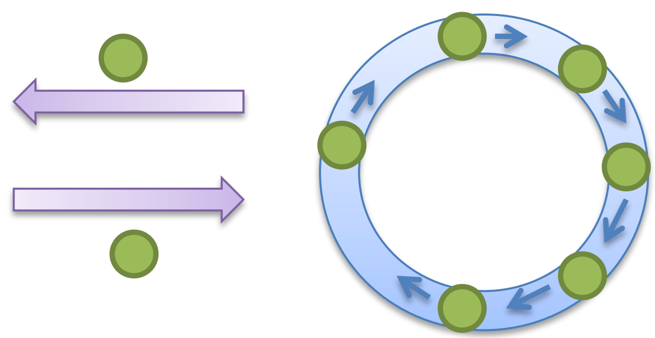
Density large-deviations of nonconserving driven models



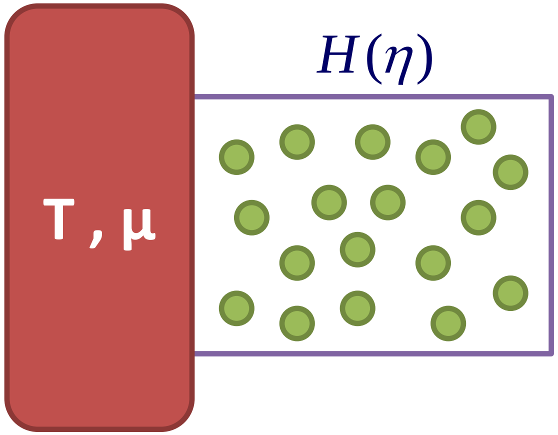
Or Cohen and David Mukamel

Weizmann Institute of Science

Statistical Mechanical Day, Weizmann Institute, June 2012

Ensemble theory out of equilibrium ?

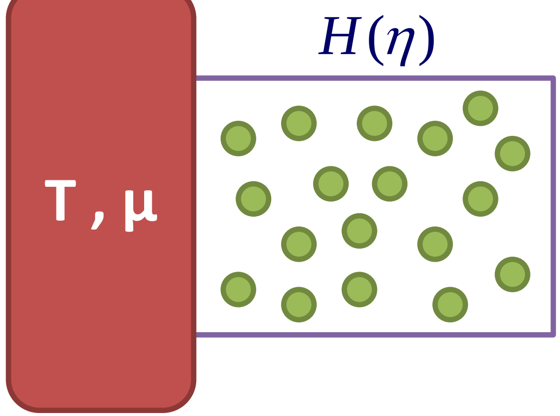
Equilibrium



$$P^{G.Can.}(\eta, N) = P_N^{Can.}(\eta) P^{G.Can.}(N)$$

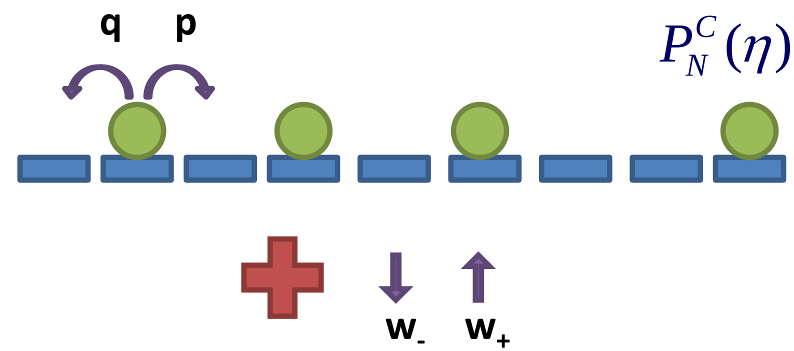
Ensemble theory out of equilibrium ?

Equilibrium



$$P^{G.Can.}(\eta, N) = P_N^{Can.}(\eta) P^{G.Can.}(N)$$

Driven diffusive systems

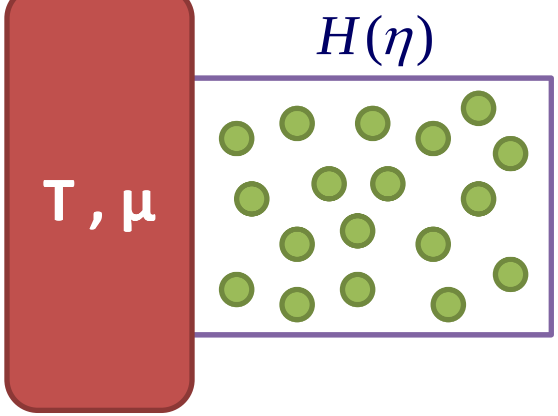


$$P^{NC}(\eta, N) = F\left[P_N^C(\eta), \frac{w_+}{w_-} \right] \ ???$$

Can we infer about the nonconserving system from the steady state properties of the conserving system ?

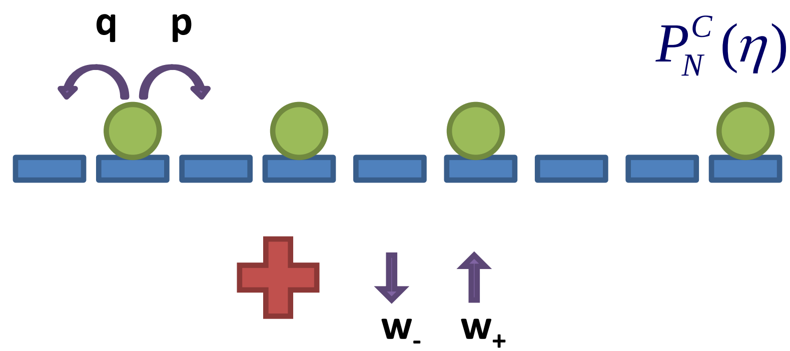
Ensemble theory out of equilibrium ?

