Part III. — Applications – Dynamical Heterogeneities in KCMs; Transport Models

Complexity Summer School

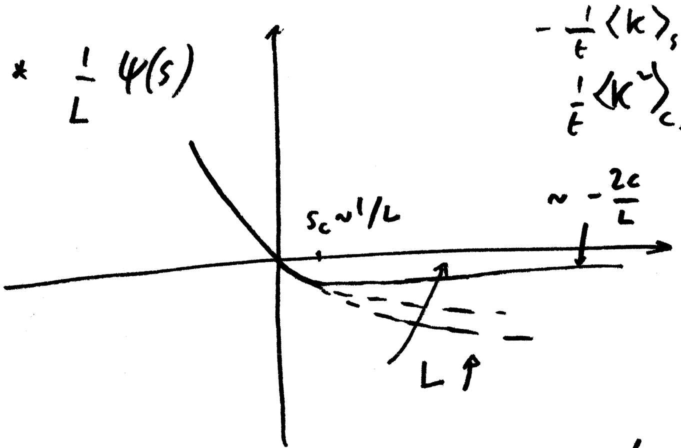
Warwick 2013

Outline:

1. Phase Coexistence in 1D & ∞D KCMs
2. 2^{nd} order phase transitions in transport models

1. Phase Coexistence in 1D & ∞D KCMs

1-a. Results for the dynamical free-energy of the 1DFA:

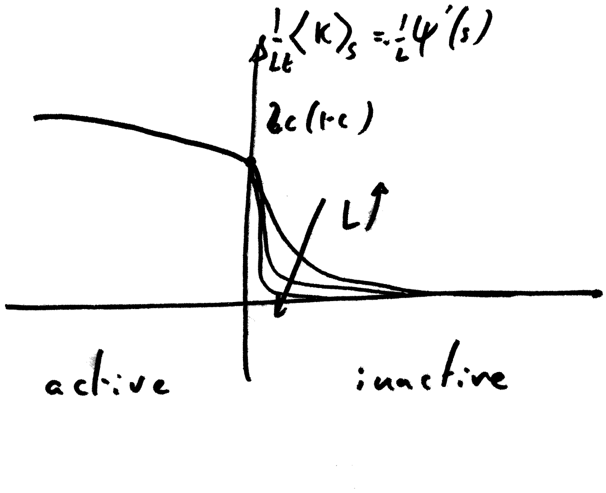


$$-\frac{1}{t}\langle K\rangle_s = \psi'(s) < 0 \quad \frac{1}{t}\langle K^2\rangle_{c,s} = \psi''(s) > 0 \Big\}: \ \psi(s) \text{ is decreasing and convex}$$

$$\big(\mathbb{W}(s)\big)_{\mathcal{C}'\mathcal{C}} = e^{-s} W(\mathcal{C}\to\mathcal{C}') - \delta_{\mathcal{C}\mathcal{C}'}\, r(\mathcal{C})$$

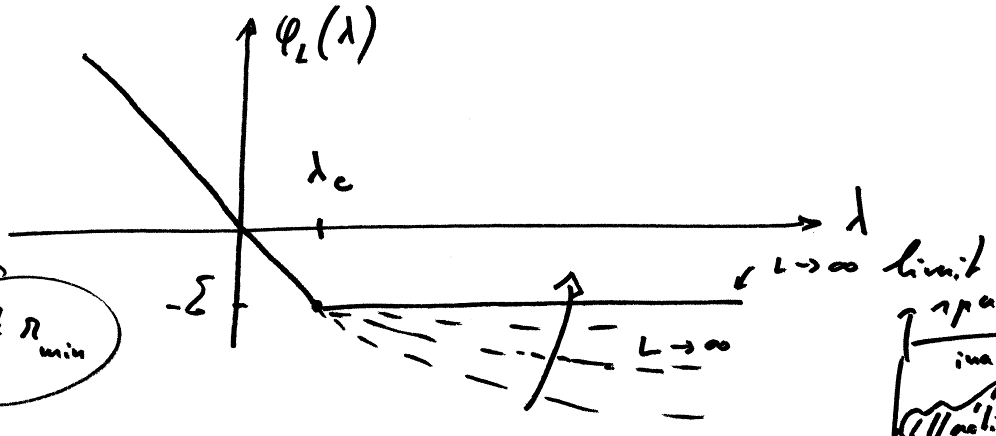
$$\lim_{s\to\infty} (\,—\,) = -\delta_{\mathcal{C}\mathcal{C}'}\, r(\mathcal{C}) \quad [\text{diagonal operator}]$$

$$\hookrightarrow \boxed{\psi(s\to\infty) = -\min_{\mathcal{C}} r(\mathcal{C}) = -2c}$$

