\max} = \frac{\rho_c^{1+\phi}}{1+\phi} \frac{(1-\delta)^{1+\phi}}{\left(1-\delta^{\frac{1}{1+\phi}}\right)^{\phi}} ,$$

$$(\rho_+ - \rho_-)^{\max} = \rho_c (1-\delta) \frac{1-\delta^{\frac{1}{\phi}}}{1-\delta^{\frac{1+\phi}{\phi}}} .$$

Asymmetric piecewise-constant periodic forcing



$$\rho_\pm(t) = \begin{cases} 1 - \tau_0/\tau \text{ or } 0, & t \in [0, \tau_0] \\ 0 \text{ or } \tau_0/\tau, & t \in [\tau_0, \tau] \end{cases}$$

- zero average bias $\int_0^\tau \Delta\rho(t) dt = 0$

$$J_{\rm av}(\alpha) = \frac{1}{\tau} \int_0^\tau J[\rho_+(t), \rho_-(t)] dt$$

Asymmetry parameter $\alpha = \tau/\tau_0 - 1$

- optimal pumping condition

Non-stationary aging regime

Slow glassy dynamics is obtained by setting $\boxed{\rho_- = \rho_+ = \rho_c}$

Looking for solution of the form $\rho_c - \rho(z,t) = f(z)\, g(t)$, we get:

$$\begin{aligned} f(z) &= \left[f^{\phi}(z) f'(z)\right]' \text{ with boundary condition: } f(\pm L) = 0, \\ g'(t) &= g^{1+\phi}(t). \end{aligned}$$

Some interesting features

Power-law critical relaxation: $\rho_c - \rho(z,t) \sim t^{-1/\phi}$

Simple aging behaviour: $B(t, t_w) = \int_{t_w}^{t} D(s)\, ds \sim \log t - \log t_w$

Triangle relation: $B(t, t_w) = B(t, s) + B(s, t_w)$

Weak-ergodicity breaking: $\lim_{t\to\infty} \lim_{t_w\to\infty} B(t + t_w, t_w) \neq \lim_{t_w\to\infty} \lim_{t\to\infty} B(t + t_w, t_w)$

Constrained lattice gases: the *equilibrium* case

2d KA model: a particle on a square lattice can jump to a NN vacancy iff it has less than 3 NN particles *before* and *after* it has jumped.

Singular diffusion at high-density (via a bootstrap percolation argument):

$$D(\rho) \sim \exp \frac{c}{1-\rho}$$

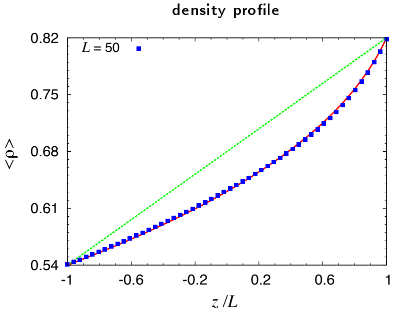
and several glassy features, e.g.:

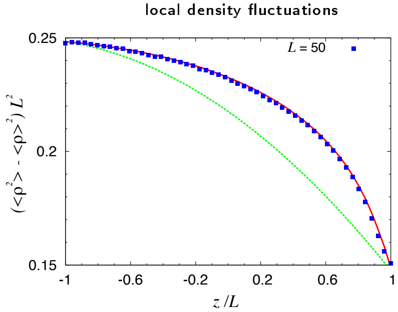
- Extensive entropy of metastable (= permanently blocked) states
- Stretched exponential relaxation, aging dynamics and heterogeneity
- Ergodicity breaking on Bethe lattice similar to Mode-Coupling Theory (*hybrid* transition and *higher-order glass singularities*)

Constrained exclusion processes: the *symmetric* case

2D KA model boundary-driven by two reservoirs at unequal densities.

No microscopic bias. Steady current driven by the density gradient.





