Statistical mechanics of the coagulation-diffusion process with a stochastic reset

Malte Henkel

Groupe de Physique Statistique
Institut Jean Lamour, Université de Lorraine **Nancy**, France

co-authors: X. Durang, H. Park (KIAS Seoul)

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Overview

1. Motivation
2. Single random walk with a reset, in $1D$
3. Coagulation-diffusion process with a reset
4. Interparticle distribution function
5. Conclusions

1. Motivation

Question : new aspects in behaviour of interacting many-body systems ?

use **exactly solvable models** as paradigms for fresh insight and as reference examples for further numerical study

non-equilibrium setting : master equation for the probability distribution $\mathbf{P}(\{\sigma\}; t)$ of a configuation $\{\sigma\}$

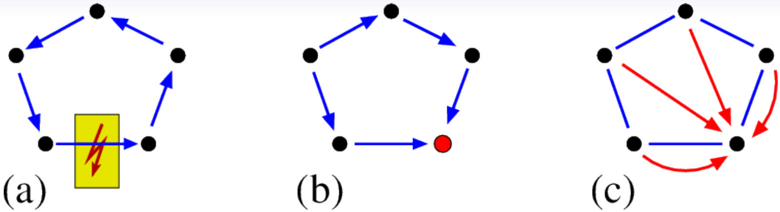
$$\frac{\partial}{\partial t}\mathbf{P}(\{\sigma\}; t) = \sum_{\{\sigma'\}} \left[w(\sigma' \to \sigma)\mathbf{P}(\{\sigma'\}; t) - w(\sigma \to \sigma')\mathbf{P}(\{\sigma\}; t) \right]$$

If **detailed balance condition**, with $\mathbf{P}_{\rm eq}(\{\sigma\}) = \lim_{t\to\infty} \mathbf{P}(\{\sigma\}; t)$

$$w(\sigma \to \sigma')\mathbf{P}_{\rm eq}(\{\sigma\}) \quad = \quad w(\sigma' \to \sigma)\mathbf{P}_{\rm eq}(\{\sigma'\}; t)$$

then relaxion towards equilibrium !

No probability currents between equilibrium configurations $\{\sigma\}, \{\sigma'\}$.



three ways (**2** old, **1** new) how to **break** detailed balance

$\Longrightarrow$ **non**-equilibrium stationary state

(a) probability currents, through coupling to external engines
(b) absorbing stationary states
(c) extra probability currents through **resets**

first case study : single random walk with reset — EVANS & MAJUMDAR 11

may lead to improved search algorithms

here : interacting many-body system with reset — **CDPR**

$=$ **C**oagulation-**D**iffusion **P**rocess with a stochastic **R**eset

2. Single random walk with a reset, in $1D$

Evans & Majumdar '11 `arxiv:1102.2704`

random walk of a single particle,
sent back to its initial position x_0 with probability r at each step

without reset

$$(\partial_t - D\partial_x^2)P(t,x) = 0$$

$$P(t,x) = (2\pi\sigma^2)^{-1/2} \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]$$

gaussian

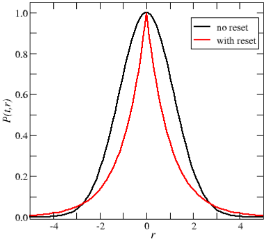
with reset rate $r > 0$

$$(\partial_t - D\partial_x^2)P(t,x) = -rP(t,x) + r\delta(x-x_0)$$

$$P(\infty,x) = \frac{\alpha}{2} \exp\left[-\alpha|x-x_0|\right]$$

laplacian

$$\alpha^2 = r/D$$



3. Coagulation-diffusion process with a reset

'coagulation' reaction : $2A \xrightarrow{D} A$, diffusion : $A + \emptyset \xleftrightarrow{D} \emptyset + A$

method of empty intervals : ben Avraham, Burschka, Doering 90,...

probability of n consecutive empty sites : $E_n(t) = \mathbf{P}(\boxed{\text{n}}; t)$