Equilibrium



$$P^{G.Can.}(\eta, N) = P_N^{Can.}(\eta) P^{G.Can.}(N)$$

Driven diffusive systems

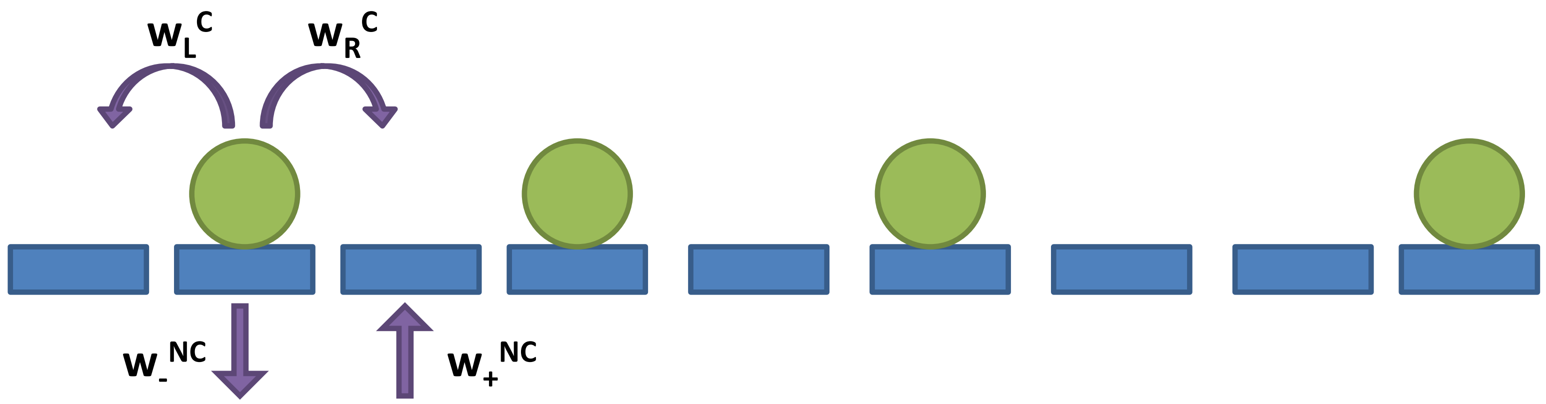


$$P^{NC}(\eta, N) = F\left[P_N^C(\eta), \frac{w_+}{w_-} \right] \text{ ???}$$

$$w_+, w_- \ll q, p$$

$$P^{NC}(\eta, N) \approx P_N^C(\eta) P^{NC}(N)$$

Generic driven diffusive model

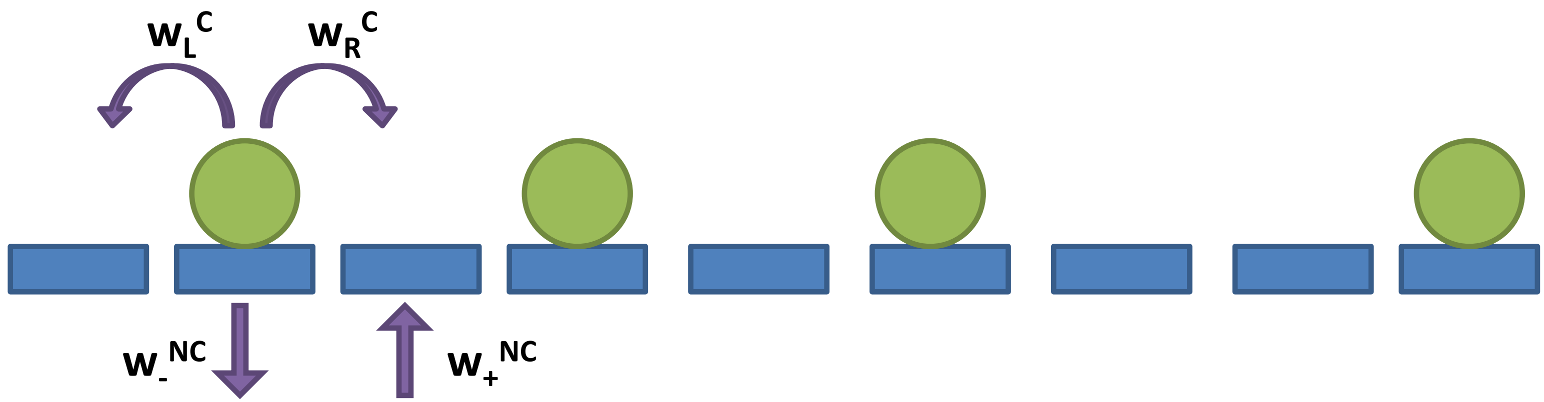


$$\partial_t P^{NC}(\eta) = \sum_{\eta' \in \Gamma_N} w^C_{\eta'\eta} P^{NC}(\eta') - w^C_{\eta\eta'} P^{NC}(\eta) + \sum_{N'=N\pm 1} \sum_{\eta' \in \Gamma_{N'}} w^{NC}_{\eta'\eta} P^{NC}(\eta') - w^{NC}_{\eta\eta'} P^{NC}(\eta)$$

conserving
(sum over η' with same N)

nonconserving
(sum over η' with N'≠N)

Generic driven diffusive model



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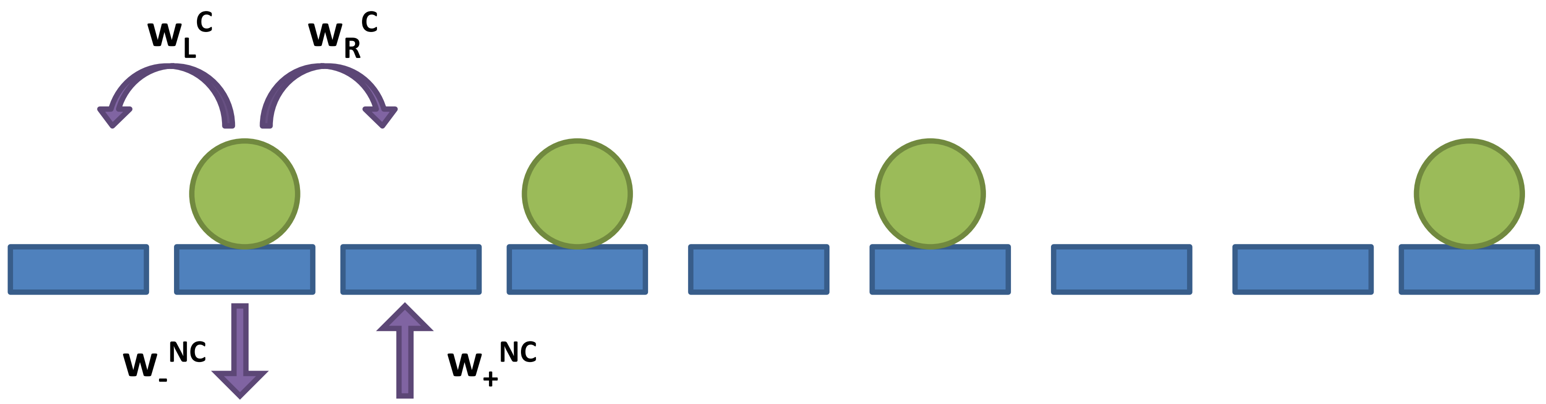
conserving
(sum over η' with same N)

nonconserving
(sum over η' with N'≠N)

Guess a steady state of the form :

$$P^{NC}(\eta, N) = P^C_N(\eta) f(N) + O\begin{pmatrix}\text{higher order} \\ \text{in } L\end{pmatrix}$$

Generic driven diffusive model



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conserving
(sum over η' with same N)

nonconserving
(sum over η' with N'≠N)

Guess a steady state of the form :

$$P^{NC}(\eta, N) = P^C_N(\eta) f(N) + O\begin{pmatrix}\text{higher order}\\ \text{in } L\end{pmatrix}$$