Green lines refer to the unconstrained dynamics, that is to the Symmetric Exclusion Process (SEP)

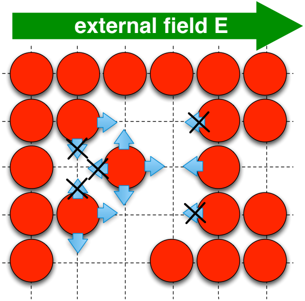
Asymmetric constrained exclusion processes

2*d* KA model bulk-driven by a constant and uniform applied force E.

Particles hop to a nearby empty site with probability:

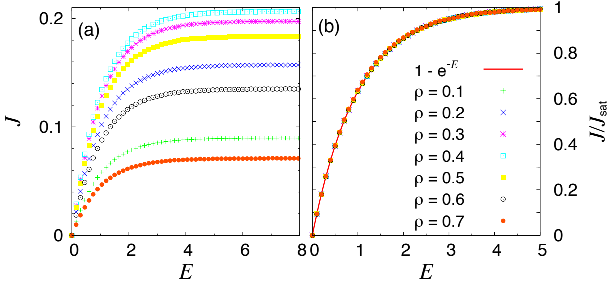
$$p = \delta(\text{constraint}) \times \min\left\{1,\, e^{\vec{E}\cdot\vec{dr}}\right\}$$

Detailed balance holds *locally* but not globally due to the periodic boundary



Positive resistance regime

Monotonic current behaviour is observed for particle density $\rho < 0.79$



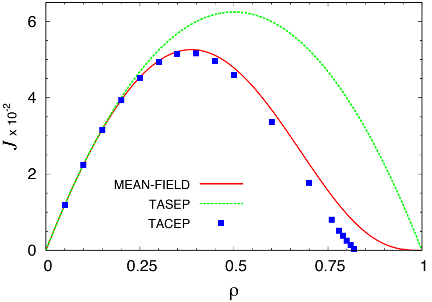
- Ohmic transport at small field, saturation at large fields, just as in ASEP
- Trivial field dependence of rescaled current $J(\rho, E)/J(\rho, \infty) = 1 - \mathrm{e}^{-E}$

For standard ASEP $J(\rho, E) = \rho(1-\rho)(1-\mathrm{e}^{-E})/4$.

The *totally asymmetric* case: $E \to \infty$

Saturation current can be approximated via a simple mean-field argument

$$J(\rho) \approx \frac{1}{4}\ \rho(1-\rho)\ (1-\rho^3)^2$$



Interplay of driving and constraints at large ρ and E

Qualitatively:

Particle moves against the field are rare

$\Downarrow$

Particles are generally more caged

$\Downarrow$

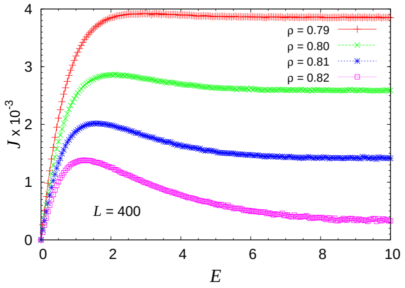
Rearrangements are more difficult

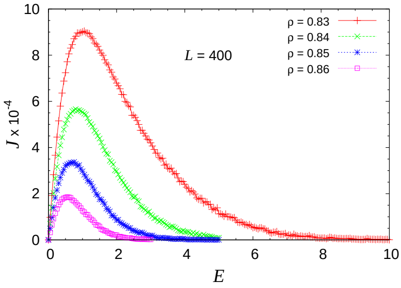
$\Downarrow$

Flow is more obstructed

Negative resistance and jamming

Non-monotonic current behaviour is observed for $\rho \geq 0.79$

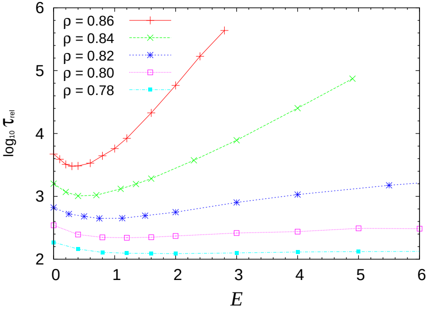




- Ohmic regime shrinks at larger density
- Apparent jamming at large fields
- Two regimes of vanishingly small current/entropy-production