$\Longrightarrow$ **closed** equation of motion **!** continuum limit $E_n(t) \to E(t,x)$

$$(\partial_t - 2D\partial_x^2)E(t,x) = 0 \;\; ; \;\; E(t,0) = 1 \;\; , \;\; E(t,\infty) = 0$$

treat non-standard boundary conditions by analytic continuation to $x < 0$:

$\boxed{E(t,-x) := 2 - E(t,x)}$ Durang, Fortin, mh ...'10

$\Longrightarrow$ slow, **algebraic**, decay of particle density

$$\rho(t) = -\,\partial_x E(t,x)|_{x=0} \sim t^{-\alpha} \;\; , \;\; \alpha = \frac{1}{2}$$

α measured in exciton kinetics on $1D$ polymers/carbon nano-tubes 1989-2013

$C_{10}H_8$: $0.52 - 0.59$, PMMA : $0.47(3)$, TMMC : $0.48(4)$, Cnano : $0.51(3)$

Kopelman *et al.*; Kroon *et al.*; Russo *et al.*; Srivastava & Kono ; Allam *et al.*

define the **CDPR** on a lattice :

1. select a reset configuration, described by empty-interval probabilities F_n
Example : if each site is occupied with proba. $p \Rightarrow F_n = (1-p)^n$
cont. limit : $F_n \to F(x) = e^{-cx}$ with $c = -\ln(1-p) \simeq p + \mathrm{O}(p^2)$

2. take a chain with $\mathcal{N}$ sites, 1 **sweep** $:= \mathcal{N}$ steps of micro dynamics

3. in each step, a single particle either **hops** to a nearest neighbour,
with proba. $\mathcal{P}_d = \mathcal{P}_g = D/(2D + r/\mathcal{N})$
or else the system is **reset** to the distribution F_n
with proba. $\mathcal{P}_r = (r/\mathcal{N})/(2D + r/\mathcal{N})$.

continuum limit : have for the empty-interval probabilities $E_n(t) \to E(t,x)$

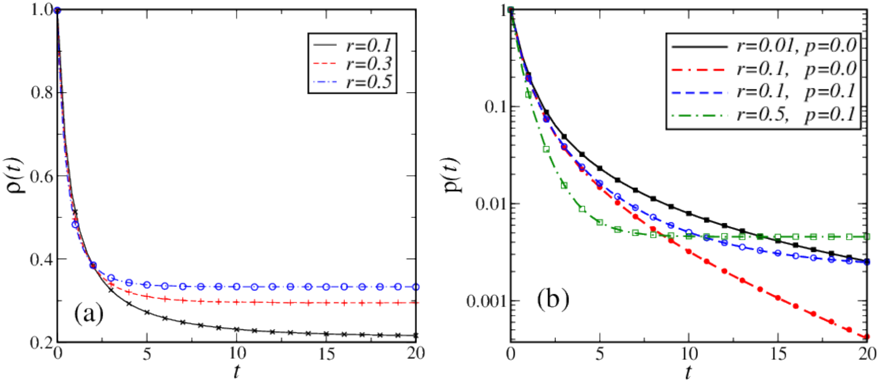
$$(\partial_t - 2D\partial_x^2)E(t,x) = r\left(F(x) - E(t,x)\right) \;\; ; \;\; E(t,0) = 1 \;\; , \;\; E(t,\infty) = 0$$

quite analogous to master equation of a single random walk with reset !

to test the equation of motion :
solve them explicitly on the discrete lattice and **compare with simulations**

particle density : $\rho(t) = 1 - E_1(t)$ **left** panel, $p = 0.5$

pair density : $p(t) = 1 - 2E_1(t) + E_2(t)$ **right** panel



perfect agreement between analytical and numerical methods

in general exponential approach towards $\rho(\infty) \neq 0$, $p(\infty) \neq 0$

