

Kinetic and stochastic models of condensation

Stefan Grosskinsky

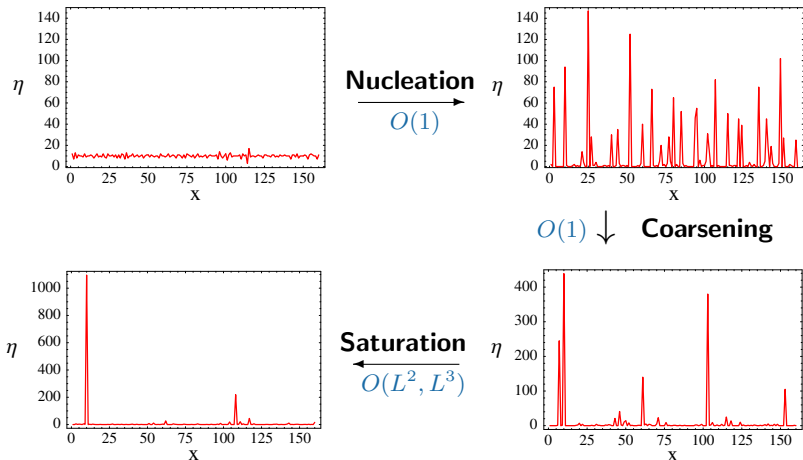
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HIM, Bonn

Dynamics of condensation

ZRP with $g(k) = 1 + b/k$, $b = 4$, $\rho_c = 1/(b - 2) = 0.5$, $\rho = 10$



hydrodynamics $O(L, L^2)$

[subcritical, Stamatakis (2015)]

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

Previous rigorous results on condensation dynamics

Stationary dynamics for ZRP (metastability)

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

$$Y^N(\eta(tN^{1+b})) \rightarrow Y_t \quad \text{RW on (subset of) } \Lambda, \quad \text{rates} \propto \text{cap}_\Lambda(x, y)$$

- L fixed, $N \rightarrow \infty$, $p(x, y)$ asymmetric [Landim (2014), Seo (2018)]

- $L, N \rightarrow \infty$, $N/L \rightarrow \rho > \rho_c$, $p(x, y)$ symmetric on rescaled torus $\subset \mathbb{T}$

$$Y^L(\eta(tL^{1+b})) \rightarrow Y_t \quad \text{Lévy-type on } \mathbb{T} \quad \begin{array}{l} \text{[Armendáriz, G., Loulakis (2017)]} \\ \text{[Bovier, Neukirch (2014)]} \end{array}$$

Nucleation/Coarsening for ZRP

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

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

Inclusion process

- L fixed, $N \rightarrow \infty$, $d = d_N \ll 1/\log N$, time scale t/d_N

Coarsening for $p(x, y)$ symmetric, $Nd_N \rightarrow \infty$ [G., Redig, Vafayi (2013)]

Stat. dynamics with multiple scales [Bianchi, Dommers, Giardiná (2017)]

Nucleation and coarsening/MF limits

Jatuviriyapornchai, G., Stoch. Proc. Appl. **129**(4), 1455-1475 (2019)

Jatuviriyapornchai, G., J. Phys. A: Math. Theor. **49**(18), 185005 (2016)

Godrèche, Drouffe, J. Phys. A: Math. Theor. **50**(1), 015005 (2016)

Godrèche, Luck, J. Phys. A: Math. Theor. **38**(33), 7215 (2005)

Y.-X. Chau, C. Connaughton, S. G., J. Stat. Mech., P11031 (2015)

J. Cao, P. Chleboun, S. G., J. Stat. Phys. **155**, 523543 (2014)

S. G., F. Redig, K. Vafayi, Electron. J. Probab. **18**, 123 (2013)

Mean-field equation

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

Empirical measures $F_k^L(\eta) = \frac{1}{L} \sum_{x \in \Lambda} \delta_{\eta_x, k} \in [0, 1]$