"Non-Newtonian" features

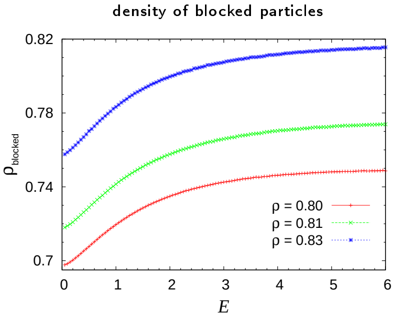
Non-monotonic field-dependence of structural relaxation time $\sim$ viscosity

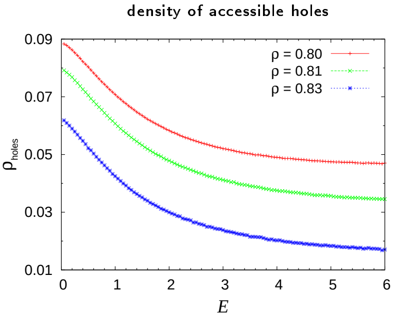


- "Thinning" regime at small E
- "Thickening" at larger E

Blocked particles and free volume

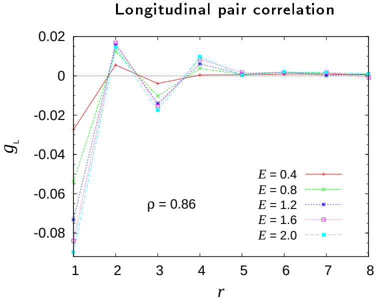
At variance with the equilibrium measure and with the ASEP, constant-density configurations are not equiprobable in NESS



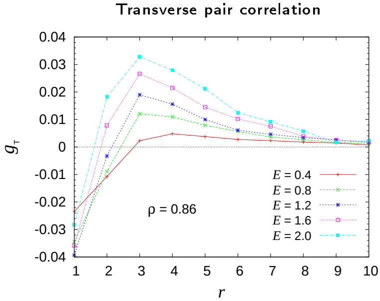


The NESS measure depends in a nontrivial manner on the applied field

Pair correlation



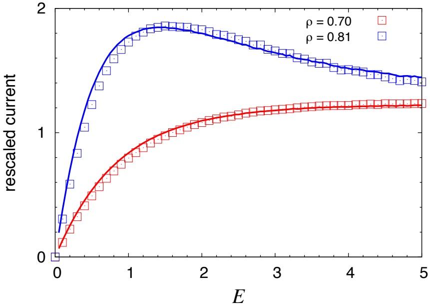
Liquid-like short-range longitudinal repulsion



Fluctuation-induced transverse attraction

A mean-field attempt

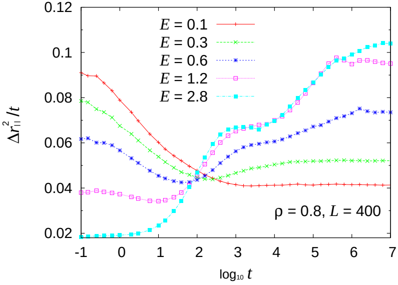
In analogy with the ASEP write $J(\rho, E) \sim (1 - \mathrm{e}^{-E})\ (1 - \rho_{\mathrm{blocked}})\ \rho_{\mathrm{hole}}$

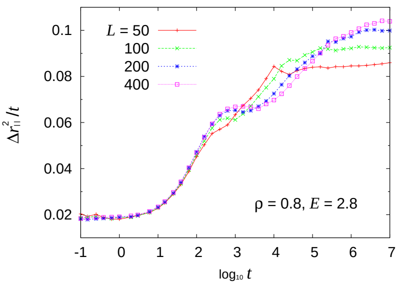


The transition between the positive and NR regimes is well described, however the approach fails as soon as $\rho > 0.81$, free particles and holes are strongly correlated

Anomalous diffusion

Time averaged longitudinal mean-square displacement





- Longitudinal diffusion is generally enhanced at late times
- Sub-diffusion regime at early times for small applied fields
- Long-lived longitudinal super-diffusion regime at larger E