It is consistent if :

$$w^{NC}_{\eta'\eta} \sim L^{-\gamma}$$

In many cases :

$$\gamma > 2$$

Slow nonconserving dynamics

To leading order in L we obtain

$$0=\sum_{N'=N\pm 1} f(N')[\sum_{\eta\in\Gamma_N}\sum_{\eta'\in\Gamma_{N'}} w^{NC}_{\eta'\eta} P^C(\eta')] - f(N)[\sum_{\eta\in\Gamma_N}\sum_{\eta'\in\Gamma_{N'}} w^{NC}_{\eta'\eta} P^C(\eta')]$$

$$0=\sum_{N'=N\pm 1} f(N')W_{N',N} - f(N)W_{N,N'}$$

Slow nonconserving dynamics

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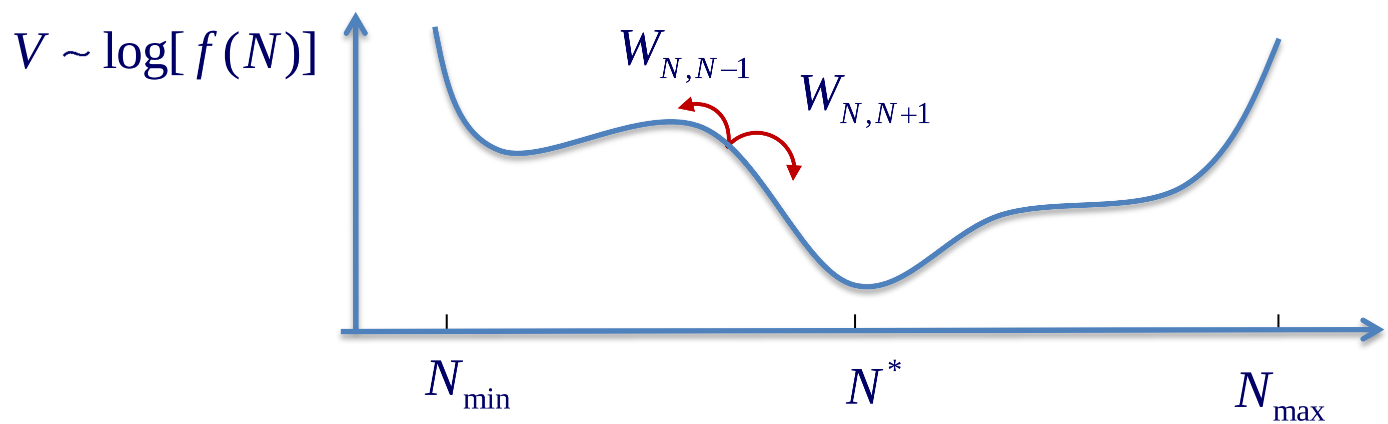


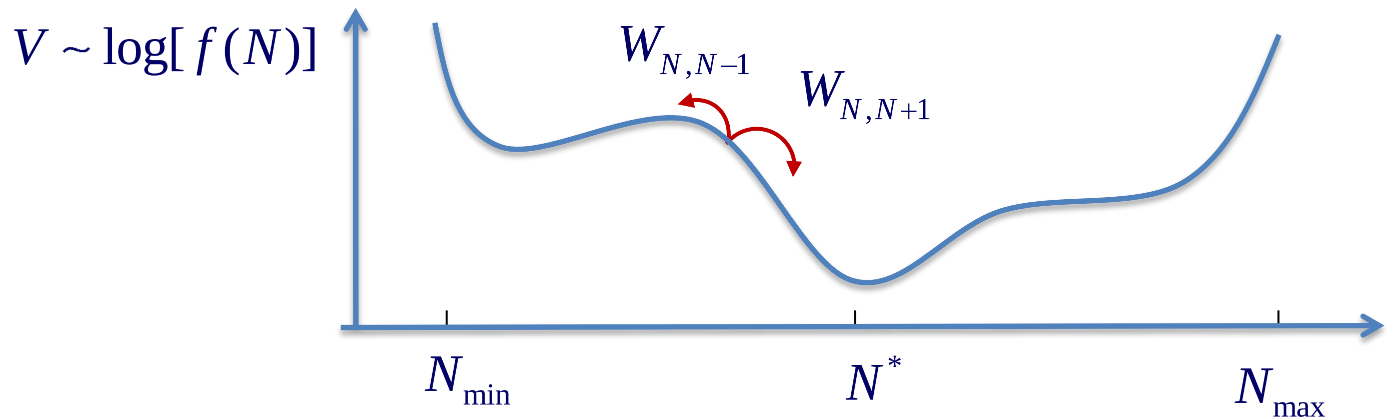
= 1D - Random walk in a potential

Slow nonconserving dynamics

To leading order in L we obtain

$$0 = \sum_{N'=N\pm1} f(N')\Big[\sum_{\eta\in\Gamma_N}\sum_{\eta'\in\Gamma_{N'}} w^{NC}_{\eta'\eta} P^C(\eta')\Big] - f(N)\Big[\sum_{\eta\in\Gamma_N}\sum_{\eta'\in\Gamma_{N'}} w^{NC}_{\eta'\eta} P^C(\eta')\Big]$$

$$0 = \sum_{N'=N\pm1} f(N')W_{N',N} - f(N)W_{N,N'}$$



= 1D - Random walk in a potential

Steady state solution :

$$f(N) = P^{NC}(N) = \prod_{N'=N_0}^{N} \frac{W_{N',N'+1}}{W_{N'+1,N'}}$$

Outline

1. **Limit of slow nonconserving**

$$w^{NC} \sim L^{-\gamma}$$

$$P^{NC}(\eta, N) \approx P_N^C(\eta) P^{NC}(N)$$

$$P^{NC}(N) = F[P_N^C(\eta), w^{NC}]$$

$$\Downarrow$$

$$\mu(N)$$

2. **Example of the ABC model**

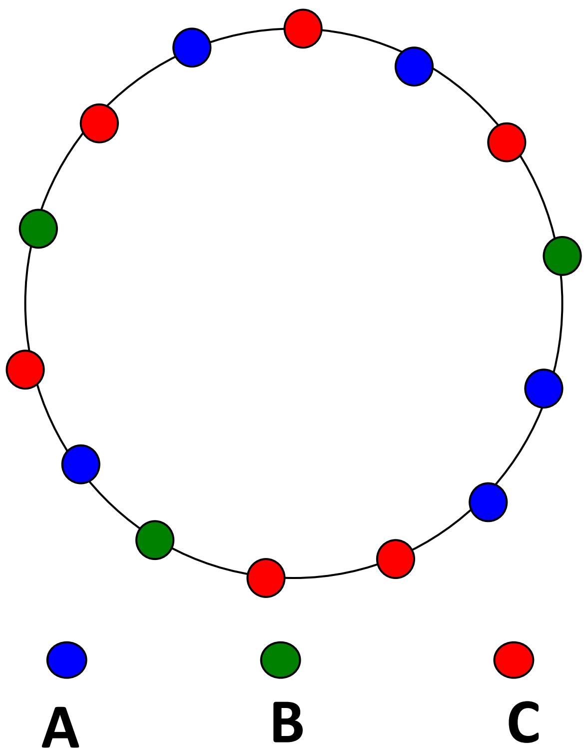
3. **Nonequilibrium chemical potential**

   (dynamics dependent !)

