Derivation of mean-field rate equations for stochastic particle systems

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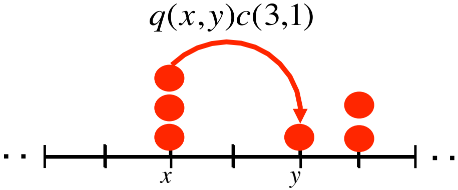
Outline

1. Introduction
   - Stochastic Particle systems
   - Condensation
   - Dynamics of condensation
2. Results
   - Main Theorem
   - Properties of solutions to MFE
   - Scaling analysis
   - Birth death chain for ZRP
3. Summary

Stochastic particle systems



Lattice: Λ of size $|\Lambda| = L$

State space: $X_L = \{0, 1, ..\}^\Lambda$

$\boldsymbol{\eta} = (\eta_x : x \in \Lambda)$

Jump rates: $q(x, y)\, c(\eta_x, \eta_y)$

q irreducible on Λ, $c(k, l) = 0 \;\Leftrightarrow\; k = 0$

Generator:

$$\mathcal{L}h(\boldsymbol{\eta}) = \sum_{x,y\in\Lambda} q(x, y)c(\eta_x, \eta_y)\big(h(\boldsymbol{\eta}^{x,y}) - h(\boldsymbol{\eta})\big)$$

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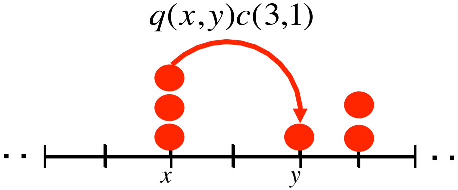

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Zero-range process (ZRP)

$$c(k, l) = g(k) = \begin{cases} 0 & \text{if} \quad k = 0, \\ 1 + \frac{b}{k^\gamma} & \text{otherwise,} \end{cases}$$

for any constant $b > 0$ and $\gamma \in (0, 1]$.

[Spitzer (1970); Andjel (1982); Cocozza-Thivent (1985); Evans (2000)]

Stationary measures

Product measures ν_ϕ with marginals

$$\nu_\phi[\eta_x = n] = \frac{1}{z(\phi)}\,\phi^n w(n) \quad \text{with} \quad w(k) = \prod_{k=1}^{n} \frac{c(1,k-1)}{c(k,0)}$$

where $0 \le \phi < \phi_c$, radius of convergence of $z(\phi) = \sum_{k\ge 0} \phi^k w(k)$

[Cocozza-Thivent (1985), Fajfrova, Gobron, Saada (2015)]

Above are stationary for a spatially homogeneous SPS if and only if

$$\frac{c(n,m)}{c(m+1,n-1)} = \frac{c(n,0)c(1,m)}{c(m+1,0)c(1,n-1)} \quad \text{for all } n \ge 1,\ m \ge 0$$

and $\quad c(n,m) - c(m,n) = c(n,0) - c(m,0) \quad$ for all $n, m \ge 0$.

Condensation

spatial homogeneity for all $x \in \Lambda$ $\sum_{y\in\Lambda} \big(q(x,y) - q(y,x)\big) = 0$

canonical measures $\pi_{L,N}$ on $X_{L,N} = \big\{\boldsymbol{\eta} \in X_L : \sum_{x\in\Lambda} \eta_x = N\big\}$

thermodynamic limit $L, N \to \infty$, $N/L \to \rho \geq 0$

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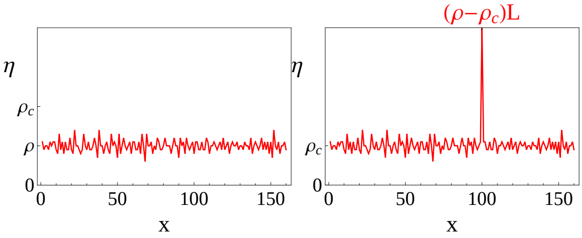
A spatially homogeneous SPS exhibits condensation with critical density ρ_c, if

$$\rho_c := \sup\big\{\rho \geq 0 : N/L \to \rho,\ \limsup_{N,L\to\infty} \pi_{L,N}(\eta_x^2) < \infty\big\} < \infty\ .$$

Condensation in ZRP

The system exhibits a phase transition in the thermodynamic limit. If $\rho > \rho_c$, the system separates into

1. a homogeneous background
2. a condensate, which is the excess mass accumulated on a single randomly located lattice site.