A) CDPR in the continuum

In the continuum limit, solve equation of motion

$$\partial_t E(t,x) = 2D\partial_x^2 E(t,x) - rE(t,x) + rF(x)\ ,\ \ E(t,0) = 1\ ,\ \ E(t,\infty) = 0$$

via the decompostion $\boxed{E(t,x) = \frac{1}{2}f(x) + b(t,x)}$ such that

$$\begin{aligned} f''(x) - \alpha^2 f(x) + 2\alpha^2 F(x) &= 0\ ;\ \ f(0) = 2\ ,\ \ f(\infty) = 0 \\ \partial_t b(t,x) - 2D\partial_x^2 b(t,x) + rb(t,x) &= 0\ ;\ \ b(t,0) = b(t,\infty) = 0 \end{aligned}$$

where $\alpha^2 := r/(2D)$. The solutions are (with $b_0(x) = E_0(x) - \frac{1}{2}f(x)$, $F(x) = e^{-cx}$)

$$\begin{aligned} f(x) &= \left(2 - \frac{\alpha}{\alpha+c}\right) e^{-\alpha x} + \frac{\alpha}{\alpha+c}\, e^{-cx} + \frac{\alpha}{\alpha-c}\left(e^{-(c-\alpha)x} - 1\right) e^{-\alpha x} \\ b(t,x) &= \sqrt{\frac{\pi}{2Dt}}\, e^{-2D\alpha^2 t} \int_0^\infty \mathrm{d}x'\ b_0(x') \left[e^{-\frac{(x-x')^2}{8Dt}} - e^{-\frac{(x+x')^2}{8Dt}}\right] \end{aligned}$$

$\Longrightarrow$ particle-density $\rho(t) = -\left.\partial_x E(t,x)\right|_{x=0}$ becomes for large times

$$\rho(t) \overset{t\to\infty}{\simeq} \frac{\alpha c}{\alpha + c} + \mathrm{O}\left(t^{-1/2} \exp\left(-2D\alpha^2 t\right)\right)$$

$\Longrightarrow$ stationary density ρ_∞ depends **monotonously** on $\alpha \sim \sqrt{r}$

B) CDPR in the continuum, with extra **input** $\emptyset \xrightarrow{\lambda} A$

solve equation of motion, with boundary conditions $E(t,0)=1,\ E(t,\infty)=0$

$$\partial_t E(t,x) = 2D\partial_x^2 E(t,x) - \lambda x E(t,x) - rE(t,x) + rF(x)$$

let $\boxed{\alpha^2 := \frac{r}{2D},\ \beta^3 := \frac{\lambda}{2D},\ \mu := \frac{\alpha^2}{\beta^3} = \frac{r}{\lambda}}$, decompose $E(t,x) = \frac{1}{2}f(x) + b(t,x)$

$\Longrightarrow$ stationary part $f(x)$ obeys

$$f''(x) - \beta^3(x+\mu)f(x) + 2\alpha^2 F(x) = 0 \ \ ; \ \ f(0)=2 \ \ , \ \ f(\infty)=0$$

with an explicitly known solution in terms of Airy functions Ai, Bi.

$\Longrightarrow$ stationary density ρ_∞ has **scaling form**, c : density of reset

$$\rho_\infty = -\frac{1}{2}\left.\frac{\partial f(x)}{\partial x}\right|_{x=0} = cP\left(\frac{c}{\beta}, \beta\mu\right)$$

$$P(u,y) = -\frac{1}{u}\frac{\mathrm{Ai}'(y)}{\mathrm{Ai}(y)} - \pi y\left(\mathrm{Bi}'(y) - \mathrm{Ai}'(y)\frac{\mathrm{Bi}(y)}{\mathrm{Ai}(y)}\right)\int_0^\infty \mathrm{d}Y\, F(uY/c)\mathrm{Ai}(Y+y)$$

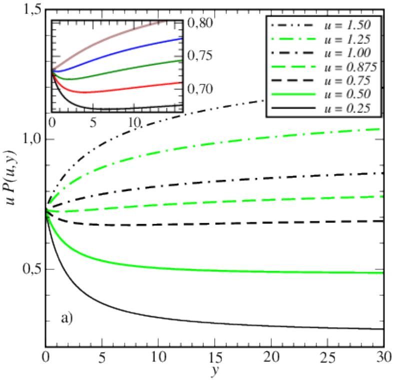
dynamics : relax. time $\frac{1}{\tau} = |a_1|\beta^2 + r$, with $\mathrm{Ai}(a_1)=0$, exponential approch to stat. state