4. **Conclusions**

ABC model

Ring of size L



Dynamics :

$$AB \underset{1}{\overset{q}{\rightleftarrows}} BA$$

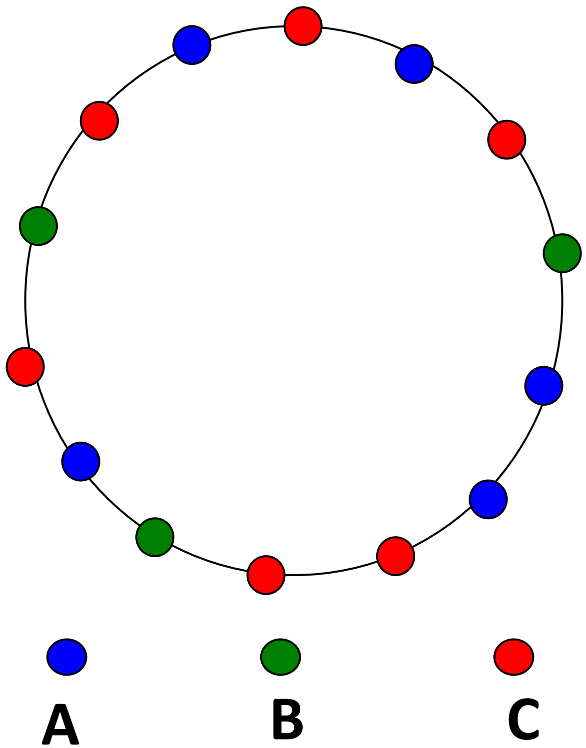
$$BC \underset{1}{\overset{q}{\rightleftarrows}} CB$$

$$CA \underset{1}{\overset{q}{\rightleftarrows}} AC$$

Evans, Kafri , Koduvely & Mukamel - Phys. Rev. Lett. 1998

ABC model

Ring of size L



Dynamics :