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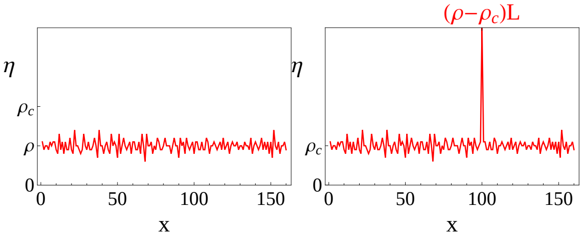


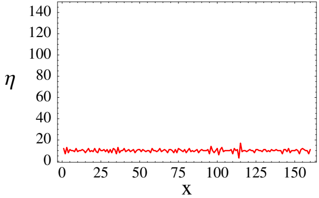
Applies to ZRP with $\phi_c = 1$, and we have with $R(\phi) = \nu_\phi(\eta_x)$

$$\rho_c = \lim_{\phi \nearrow \phi_c} R(\phi) \in [0, \infty] \ .$$

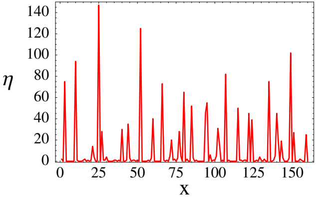
$\rightarrow$ Condensed phase concentrates on a single lattice site.

Dynamics of condensation

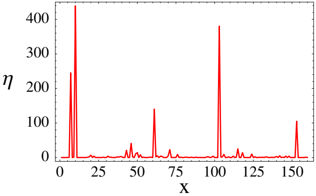
ZRP with $g(k) = 1 + b/k$, $b = 2.5$, $\rho_c = 1/(b-2) = 2$, $\rho = 10$



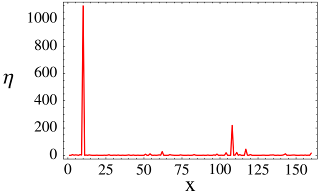
Nucleation $O(1)$



$O(1)$ ↓ **Coarsening**



Saturation $O(L^2, L^3)$



stationary dynamics of condensate $O(L^{1+b})$

Previous results on condensation dynamics

Stationary dynamics for ZRP

- L fixed, $N \to \infty$, $q(x, y)$ reversible [Beltrán, Landim (2010,11,12,15)]

$$Y^N\big(\eta(tN^{1+b})\big) \to Y_t \quad \text{RW on (subset of) } \Lambda$$

- L fixed, $N \to \infty$, $q(x, y) = \delta_{y,x+1}$ with PBC [Landim (2014)]
- $L, N \to \infty$, $N/L \to \rho > \rho_c$, $q(x, y)$ symmetric on rescaled torus $\subset \mathbb{T}$

$$Y^L\big(\eta(tL^{1+b})\big) \to Y_t \quad \text{Lévy-type on } \mathbb{T}$$

[Armendáriz, G., Loulakis (2017)]

Nucleation/Coarsening for ZRP

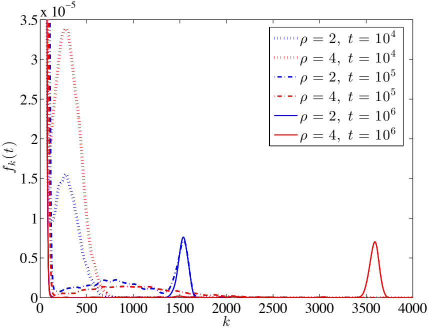
- L fixed, $N \to \infty$, $q(x, y)$ irreducible [Beltrán, Jara, Landim (2017)]