- Assume**
- **complete graph** $p(x,y) = 1/(L-1)$
 - **jump rates** $u(k,l) \leq C_1 k(C_2 + l)$
 - **initial conditions** $\eta(0)$ such that $F_k^L(\eta(0)) \rightarrow f(0)$ on \mathbb{N}_0
 $m_0(0) = 1$, $m_1(0) = \sum_k k f_k(0) = \rho < \infty$, $m_2(0) < \infty$

and $\alpha_1, \alpha_2 > 0$ such that for all $L \geq 1$

$$\eta(0) \in \Omega_\alpha := \left\{ \eta : \frac{1}{L} \sum_{x \in \Lambda} \eta_x < \alpha_1, \frac{1}{L} \sum_{x \in \Lambda} \eta_x^2 < \alpha_2 \right\}$$

→ for example $\eta_x(0) \sim f(0)$ i.i.d. bounded

Mean-field equation

Theorem – LLN for empirical process

Under above assumptions, for all $k \in \mathbb{N}_0$ the empirical processes

$(F_k^L(\eta(t)) : t \geq 0)$ converge weakly on path space to $(f_k(t) : t \geq 0)$ as $L \rightarrow \infty$, which are given as the unique solution of the **mean-field (rate) equation**

$$\begin{aligned} \frac{d}{dt} f_k(t) = & \sum_{l \geq 0} \left(u(k+1, l) f_l(t) f_{k+1}(t) + u(l, k-1) f_l(t) f_{k-1}(t) \right) \\ & - \sum_{l \geq 0} (u(k, l) + u(l, k)) f_l(t) f_k(t) \quad \text{for all } k \geq 0, \quad (\text{MFE}) \end{aligned}$$

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

Mean-field equation

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

- This implies in particular uniqueness of the solution to (MFE) for given $f(0)$,
- as well as convergence of expectations,

$$f_k^L(t) := \mathbb{E}^L [F_k^L(\eta(t))] = \frac{1}{L} \sum_{x \in \Lambda} \mathbb{P}^L [\eta_x(t) = k] \rightarrow f_k(t).$$

Propagation of chaos

Assume in addition symmetry of initial conditions, i.e.

the law of $\{\eta_x(0) : x \in \Lambda\}$ is permutation invariant for each $L \geq 1$.

Corollary – Propagation of chaos

(see e.g. [e.g. dai Pra (2017)])

Under the conditions of the Theorem and above, for any finite-dimensional marginal with distinct $x_1, \dots, x_m \in \Lambda$, $m \geq 1$, we have for any $T > 0$

$(\eta_{x_i}(t) : t \in [0, T])$ converge to independent birth-death chains ,

with (non-linear) master equation (MFE) and generator

$$\mathcal{L}_{f(t)} h(k) = \alpha_k(t)[h(k+1) - h(k)] + \beta_k(t)[h(k-1) - h(k)] ,$$

with rates $\alpha_k(t) = \sum_{l \geq 0} u(l, k) f_l(t)$ and $\beta_k(t) = \sum_{l \geq 0} u(k, l) f_l(t)$.

[Gärtner (1988) WASEP; Rezakhanlou (1994) SSEP and ZRP, (1996) multi-type model ...]

Proof of main result

- 1 existence of limits $t \mapsto f(t)$ via tightness
- 2 limits are solutions of (MFE)
- 3 uniqueness of solutions of (MFE)

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Moments. $m_n^L(t) := \mathbb{E}^L \left[\sum_{k \geq 0} k^n F_k^L(\eta(t)) \right] = \sum_{k \geq 0} k^n f_k^L(t)$

$$m_0^L(t) \equiv 1 \quad \text{and} \quad m_1^L(t) \equiv m_1^L(0) \xrightarrow{L \rightarrow \infty} \rho .$$

Lemma. $C > 0$ such that $m_2^L(t) \leq (\alpha_2 + Ct)e^{Ct}$ for all $t \geq 0$, $L \geq 1$,

using $\frac{d}{dt} \mathbb{E}^L [F_k^L(\eta(t))] = \mathbb{E}^L [\mathcal{L}F_k^L(\eta(t))]$ and Gronwall .