$$AB \underset{1}{\overset{q}{\rightleftarrows}} BA$$

$$BC \underset{1}{\overset{q}{\rightleftarrows}} CB$$

$$CA \underset{1}{\overset{q}{\rightleftarrows}} AC$$

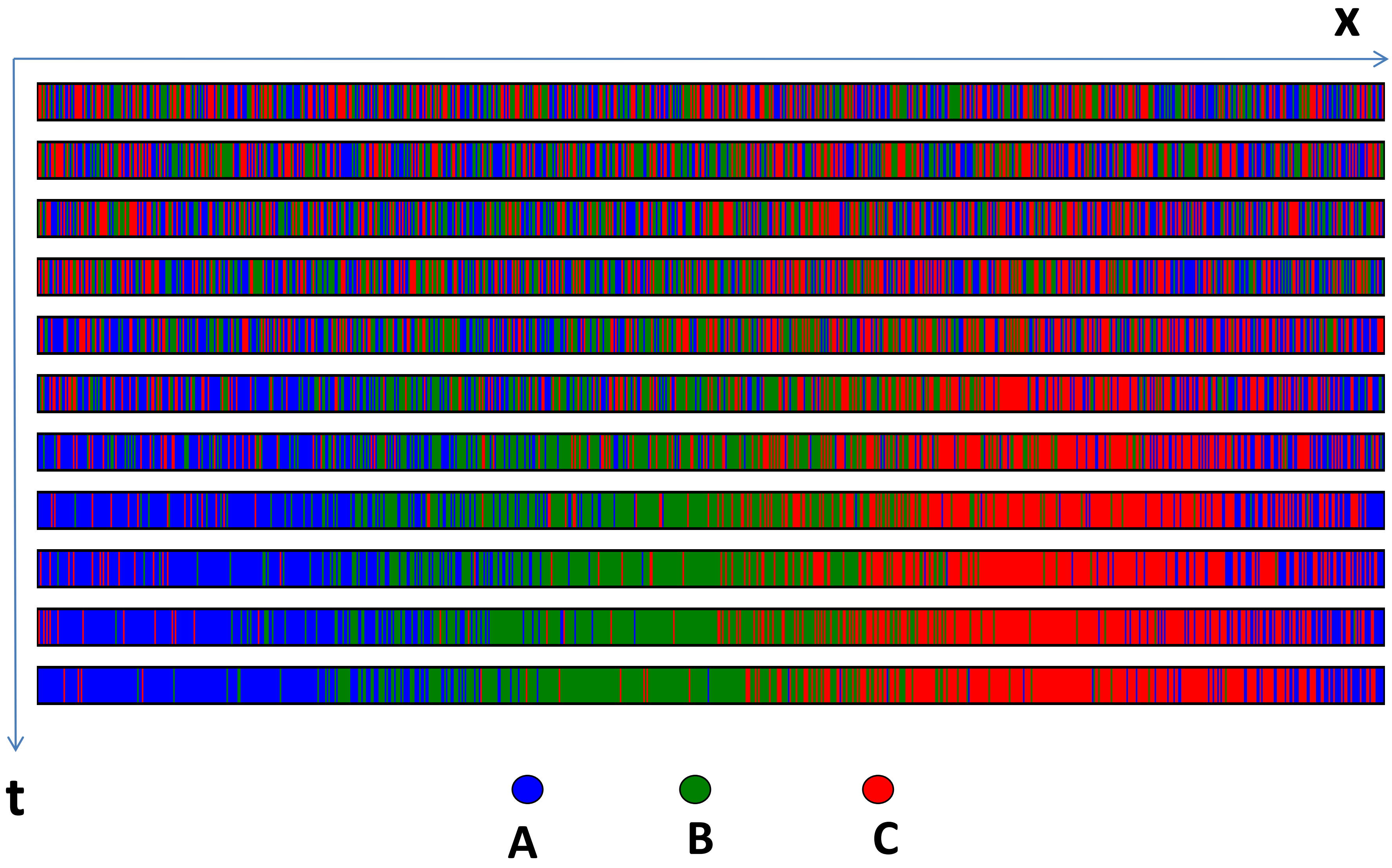
$L \to \infty$

q=1 **ABBCACCBACABACB**

q<1 **AAAAABBBBBCCCCC**

Evans, Kafri , Koduvely & Mukamel - Phys. Rev. Lett. 1998

ABC model



Evans, Kafri , Koduvely & Mukamel - Phys. Rev. Lett. 1998

Phase transition

Weakly asymmetric
thermodynamic limit

$$q = \exp(-\frac{\beta}{L})$$

$$P[\rho_\alpha] \propto e^{-L\beta F[\rho_\alpha]} \qquad \alpha = A, B, C$$

Clincy, Derrida & Evans - *Phys. Rev. E* 2003

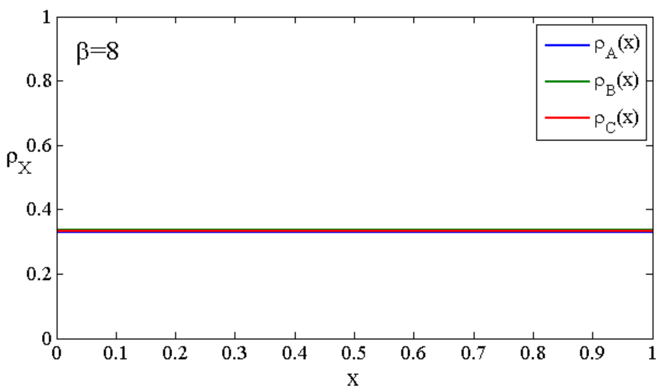
Phase transition

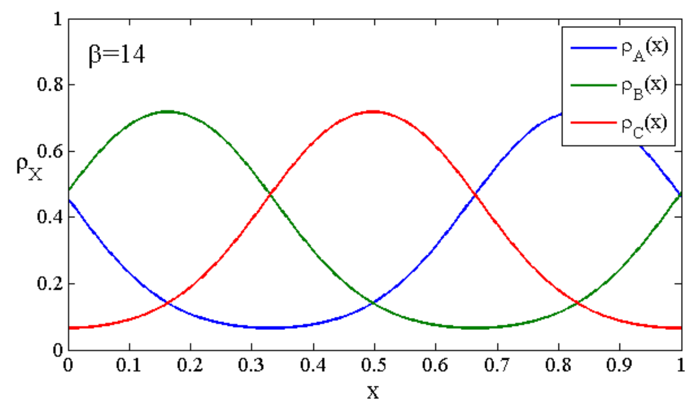
Weakly asymmetric
thermodynamic limit

$$q = \exp(-\frac{\beta}{L})$$

$$P[\rho_\alpha] \propto e^{-L\beta F[\rho_\alpha]} \qquad \alpha = A, B, C$$

For low β's $\rho^*_\alpha(x) = r_\alpha = N_\alpha / L$





2nd order phase transition at $\beta_c = 2\pi\sqrt{3} / \sqrt{1 - \sum_\alpha (\frac{1}{3} - r_\alpha)^2}$

Clincy, Derrida & Evans - *Phys. Rev. E* 2003

Nonconserving ABC model

(1)

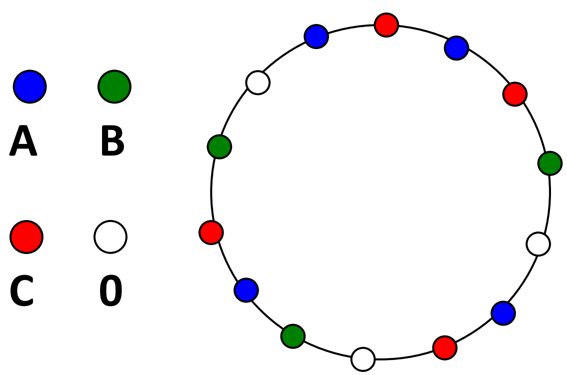
$$AB \underset{1}{\overset{q}{\rightleftarrows}} BA$$

$$BC \underset{1}{\overset{q}{\rightleftarrows}} CB$$

$$CA \underset{1}{\overset{q}{\rightleftarrows}} AC$$

(2)

$$0X \underset{1}{\overset{1}{\leftrightarrows}} X0 \qquad X = A, B, C$$



(1) + (2)

Conserving model
(canonical ensemble)

Nonconserving ABC model

1

$AB \underset{1}{\overset{q}{\rightleftharpoons}} BA$

$BC \underset{1}{\overset{q}{\rightleftharpoons}} CB$

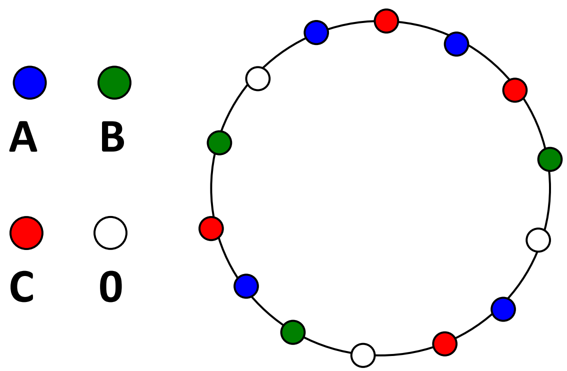
$CA \underset{1}{\overset{q}{\rightleftharpoons}} AC$

2

$0X \underset{1}{\overset{1}{\rightleftharpoons}} X0 \quad X = A, B, C$

3

$ABC \underset{p}{\overset{pe^{-3\beta\mu}}{\rightleftharpoons}} 000$



1 + 2 — **Conserving model**
(canonical ensemble)

1 + 2 + 3 — **Nonconserving model**
(grand canonical ensemble)

Lederhendler & Mukamel - *Phys. Rev. Lett.* 2010

Conserving steady-state

Hydrodynamic equations :

$$\rho_A\left(\frac{i}{L}\right) = \langle A_i \rangle \qquad \langle A_i B_{i+1} \rangle \cong \langle A_i \rangle \langle B_{i+1} \rangle$$

Drift Diffusion

$$\frac{d\rho_A}{dt} = \frac{1}{L^2}\frac{d}{dx}\left[\beta\rho_A\left(\rho_B - \rho_C\right) + \frac{d\rho_A}{dx}\right]$$

Nonequal densities : Cohen & Mukamel - *Phys. Rev. Lett.* 2012
Equal densities : Ayyer et al. - J. Stat. Phys. 2009

Conserving steady-state

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Drift   Diffusion

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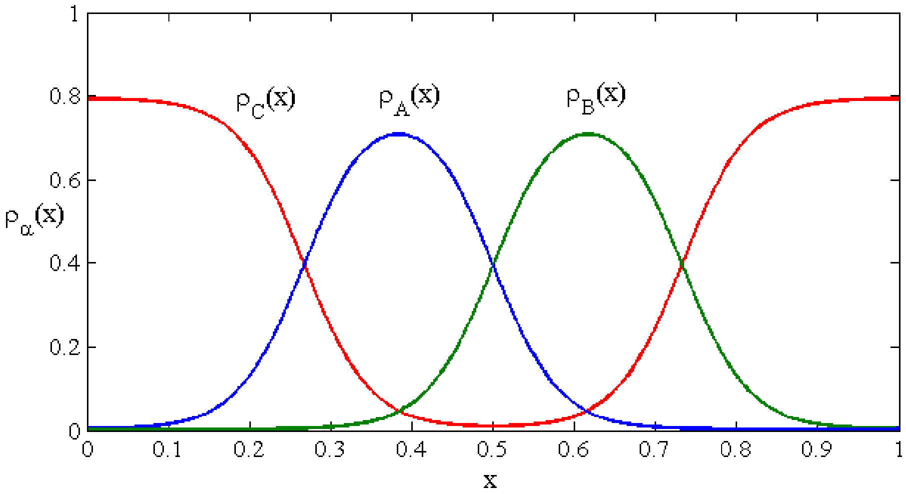
Steady state can be solved analytically