$\Longrightarrow$ **non-monotonous** dependence of ρ_∞ on c, α, β **!**

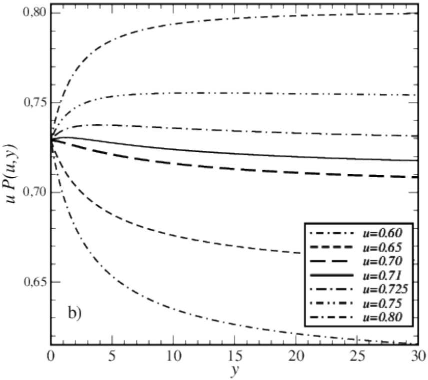
interpretation : $u = c/\beta \approx \dfrac{\text{density of reset}}{\text{stat. density without reset}}$,

$$y = (\alpha/\beta)^2 = \frac{\text{scaled reset rate}}{\text{scaled input rate}}$$

left panel $F(x) = e^{-cx}$



right panel $F(x) = \mathrm{erfc}\left(\frac{\sqrt{\pi}}{2}cx\right)$



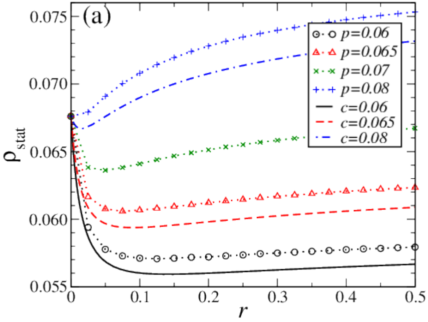
left : if $u < u_c \simeq 0.93$, then $uP(u,y)$ has a **minimum** at some $y^* \neq 0$

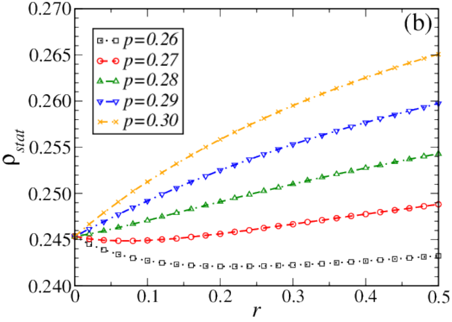
if $u > u_c$, then $uP(u,y)$ increases monotonously with y

right : if $u \approx 0.70 - 0.75$, then $uP(u,y)$ has a **maximum** at some $y^* \neq 0$

qualitatively similar for simulations on discrete chain, $F(x) = e^{-cx}$
and two values of the input rate λ,
p is the occupation probability of a site after reset

left panel $\lambda = 0.0008$ right panel $\lambda = 0.04$





full lines : exact solution in the continuum

4. Interparticle distribution function (IPDF)

on discrete chain $\mathcal{D}_n$: proba. that distance to nearest particle is n

$$\text{in the continuum limit :} \quad \mathcal{D}_n \to \mathcal{D}(x) = \frac{1}{2\rho_\infty} \frac{\partial^2 f(x)}{\partial x^2}$$

several **examples** of the stationary empty-interval probability $E(\infty, x)$
and the stationary IPDF $\mathcal{D}(x)$;
for later comparison in systems with a reset :

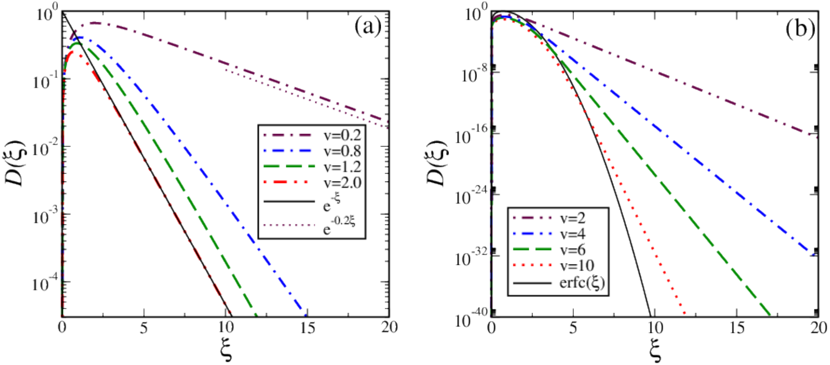
	system	$E(\infty,x)$	$\mathcal{D}(x)$
(a)	uncorrelated	$\exp(-cx)$	$c\exp(-cx)$
(b)	coagulation-diffusion	$\mathrm{erfc}\left(\frac{1}{2}\sqrt{\pi}\,cx\right)$	$\frac{1}{2}\pi c^2\, x \exp\left(-\frac{\pi}{4}c^2x^2\right)$
(c)	with particle-input	$\mathrm{Ai}\,(\beta x)/\mathrm{Ai}\,(0)$	$\beta^2 x \mathrm{Ai}\,(\beta x)/\lvert\mathrm{Ai}\,'(0)\rvert$