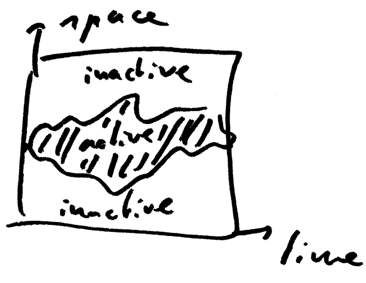


} 1^{st} order jump in the (dynamical) order parameter

* <u>Finite-size effects</u>. $s = \frac{\lambda}{L}$ $\quad \varphi_L(\lambda) = \Psi_L\left(\frac{\lambda}{L}\right)$



⚠ $\Sigma \neq r_{min}$



$\lambda > \lambda_c$: $\varphi(\lambda) = -\Sigma + \left(\frac{\lambda}{L}\right)^{2/3} + \dots$

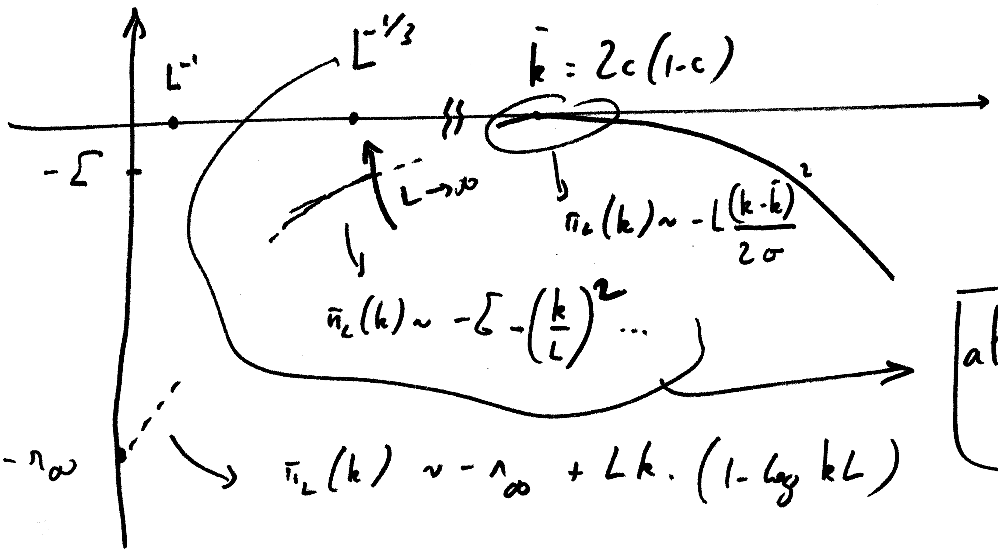
$-\Sigma$ → optimal configuration is a bubble

[Σ is a surface tension]

$\left(\frac{\lambda}{L}\right)^{2/3}$ → finite-size scaling. The boundary of the bubble is a random walk

↳ Finite-size scaling of Ψ tells us about the nature of the interface between active & inactive regions

* <u>Finite-size scaling in 'direct space'</u>: $P(K = kt) \sim e^{t\,\pi_L(k)}$



→ atypical fluctuations

1-6- A "mean-field" picture: FA on a complete graph.

$1 \leq n \leq L$ = # of active sites

$$\begin{cases} W(n \to n+1) = \underset{\text{activation rate}}{c} \ \underset{\text{\# activable sites}}{(L-n)} \ \underset{\text{\# active neighbors (Kinetic Constraint)}}{n} \\ W(n \to n-1) = \underset{\text{inactiva}^{\circ}\text{ rate}}{(1-c)} \ \underset{\text{\# sites that can be desactivated}}{n} \ \underset{\text{\# active neighbors}}{(n-1)} \end{cases}$$

(Important to avoid absorbing state n=0)

$r(n) = W(n \to n+1) + W(n \to n-1)$

Rk: this is an example of one-step process; see Tobia's lecture.