Proof of main result

1. Tightness. For each bounded $h : \mathbb{N}_0 \rightarrow \mathbb{R}$ the law of

$$t \mapsto H(\eta(t)) := \sum_{k \geq 0} h_k F_k^L(\eta(t))$$

on path space $D_{[0, \infty)}(\mathbb{R})$ is tight as $L \rightarrow \infty$.

Using a version of **Aldous' criterion**, $|\sum_k h_k F_k^L(\eta)| \leq \|h\|_\infty$ and Markov's inequality we need to establish

$$\limsup_{L \rightarrow \infty} \sup_{t < \delta} \sup_{\zeta \in \Omega_\alpha} \mathbb{E}_\zeta^L [|H(\eta(t)) - H(\zeta)|] \rightarrow 0 \quad \text{as } \delta \rightarrow 0^+ .$$

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Itô's formula $M_h(t) := H(\eta(t)) - H(\eta(0)) - \int_0^t \mathcal{L}H(\eta(s)) ds$

is a local m'gale with pred. QV $\langle M_h \rangle(t) = \int_0^t [\mathcal{L}H^2 - 2H\mathcal{L}H](\eta(s)) ds .$

$$\begin{aligned} \mathcal{L}H(\eta) = & \sum_{k \geq 0} h_k \left[F_{k-1}^L(\eta) \sum_{l \geq 1} u(l, k-1) F_l^L(\eta) + F_{k+1}^L(\eta) \sum_{l \geq 0} u(k+1, l) F_l^L(\eta) \right. \\ & \left. - F_k^L(\eta) \sum_{l \geq 0} (u(k, l) + u(l, k)) F_l^L(\eta) \right] (1 + 1/L) + \Delta_L(\eta) \end{aligned}$$

Proof of main result

$$\mathbb{E}^L [|H(\eta(t)) - H(\eta(0))|] \leq \underbrace{\int_0^t \mathbb{E}^L |\mathcal{L}H(\eta(s))| ds}_{(1)} + \underbrace{\mathbb{E}^L [[M_h](t)]}_{(2)}.$$

with estimates

$$(1) \leq t \|h\|_\infty \left(4C_1 \alpha_1 (\alpha_1 + C_2) + \frac{C}{L} (1+t) e^{Ct} \right)$$

$$(2) \leq t \|h\|_\infty^2 \frac{1}{L} \left(4C_1 \alpha_1 (\alpha_1 + C_2) + \frac{C}{L} (1+t) e^{Ct} \right)$$

Both vanish as $t \leq \delta \rightarrow 0$ uniformly in L which implies **tightness**.

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2. Estimate for (2) implies $\mathbb{E}^L [[M_h](t)] \rightarrow 0$ as $L \rightarrow \infty$ for all $t \geq 0$, so the martingale vanishes and each limit **solves a weak version of (MFE)**

$$\sum_{k \geq 0} h_k (f_k(t) - f_k(0)) = \int_0^t \sum_{k \geq 0} h_k (\mathcal{L}_{f(s)}^\dagger f(s))_k ds.$$

Proof of main result

3. Uniqueness of solutions of (MFE)

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

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

Gronwall estimate $m_2^L(t) \leq (\alpha_2 + Ct)e^{Ct}$ for all $t \geq 0$.