$$\rho_\alpha(x, r)$$



Nonequal densities : Cohen & Mukamel - *Phys. Rev. Lett.* 2012
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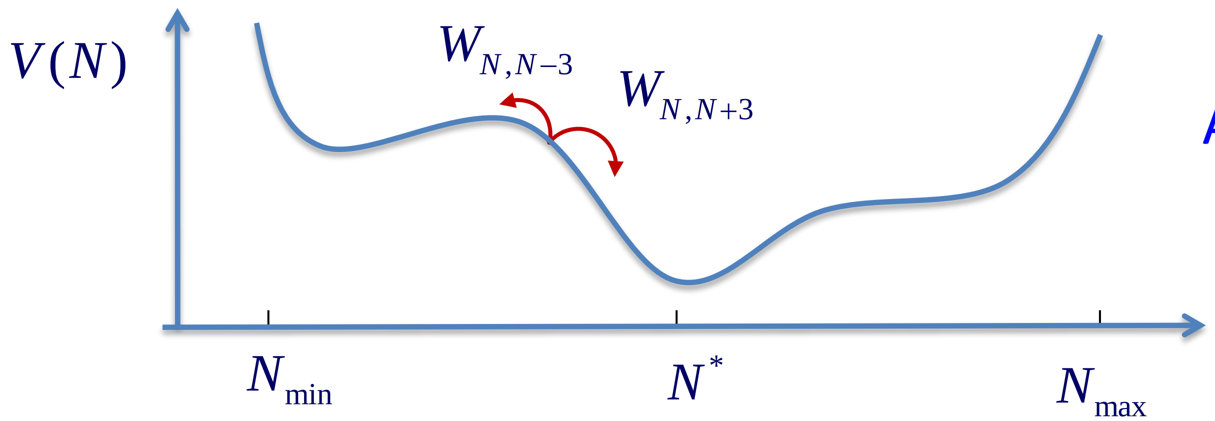
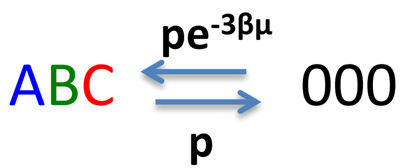
Slow nonconserving model

Slow nonconserving limit

$$p \sim L^{-\gamma} \;, \quad \gamma > 2$$





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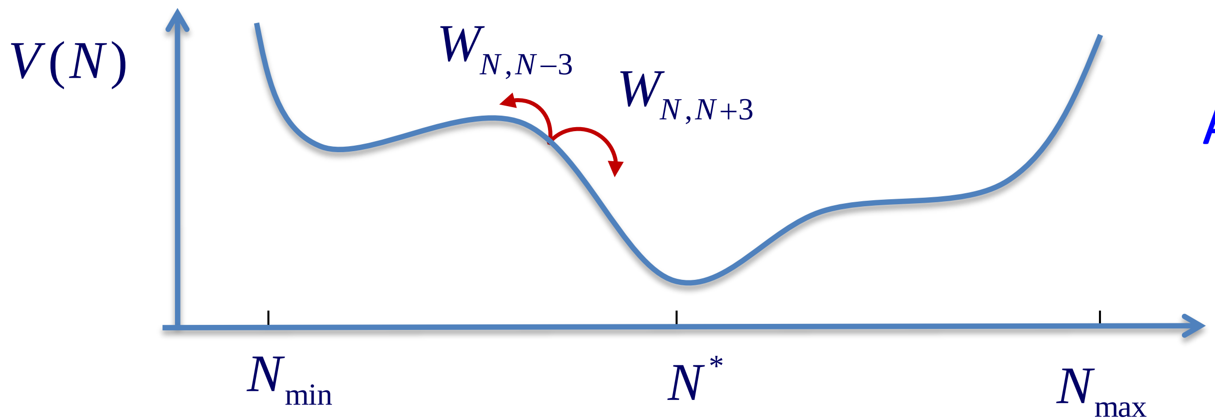
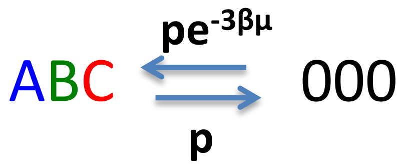
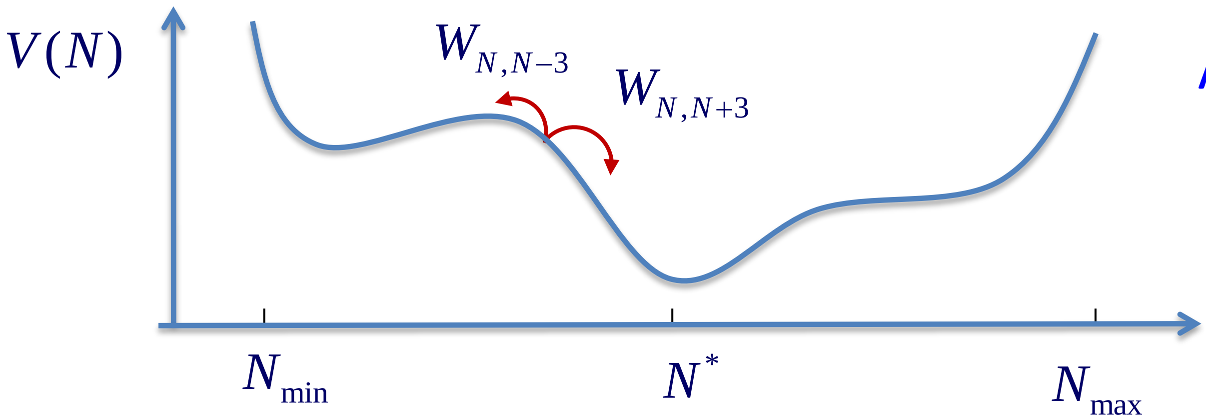




$$W_{N,N+3} = \sum_{\eta \in \Gamma_N} \sum_{\eta' \in \Gamma_{N+1}} w_{\eta\eta'}^{NC} P^C(\eta') \approx \int_0^1 dx (\rho_0^*(x, \frac{N}{L}))^3$$

saddle point approx.

Slow nonconserving model



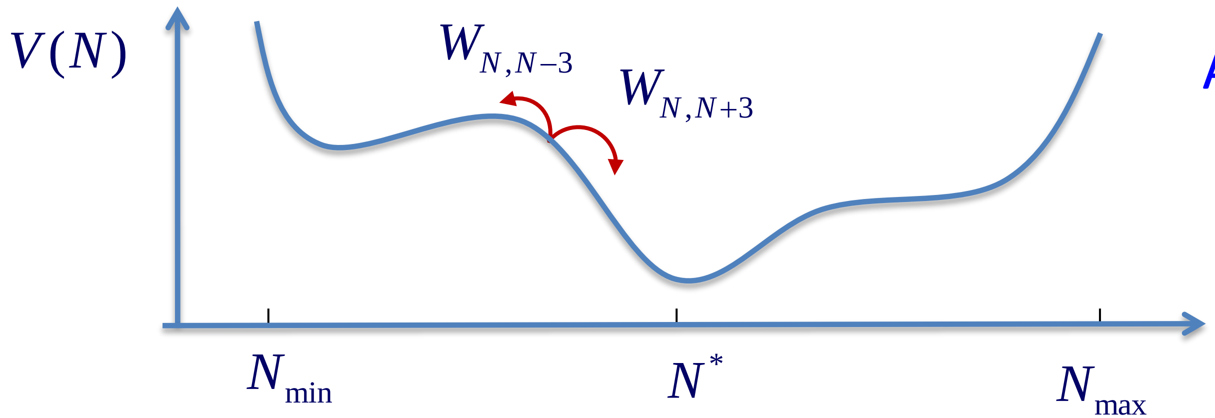
ABC $\underset{p}{\overset{pe^{-3\beta\mu}}{\rightleftarrows}}$ 000

$$r = \frac{N}{L}$$

$$\mu_S(r) = \frac{1}{3\beta}\log\left[\frac{\int_0^1 dx(\rho_0^*(x,r))^3}{\int_0^1 dx\,\rho_A^*(x,r)\rho_B^*(x,r)\rho_C^*(x,r)}\right]$$

$$P^{NC}(r) \sim \exp[-L\beta(\int^r dr'\mu_S(r') - \mu r)] \equiv e^{-L\beta G_\mu(r)}$$