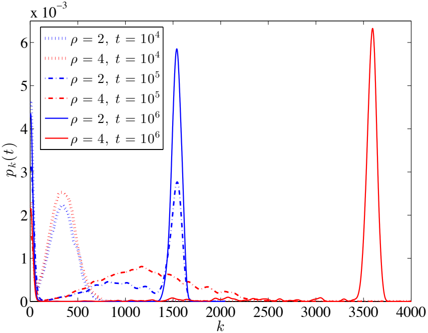
$$\boldsymbol{\eta}(tN^2)/N \to \mathbf{X}_t \quad \text{absorbed diffusion on } \Delta_L$$

Mean-field equation

Single-site marginal and size-biased version

$$f_k^L(t) := \mathbb{P}[\eta_x(t) = k] \ , \quad p_k^L(t) = \frac{k\, f_k^L(t)}{\rho}$$





ZRP with $g(k) = 1 + b/k,\ b = 4,\ \rho_c = 0.5,\ L = 1024$

Mean-field equation

SPS with generator $\mathcal{L}h(\boldsymbol{\eta}) = \sum_{x,y\in\Lambda} p(x,y)c(\eta_x,\eta_y)\big(h(\boldsymbol{\eta}^{x,y}) - h(\boldsymbol{\eta})\big)$

Assume

- $q(x,y) = 1/(L-1)$ (complete graph) ,
- $c(k,l) \leq \bar{C}$ (uniformly bounded rates)
- $\eta_x(0) \sim f(0)$ (i.i.d. initial conditions with density ρ)

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Theorem

Under above assumptions $f_k^L(t) \to f_k(t)$ for all $k \in \mathbb{N}_0$ and $t \geq 0$ where $f(t) = (f_k(t) : k \in \mathbb{N}_0)$ is the unique solution of the MF equation

$$\frac{d}{dt} f_k(t) = \sum_{l\geq 0}\Big(c(k+1,l) f_l(t) f_{k+1}(t) + c(l,k-1) f_l(t) f_{k-1}(t)\Big) - \sum_{l\geq 0}\big(c(k,l)+c(l,k)\big) f_l(t) f_k(t) \quad \text{for all } k \geq 0 , \tag{MFE}$$

with initial condition $f(0)$ given above.

Mean-field equation

Corollary

The single-site process $\big(\eta_x(t) : t \geq 0\big)$ converges weakly on path space to a (non-linear) birth-death chain on $\mathbb{N}_0$ with rates

$$\beta_k(t) = \sum_{l \geq 0} c(l,k) f_l(t) \quad \text{and} \quad \mu_k(t) = \sum_{l \geq 0} c(k,l) f_l(t) \ .$$

Proof. 1. Law $\mathbb{Q}^L$ of $t \mapsto \eta_x(t)$ is tight on $D([0,\infty), \mathbb{N}_0)$ by a standard application of Aldous' criterion

$\Rightarrow$ Existence of limit points $\mathbb{Q}$ and $t \mapsto f(t) = \mathbb{Q}[\eta_x(t) = .]$

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$$\Rightarrow \quad \text{Existence of limit points } \mathbb{Q} \text{ and } t \mapsto f(t) = \mathbb{Q}[\eta_x(t) = .]$$

2. Limit $f(t)$ solves MFE: Apply generator $\mathcal{L}$ to $\mathbb{I}_{\eta_x = k}(\boldsymbol{\eta})$ to get

$$\begin{aligned} \frac{d}{dt} f_k^L(t) = \sum_{l\geq 0} \Big(& c(k{+}1,l)\, \mathbb{P}^L[\eta_x(t) = k{+}1, \eta_y(t) = l] \\ & + c(l,k{-}1)\, \mathbb{P}^L[\eta_x(t) = k{-}1, \eta_y(t) = l] \Big) \\ & - \sum_{l\geq 0} \big(c(k,l) + c(l,k)\big) \mathbb{P}^L[\eta_x(t) = k, \eta_y(t) = l] \end{aligned}$$