- Consider $f(t), \hat{f}(t)$ with $f(0) = \hat{f}(0) \in \mathcal{P}(\mathbb{N}_0)$ and establish Gronwall for

$$\theta(t) := \sum_{k \geq 0} (k+1) |\Delta_k(t)| \quad \text{where} \quad \Delta_k(t) := f_k(t) - \hat{f}_k(t).$$

[Esenturk (2017), Schlichting (2018)], following classical proof [Ball, Penrose (1986)]

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Extensions. multiple particle jumps and quantitative bounds

systematic error $\left| \mathbb{E}^L \left[H(\eta(t)) - \sum_{k \geq 0} h_k f_k(t) \right] \right| \leq C e^{Ct} \frac{\|h\|_\infty}{L}$

random error $\mathbb{E}^L \left[\left| H(\eta(t)) - \mathbb{E}^L[H(\eta(t))] \right|^2 \right]^{1/2} \leq C e^{Ct} \frac{\|h\|_\infty}{\sqrt{L}}$

Scaling analysis for ZRP

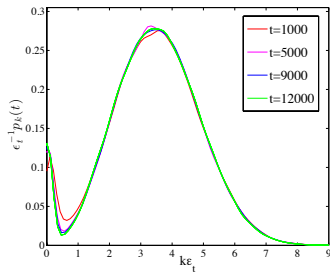
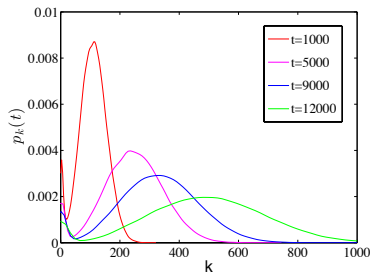
Scaling ansatz for phase separated solution with $m_1(t) = \rho > \rho_c$

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

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

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

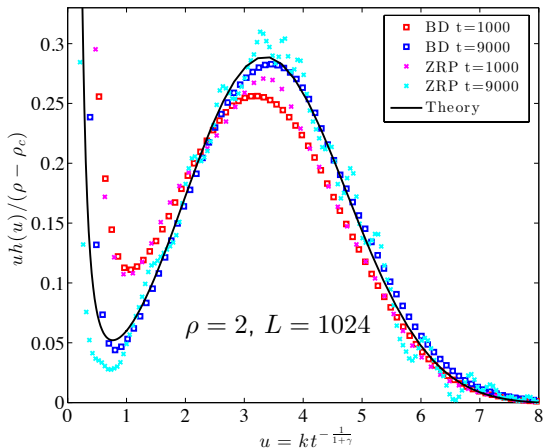
ZRP with rates $g(k) = 1 + b/k$, $b = 4$, $\rho_c = 1/2$, $\rho = 10$



Scaling analysis for ZRP

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

[Godr che (2003); J., G. (2016); Godr che, Drouffe (2016)]



Coarsening scaling law for ZRP

ZRP with rates $g(k) = 1 + b/k$ with $\rho_c = 1/(b - 2)$.

Provided we can rigorously establish the scaling solution $f(t)$ for $m(0) = \rho > \rho_c$, we would have for the empirical measures with $\epsilon_t = t^{-1/2}$

$$\lim_{t \rightarrow \infty} \lim_{L \rightarrow \infty} \frac{1}{\epsilon_t^L} F_{[u/\epsilon_t]}^L(\boldsymbol{\eta}(t)) = h(u),$$

where h solves $h''(u) + \left(\frac{u}{2} - A + \frac{b}{u}\right)h'(u) + \left(1 - \frac{b}{u^2}\right)h(u) = 0$.

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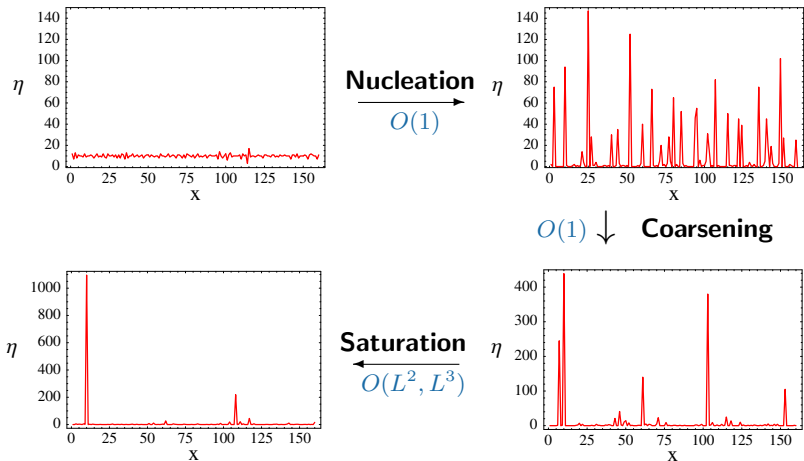
For size-biased samples $\bar{\eta}_x$ of occupation numbers this means