Exercices:

- $P_{eq}(n) = \binom{L}{n} c^n (1-c)^{L-n}$ is the steady-state (equilibrium distribution)

[Show that $W(n \to n+1)\, P_{eq}(n) = W(n+1 \to n)\, P_{eq}(n+1)$]

This 'detailed balance' condition implies that $P_{eq}(n)$ is the steady-state solu° of the master equation

- $\mathbb{W}^{sym}(s) = P_{eq}^{-1/2}(\hat{n})\, \mathbb{W}(s)\, P_{eq}^{1/2}(\hat{n})$ is a symmetric matrix

of elements $\left(\mathbb{W}^{sym}(s)\right)_{nn'} = e^{-s}\left\{\sqrt{W(n \to n+1)W(n+1 \to n)}\ \delta_{n'n+1} + \sqrt{W(n \to n-1)W(n-1 \to n)}\ \delta_{n'n-1}\right\}$
$- r(n)\, \delta_{nn'}$

- Use the following theorem: for a symmetric matrix $\mathbb{W}^{sym}$

$$\psi(s) = \max \mathrm{Sp}\, \mathbb{W}^{sym} = \max_{|P\rangle \neq 0} \frac{\langle P | \mathbb{W}^{sym} | P \rangle}{\langle P | P \rangle} \quad (*)$$

with $|P\rangle = \sum_{1 \leq n \leq L} P(n)\,|n\rangle$ and $\underbrace{P(n) = e^{L f(n/L)}}_{\text{large deviation scaling}}$

substitute this form of $P(n)$ into $(*)$ to show that

(Remark: the spectrum of $\mathbb{W}(s)$ and of $\mathbb{W}^{sym}(s)$ are the same:

$\underset{\text{eigv of } \mathbb{W}^{sym}(s) \text{ of eigv. } \lambda}{P_{eq}^{-1/2}\, \mathbb{W}(s)\, P_{eq}^{1/2}\, |\lambda\rangle = \lambda |\lambda\rangle} \iff \mathbb{W}(s)\, \underset{\text{eigv. of } \mathbb{W}(s) \text{ of eigv. } \lambda}{\left(P_{eq}^{1/2}|\lambda\rangle\right)} = \lambda \left(P_{eq}^{1/2}|\lambda\rangle\right)$)

$$\frac{1}{L}\Psi(s) \underset{L\to\infty}{\sim} \max_{f} \frac{\sum_n \left[\sqrt{w^+w^-}\left(e^{2f'(\rho)} + e^{-2f'(\rho)}\right) - n\right] e^{2L f(\rho)}}{e^{2L f(\rho)}}$$

$$\left(\begin{array}{c}\rho = \frac{n}{L} \\ 0<\rho<1\end{array}\right) \quad \begin{array}{c} w_{\pm}(n) = W(n \to n\pm 1) \\ \downarrow \\ w^{+}(\rho)\end{array}$$

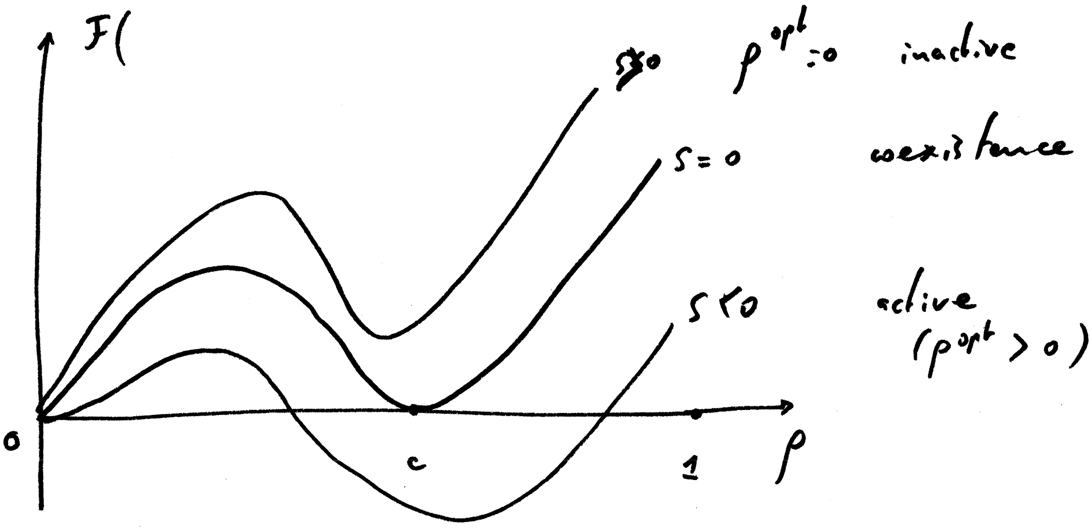
in the large L limit, extremal values of f dominate, & verify $f'(\rho) = 0$