Mean-field equation – Proof

Factorization Lemma

For $x \neq y \in \Lambda$ and all $t \geq 0$ we have uniformly in $k, l \in \mathbb{N}_0$

$$\mathbb{P}^L[\eta_x(t) = k, \eta_y(t) = l] \to f_k(t)\, f_l(t) \quad \text{as } L \to \infty \ .$$

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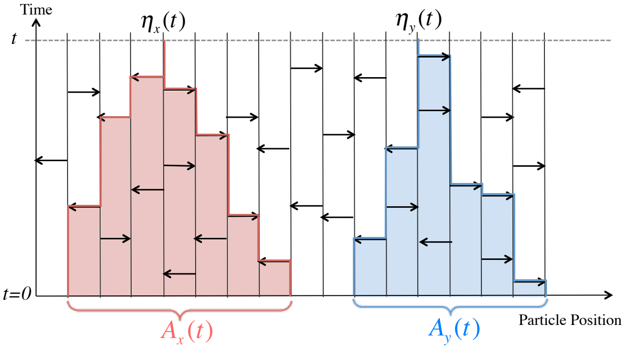
Graphical construction given by i.i.d. $PP_{xy}\big(\frac{\bar{C}}{L-1}\big)$; use to define

$$A_x(t) = \big\{z \in \Lambda : (z,0) \to (x,t)\big\} \subset \Lambda \quad \text{for all } x$$



Mean-field equation – Proof

Proof of Theorem. 1. Existence of limit points $(f(t) : t \geq 0)$

2. Limits points are solutions of (MFE)

3. Uniqueness of solutions of (MFE)

Mean-field equation – Proof

Proof of Theorem. 1. Existence of limit points $(f(t) : t \geq 0)$

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3. Uniqueness of solutions of (MFE)

We have $f_k^L(t) \in [0,1]$ and $\sum_k f_k^L(t) = 1$ for all $L \geq 0$, so

$$f_k(t) \in [0,1] \quad \text{and} \quad \sum_k f_k(t) \leq 1 \ .$$

Consider two solutions $f(t), \hat{f}(t)$ of above type with $f(0) = \hat{f}(0) \in \mathcal{P}(\mathbb{N}_0)$. Then

$$\frac{d}{dt} \|f(t) - \hat{f}(t)\|_2^2 \leq 16\bar{C} \|f(t) - \hat{f}(t)\|_2^2$$

which implies $f(t) = \hat{f}(t)$ for all $t \geq 0$ by Gronwall.

Properties of solutions to MFE

$(Y_t : t \geq 0)$ non-linear BD chain with master equation (MFE) and generator

$$\mathcal{L}_{BD}h(k) = \beta_k(t)\big(h(k+1) - h(k)\big) + \mu_k(t)\big(h(k-1) - h(k)\big)$$

- **moments** $m_i(t) = \sum_{k \geq 0} k^i f_k(t)$

  $m_0(t) \equiv m_0(0)$ and $m_1(t) \equiv m_1(0)$ are conserved.

  in general $(Y_t : t \geq 0)$ is not a martingale , $\mathcal{L}_{BD}k = \beta_k(t) - \mu_k(t)$

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- **stationary solutions.** marginals of invariant product measures

  $f_k^\phi := \nu_\phi[\eta_x = k]$ for all $m_1 = R(\phi) \leq \rho_c$

- **ergodicity.** we expect $f(t) \to f^\phi$ as $t \to \infty$, if $m_1(0) = R(\phi) \leq \rho_c$

  for $\rho = m_1(0) > \rho_c$ we expect as $t \to \infty$ (phase separated solution)