Slow nonconserving model



$$ABC \underset{p}{\overset{pe^{-3\beta\mu}}{\rightleftarrows}} 000$$

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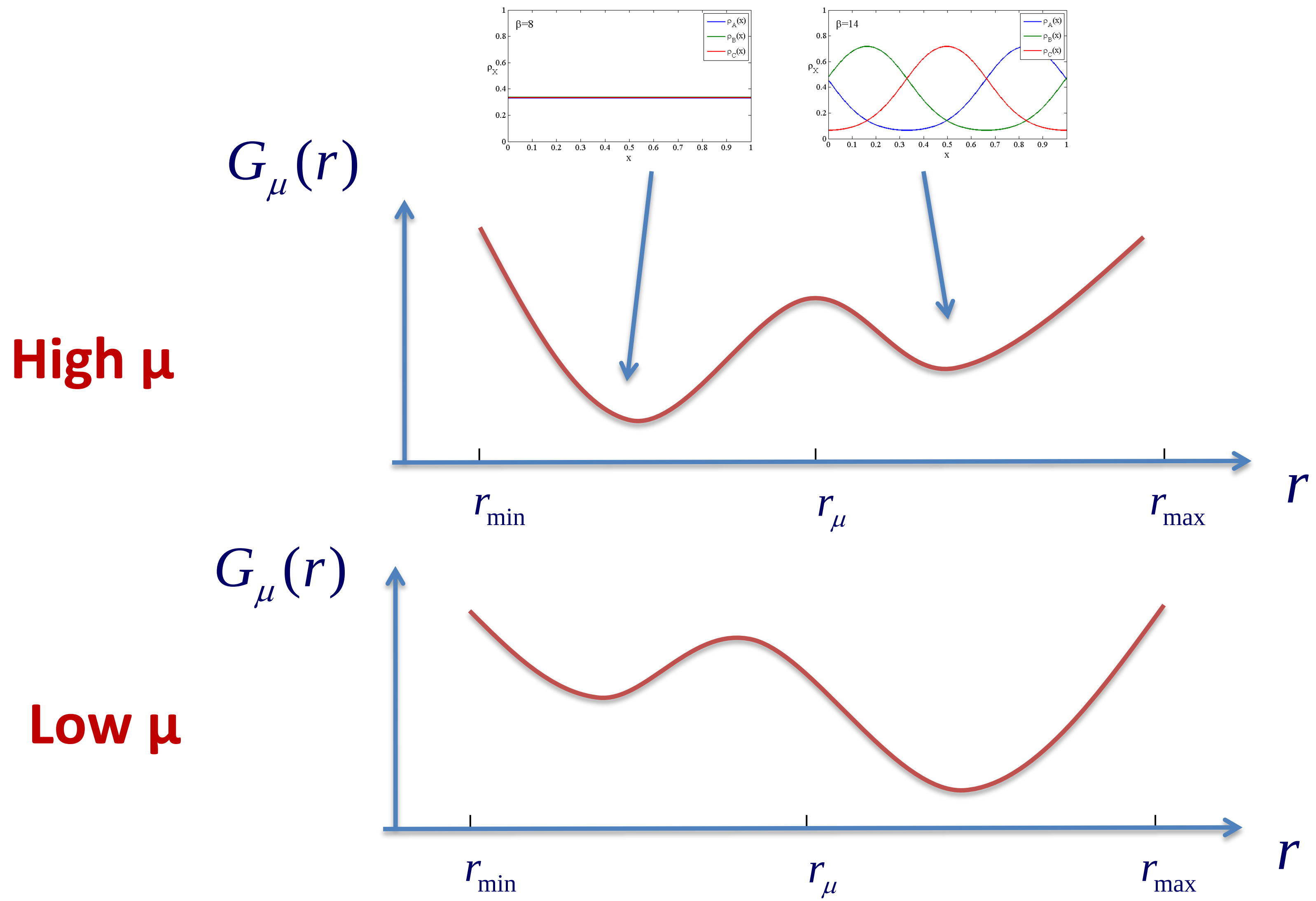
$$P^{NC}(r) \sim \exp[-L\beta(\int^r dr'\mu_S(r') - \mu r)] \equiv e^{-L\beta G_\mu(r)}$$

This is similar to equilibrium : $P^{G.Can}(r) = \exp[-L\beta(F(r,\beta) - \mu r)]$

Large deviation function of r



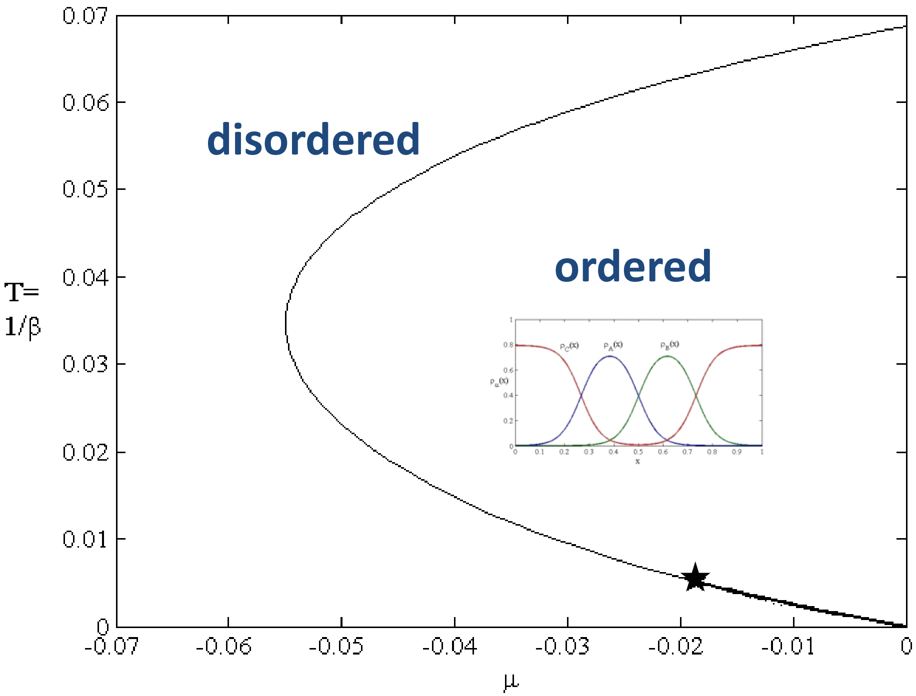
First order phase transition (only in the nonconserving model)