3. Steady state fluctuation relation

A symmetry property of the PDF of entropy production W_τ over long time τ

$$\boxed{\frac{\Pi_\tau(+W_\tau)}{\Pi_\tau(-W_\tau)} = \mathrm{e}^{W_\tau}}$$

i.e., when Π_τ satisfies the time scaling of the large-deviation regime ($\tau \to \infty$)

$$\boxed{\Pi_\tau(W_\tau) = \mathrm{e}^{\tau\pi(W_\tau/\tau)}}$$

For vanishing driving forces you get fluctuation-dissipation theorem

$$2\ \langle W_\tau \rangle = \langle W_\tau^2 \rangle - \langle W_\tau \rangle^2$$

Two serious problems

- W_τ is extensive in time and space, and monotonic in the driving force
- How large τ must be? the large-deviation regime may be out of reach

Entropy production

Consider the action functional

$$W_\tau(\{\sigma\}) = \log \frac{k(\sigma_0,\sigma_1)\cdots k(\sigma_{\tau-1},\sigma_\tau)}{k(\sigma_\tau,\sigma_{\tau-1})\cdots k(\sigma_1,\sigma_0)}$$

where $k(\sigma,\sigma') \geq 0$ are the transition probabilities for $\sigma \to \sigma'$.
Detailed balance locally holds, and for mobile particles:

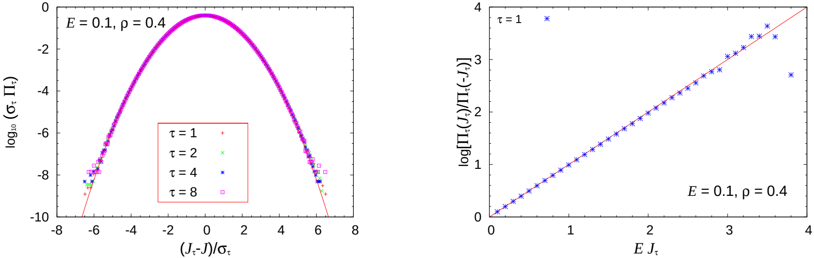
$$\log \frac{k(\sigma,\sigma')}{k(\sigma',\sigma)} = \log \frac{\min\left\{1,\, \mathrm{e}^{\vec{E}\cdot\vec{dr}}\right\}}{\min\left\{1,\, \mathrm{e}^{-\vec{E}\cdot\vec{dr}}\right\}} = \vec{E}\cdot\vec{dr} = 0,\, \pm E$$

So, the action functional W_τ represents the thermodynamic entropy production:

$$\boxed{W_\tau = E\ J_\tau}$$

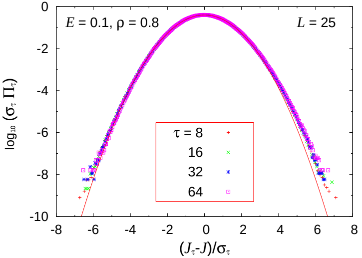
Current fluctuations I: Low-density Ohmic regime

Current fluctuations are generally Gaussian



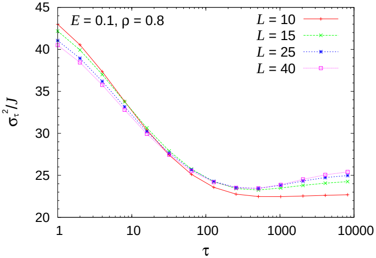
FR is always satisfied

Current fluctuations II: High-density Ohmic regime



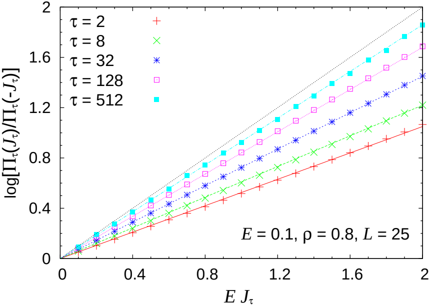
- small non-Gaussian tail develops
- no τ-dependence in rescaled PDF