  $f(t) \to f^{\phi_c}$ but also $m_1(t) \equiv \rho > \rho_c$

Scaling analysis for ZRP

Scaling ansatz for phase separated solution with $m_1(t) = \rho > \rho_c$

$$f_k(t) = f_k^{\text{bulk}}(t) + \epsilon_t^2 h(k\epsilon_t) \quad \text{as } t \to \infty$$

with scale $\epsilon_t \to 0$ and scaling function $h(u)$, $u > 0$, and $h(u) \to 0$ as $u \to \infty$

We have $f^{\text{bulk}}(t) \to f^{\phi_c}$ and $\displaystyle\sum_{k > \epsilon_t^{-1/2}} k\epsilon_t^2 h(k\epsilon_t) \to \int_{u>0} uh(u)\, du = \rho - \rho_c$.

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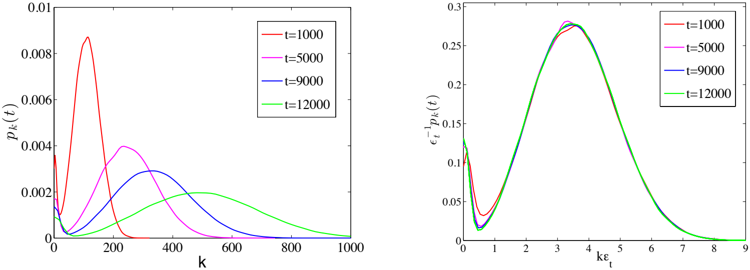
ZRP with rates $g(k) = 1 + b/k$, $b = 4$, $\rho_c = 1/2$, $\rho = 10$



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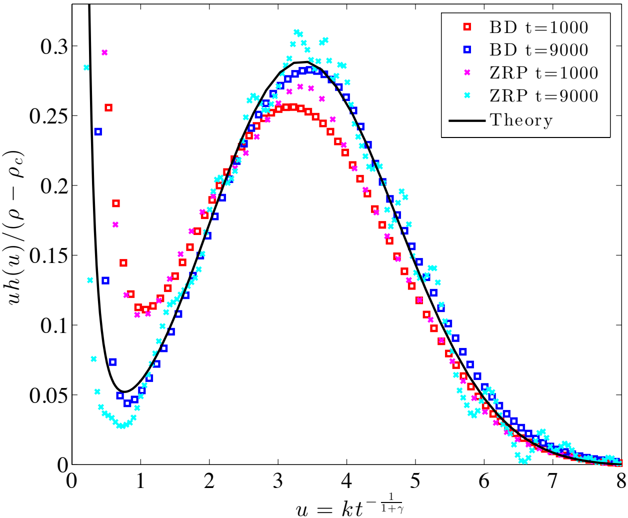
ZRP with rates $g(k) = 1 + b/k$, $\phi_c = 1$. With $\bar{g}(t) := \sum_{k \geq 0} g(k) f_k(t)$ we get

$$\frac{d}{dt} f_k(t) = g(k+1) f_{k+1}(t) + \bar{g}(t) f_{k-1}(t) - \big(g(k) + \bar{g}(t)\big) f_k(t) \ .$$

Under scaling ansatz we have $\bar{g}(t) = 1 + A\epsilon_t$, and (MFE) leads to

$$\epsilon_t = t^{-1/2} \ , \quad h''(u) + \Big(\frac{u}{2} - A + \frac{b}{u}\Big) h'(u) + \Big(1 - \frac{b}{u^2}\Big) h(u) = 0$$

Scaling analysis for ZRP



ZRP with $b = 4$, $\rho = 2$, $L = 1024$, 500 realizations

Birth death chain related to $f_k(t)$

Simulate m copies $(Y_t^i : t \geq 0)$ of the BD chain with generator

$$\mathcal{L}H(Y) = \sum_{i=1}^{m} g(Y^i)[H(Y - e^i) - H(Y)] + \bar{g}(t)[H(Y + e^i) - H(Y)],$$

with approximated rates $\bar{g}(t) \approx \langle g \rangle_m = \frac{1}{m} \sum_{i=1}^{m} g(Y_t^i)$.