$$\lim_{t \rightarrow \infty} \lim_{L \rightarrow \infty} \epsilon_t \bar{\eta}_x(t) = \begin{cases} 0, & \text{with prob. } \rho_c/\rho \\ U, & \text{with prob. } 1 - \rho_c/\rho \end{cases},$$

where U has density $uh(u)/(\rho - \rho_c)$.

Dynamics of condensation

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hydrodynamics $O(L, L^2)$

[subcritical, Stamatakis (2015)]

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

Stationary dynamics/metastability

Seo, CMP **366**(2), 781839 (2019)

Landim CMP **330**(1), 132 (2014)

Armendáriz, G., Loulakis. PTRF **169**(12), 105-175 (2017)

Bovier, Neukirch (2014)

Beltrán Landim PTRF **152**(3-4), 781807 (2012)

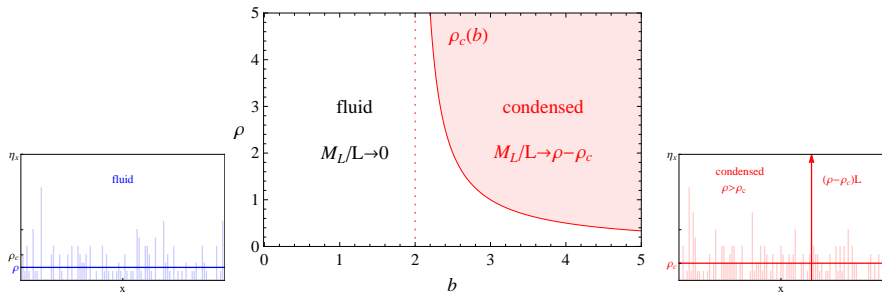
Canonical measures and condensation

fixed number of particles N : $\pi_{L,N}[\cdot] = \frac{\nu_\phi[\cdot \cap \sum_x \eta_x = N]}{\nu_\phi[\sum_x \eta_x = N]}$

Equivalence of ensembles

In the thermodynamic limit $L, N \rightarrow \infty$, $N/L \rightarrow \rho$

$$\pi_{L,N} \rightarrow \nu_\phi \quad \text{where} \quad \begin{cases} R(\phi) = \rho, & \rho \leq \rho_c \\ \phi = \phi_c, & \rho \geq \rho_c \end{cases} .$$



[Jeon, March, Pittel '00; G., Schütz, Spohn '03; Armendáriz, Loulakis '09 with G. '13; Chleboun, G. '14]

Metastability

Stationary dynamics of the condensate

$\Lambda = \mathbb{T}_L$, $g(k) = \mathbb{1}_{k>0}(1 + \frac{b}{k})$, $b > 21$ (!), $p(x, y)$ NN symmetric

$M_L(\boldsymbol{\eta}) = \max_{x \in \Lambda} \eta_x$, $\psi_L(\boldsymbol{\eta}) = \min \{x \in \Lambda : \eta_x = M_L(\boldsymbol{\eta})\}$