- Relative fluctuations decrease
- Some finite-size effects



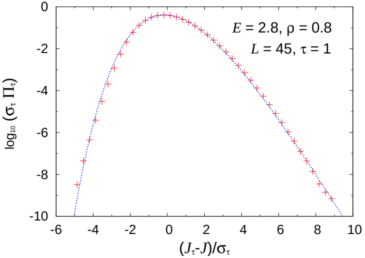
FR in the high-density Ohmic regime

Observable deviations from FR



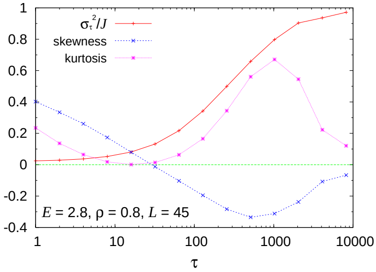
FR is eventually recovered, provided system size is not too large

Current fluctuations in the NR regime



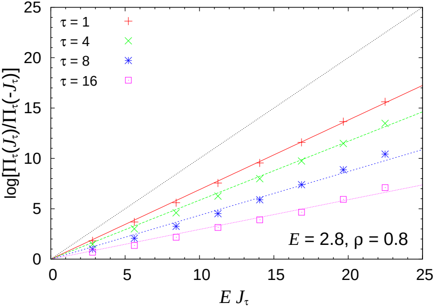
- non-Gaussian fluctuations
- generally skewed PDF

- strong τ-dependence of PDF
- relative fluctuations increase
- slow approach to asymptopy



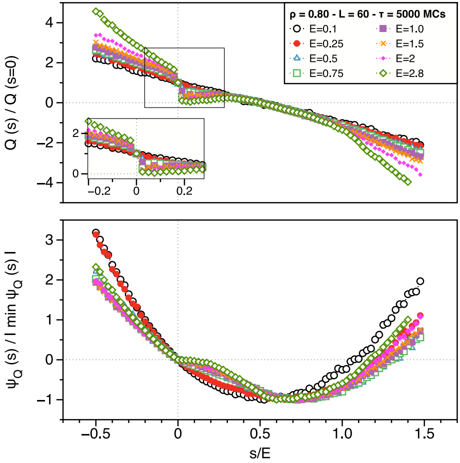
Steady-state FR in the NR regime

Time-reversal symmetry of FR is respected, but...



deviations from FR tend to increase at longer times

Asymmetric and singular LDF at large density and field



Conclusions and some open problems

Driven diffusive systems with glassy dynamics generally exhibit:

- Non-monotonic transport
- Non-Newtonian features
- Non-Gaussian fluctuations
- Anomalous (sub and super) diffusion
- Observable deviations from FR
- Physical irrilevance of large-deviation regime

–> Going beyond the non-linear diffusion model

–> Effective fluctuating hydrodynamic description

–> Phase diagram of TACEP with open boundaries

–> Exploring surface growth problems (ASEP $\leftrightarrow$ KPZ, ACEP $\leftrightarrow$?)

–> Constraints with nonuniform drive (rheology)

Related papers

- L Peliti and M Sellitto, *Aging in a simple model of structural glass*, J. Physique VI **8**, 49 (1998)
- M. Sellitto, *Fluctuations of entropy production in driven lattice glasses*, cond-mat/9809186 (unpublished)
- M Sellitto, *Driven lattice-gas as a ratchet and pawl machine*, Phys. Rev. E **65** 020101 (2002)
- M Sellitto, *Asymmetric exclusion processes with constrained dynamics*, Phys. Rev. Lett. **101**, 048301 (2008)
- M Sellitto, *Fluctuation relation and heterogeneous superdiffusion in glassy transport*, Phys. Rev. E **80**, 011134 (2009)
- F Turci, E Pitard, M Sellitto, *Driving kinetically constrained models into non-equilibrium steady states: structural and slow transport properties*, Phys. Rev. E **86**, 031112 (2012)

Relevant spatial structures