Inequivalence of ensembles

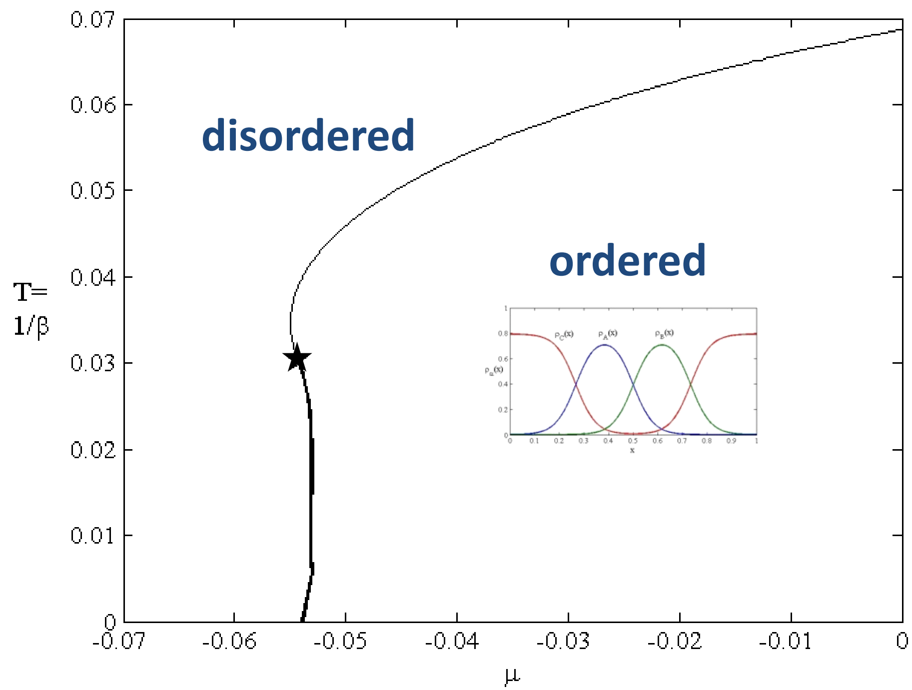
For $N_A = N_B \neq N_C$:

$$r_A = r_B = \frac{r}{3} - \Delta, \quad r_C = \frac{r}{3} + 2\Delta \qquad \Delta = 0.01$$

Conserving = Canonical

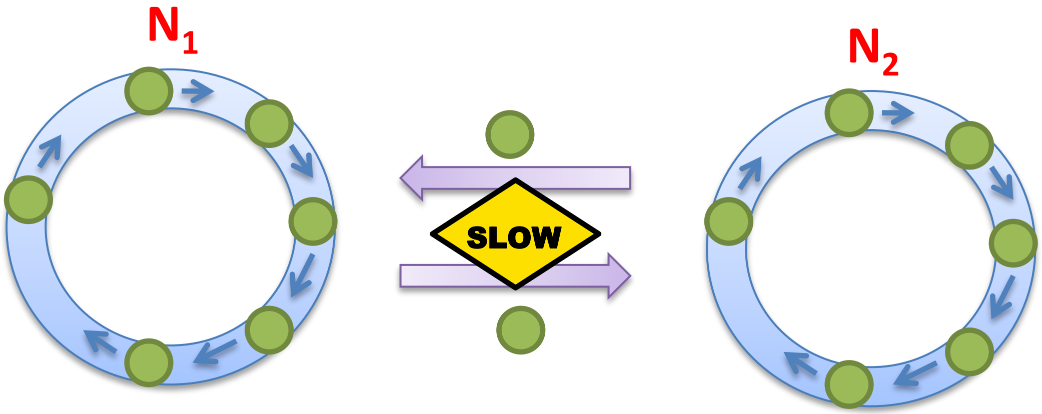


Nonconserving = Grand canonical



—— 1st order transition   **— 2nd order transition**   **★ tricritical point**

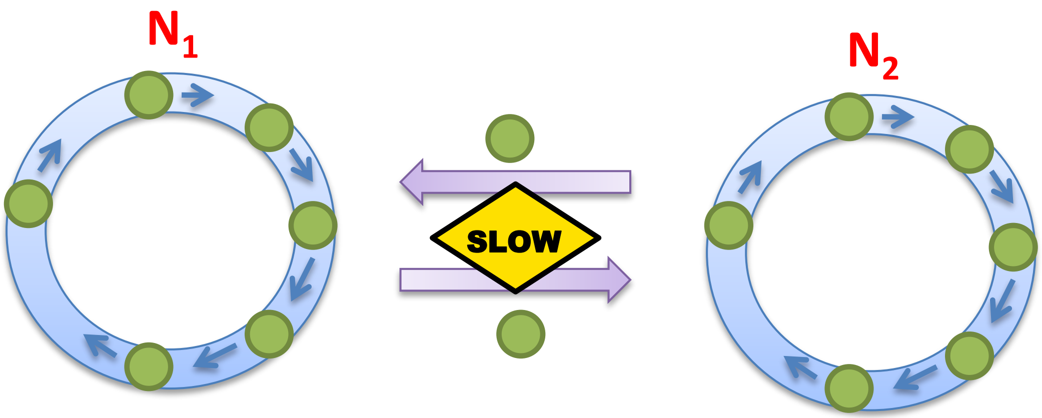
Why is $\mu_S(N)$ the chemical potential ?



$$\mu_S(N_1/L_1) = \mu_S(N_2/L_2)$$

$$N = N_1 + N_2$$

Why is $\mu_S(N)$ the chemical potential ?



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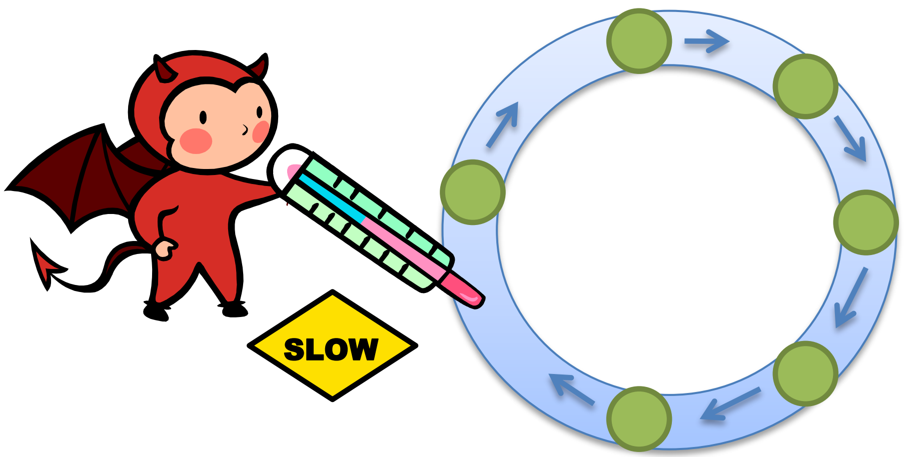
$$N = N_1 + N_2$$



Gauge measures

$$\mu_S(N/L)$$

Conclusions

1. Slow nonconserving dynamics
2. Example to ABC model
3. 1st order phase transition for nonmonotoneous μ(r) and inequivalence of ensembles.
4. Nonequilibrium chemical potential (dynamics dependent !)

Thank you !
Any questions ?