A) IPDF without input $\Longrightarrow$ scaling form

$\mathcal{D}(x) = \alpha D(\xi, v)$, with $\xi := cx$ and $v := \alpha/c$

$$D(\xi,v) = \frac{\alpha}{\rho_\infty}\left[e^{-v\xi} - F\left(\frac{\xi}{c}\right) + \frac{v}{2}\left[\int_0^\xi \mathrm{d}Y\, F\left(\frac{Y}{c}\right) e^{v(Y-\xi)} + \int_\xi^\infty \mathrm{d}Y\, F\left(\frac{Y}{c}\right) e^{v(\xi-Y)} - \int_0^\infty \mathrm{d}Y\, F\left(\frac{Y}{c}\right) e^{-v(Y+\xi)}\right]\right]$$

left panel : $F(x) = e^{-cx}$ right panel : $F(x) = \mathrm{erfc}\left(\frac{1}{2}\sqrt{\pi}\, cx\right)$



small interval size ξ : **local correlations**, according to micro-dynamics

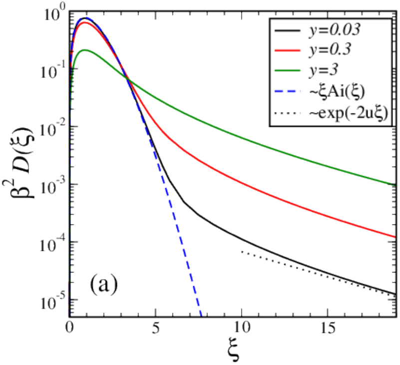
large interval size ξ : correlations remain those imposed by reset

B) IPDF with input $\Longrightarrow$ scaling form

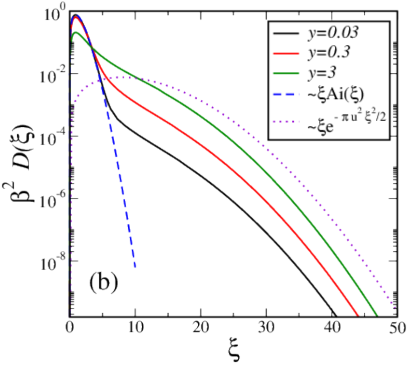
$$\mathcal{D}(x) = \frac{\beta^2}{\rho_\infty} D(\xi, u, y) \ , \ \xi := \beta x \ , \ u := c/\beta \ , \ y := \beta\mu$$

with an explicitly known scaling function.

left panel : $F(x) = e^{-cx}$, $u = 0.1$



right panel : $F(x) = \mathrm{erfc}\left(\frac{1}{2}\sqrt{\pi}\, cx\right)$, $u = 0.1$



5. Conclusions

stochastic reset brings systems out of detailed balance in a new, yet unexplored way

find new types of non-equilibrium stationary states

rapid relaxation with a **finite** relaxation time $\tau < \infty$

if CDPR and also input, find unexpected non-trivial dependence of particle density on reset and input rates

CDPR is first example of interacting many-body system with a reset

physical picture : the reset rate r introduces a new time scale $\tau_r \sim \alpha^{-2}$,
and a new **length scale** $\xi_r \sim \alpha^{-1}$.
ξ_r separates un-modified dynamics for scales $\lesssim \xi_r$
and reset distribution for scales $\gtrsim \xi_r$.

Open question : can one use this as an efficient means to rapidly relax a system to its stationary state ?