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Theorem

Let $\boldsymbol{\eta}_0 \sim \pi_{L,N}$ and consider the thermodynamic limit $L, N \rightarrow \infty$ with $L/N \rightarrow \rho > \rho_c$. On the scale $\theta_L = L^{1+b}$, $(\frac{1}{L}\psi_L(\boldsymbol{\eta}_{\theta_L t}) : t \geq 0)$ converges weakly on path space $D([0, \infty), \mathbb{T})$ to a Markov process $(Y_t : t \geq 0)$ with stationary, independent increments and generator

$$\mathcal{L}_{\mathbb{T}} f(u) = \int_{\mathbb{T} \setminus \{0\}} (f(u+v) - f(u)) \frac{C_{b,\rho}}{|v|(1-|v|)} dy$$

for all $f \in C^1(\mathbb{T})$.

$$C_{b,\rho} = \left(\frac{b-1}{b}\right)(\rho - \rho_c)^b \left(\Gamma(1+b) \int_0^{\rho-\rho_c} z^b (\rho - \rho_c - z)^b dz\right)^{-1}$$

Method of proof

Potential theory. [Bovier, Eckhoff, Gaynard, Klein (2001,2002) ... Bovier, den Hollander (2015)]

- **potential wells** $\mathcal{E}_x \subset \{\eta : \psi_L(\eta) = x\}$, $\pi_{L,N}(\cup_{x \in \Lambda} \mathcal{E}_x) \rightarrow 1$
time spent outside wells can be ignored
- **effective rates** $R_L(x, y) = \mathbb{E}_{\pi_{L,N}|\mathcal{E}^x} \sum_{\zeta} r(\cdot, \zeta) \mathbb{P}_{\zeta}(\eta_{\tau} \in \mathcal{E}_y)$
sharp bounds via capacities $\simeq C_{b,\rho} \text{cap}_{\Lambda}(x, y) L / \theta_L$
→ bounds match only after regularization!

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Martingale approach. [Landim, Beltran (2011,2012) ...]

- **tightness** of $Y_t^L := \frac{1}{L} \psi_L(\eta_{\theta_L t})$ as $L \rightarrow \infty$
involves uniform upper bounds on rates (coupling)
- **martingale problem** for all $f \in C^1(\mathbb{T})$

$$f(Y_t^L) - f(Y_0^L) - \int_0^t \mathcal{L}f(Y_s^L) ds \quad \text{is a martingale}$$

- **equilibration** replace $\psi_L(\eta_{\theta_L t})$ with a process on Λ with rates R_L
show that $t_{\text{rel}} \leq CL^4$ and $t_{\text{mix}}(\epsilon) \leq CL^5 \log \frac{1}{\epsilon} \ll \theta_L$ on the well

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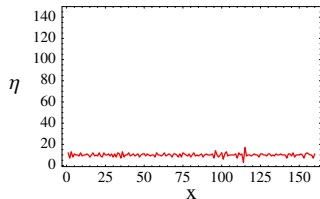
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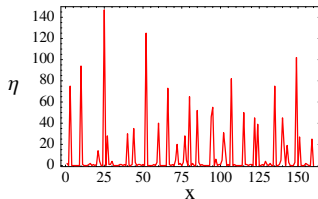
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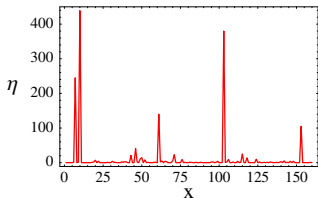
ZRP with $g(k) = 1 + b/k$, $b = 4$, $\rho_c = 1/(b - 2) = 0.5$, $\rho = 10$



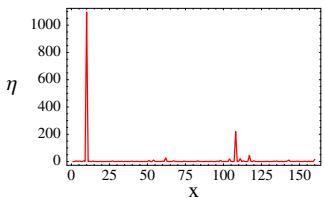
Nucleation
 $\xrightarrow{O(1)}$



$O(1) \downarrow$ **Coarsening**



Saturation
 $\xleftarrow{O(L^2, L^3)}$



hydrodynamics $O(L, L^2)$

[subcritical, Stamatakis (2015)]

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