- the total particle number $H(Y_t) = \sum_{i=1}^{m} Y_t^i$ is a (non-negative) martingale with QV linear in time
- absorbing state $Y_i = \mathbf{0}$ affects sampling at times of order m^2
- vanishing volume fraction of condensed phase (poor statistics)

Size-biased BD chain

Size-biased dynamics $(X_t : t \geq 0)$ on state space $\mathbb{N}$.
$p_k(t) = k\, f_k(t)/\rho$, $k \geq 1$, use (MFE) to get

$$\frac{d}{dt}p_k(t) = \frac{k}{k+1}g(k+1)p_{k+1}(t) + \frac{k}{k-1}\bar{g}(t)p_{k-1}(t) - \left(\frac{k-1}{k}g(k) + \frac{k+1}{k}\bar{g}(t)\right)p_k(t) + \frac{1}{k}(\bar{g}(t) - g(k))p_k(t).$$

$$\frac{d}{dt}p_1(t) = \frac{1}{2}g(2)p_2(t) - 2\bar{g}(t)p_1(t) + \sum_{k\geq 2}\frac{1}{k}(g(k) - \bar{g}(t))p_k(t),$$

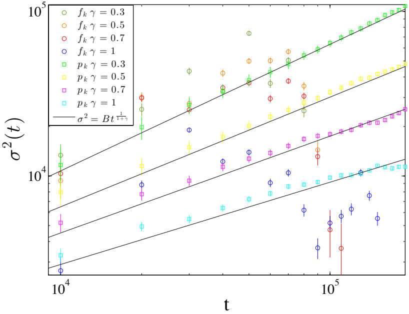
using $f_0(t) = 1 - \rho \sum_{k\geq 1} p_k(t)/k$.

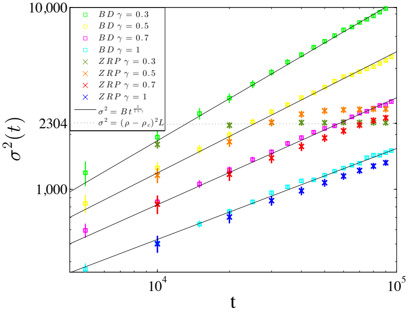
$\rightarrow$ BD chain with long-range jumps $k \rightarrow 1$ and diagonal terms

- **no** additional conservation law
- **no** absorbing state for m copies $(X_t^i : t \geq 0)$
- $X_t^i \rightarrow X_t$ as $m \rightarrow \infty$ uniformly in t
- $m_2(t) = \mathbb{E}[\eta_x^2(t)]$ is well approximated by $\frac{1}{m}\sum_{i=1}^m X_t^i$.

Scaling analysis for ZRP

ZRP with $g(k) = 1 + b/k^{\gamma}$, $b = 4$, $\gamma \in (0, 1]$, $\rho = 10$ and 2





$$\frac{d}{dt} m_2(t) \simeq (2\rho + 2) \underbrace{(\bar{g}(t) - 1)}_{= A\epsilon_t^{\gamma}}$$

Follows from $\mathcal{L}_{BD} k^2$ and with $\epsilon_t = t^{-1/(1+\gamma)}$ leads to $m_2(t) \simeq Bt^{1/(1+\gamma)}$

Summary

Results so far

- derivation of (MFE) for SPS with bounded rates (and actually with sublinear rate recently published in [S.G.,W.J (2018)])
- heuristic scaling analysis of (MFE)
- size-biased BD chains for ZRP provide efficient sampling tool

Work in progress

- rigorously establish scaling solution and coarsening scaling law for ZRP and IP
- generalised version of size-biased BD chain
- consider explosive condensation models with $c(k,l) = k^\gamma(d + l^\gamma)\ , \quad \gamma \geq 1$

Thank you!