↳ this "optimization principle" is thus independent of f and writes

$$\frac{1}{L}\Psi(s) \underset{L\to\infty}{=} -\min_{\rho} \mathcal{F}(\rho, s)$$

$\mathcal{F}(\rho,s)$ ↳ "Landau free energy" (dynamical)

$$\mathcal{F}(\rho,s) = \rho\cdot\left(c(1-\rho)+\rho(1-c)\right) - 2e^{-s}\rho\sqrt{c(1-c)\rho(1-\rho)}$$



Akin to static 1st order phase transition

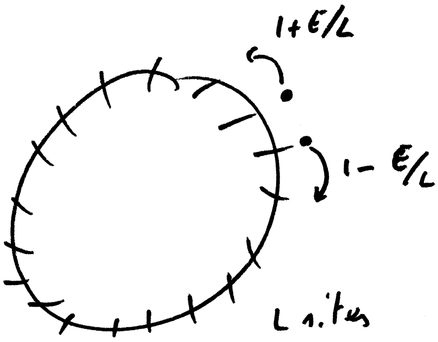
<u>Remark</u>: in this mean-field-like approach, the optimal distribution $|P\rangle$ is taken to be characterized entirely by its density ρ.

[instead of optimizing over a full distribution, one optimizes over a single number, the order parameter ρ — this is the central idea of mean-field approaches].

2 – 2ND ORDER PHASE TRANSITIONS IN TRANSPORT MODEL –

Weakly Asymmetric SEP
↓

2-a- Current fluctuations in a periodic WASEP



slight asymmetry ~ $1/L$ b/w ↻ & ↺

E is a "field"

$0 < x < 1$ spatial coord.

↓ local

Macroscopic description with a field $\rho(x,t)$ = density field

"small" multiplicative white noise

$$\partial_t \rho = -\nabla_x J \quad , \quad J = -D\nabla_x \rho - E\rho(1-\rho) + \frac{1}{\sqrt{L}}\sqrt{\rho(1-\rho)}\;\eta$$

↑ white noise

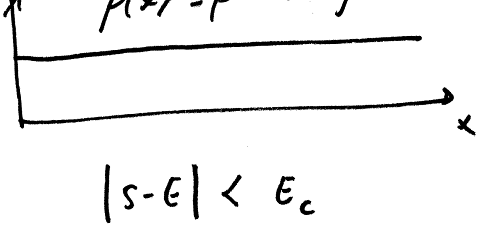
Representation of this Langevin evolution with an action

$$\langle e^{-sQ} \rangle \sim \int \mathcal{D}\rho \; e^{-L\,S[\rho;s]}$$

($S[\rho;s]$: action)

Q: total current on $[0,t]$

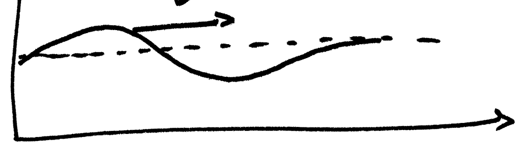
$\int \mathcal{D}\rho \, e^{-L S[\rho;s]}$: dominated by the saddle point



$|s-E| < E_c$

optimal profile is flat, uniform, stationary

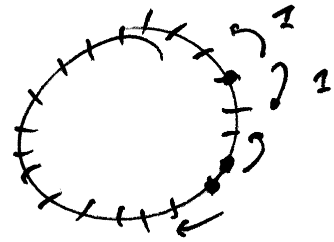
this allows to generate higher values of the current



$|s-E| > E_c$

optimal profile is non-uniform, moving at constant velocity v

2.6. Activity fluctuations in a periodic SSEP



fixed # particles, mean density ρ_0

K = # events on histories $[0,t]$

in the same way: $\langle e^{-sK} \rangle \sim \int \mathcal{D}\rho(x,t)\, e^{-L \int_0^t \{-\mathcal{H}(\rho(x,t))\}\, d\tau}$ ← action density

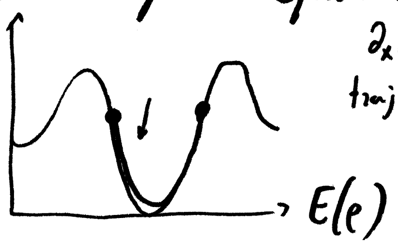
Optimal path obtained by saddle-point evaluation

Path are stationary $\rho(x)$.

Saddle point equation take the form

$\partial_x \rho = -E'(\rho)$

trajectories $\rho(x)$ with x being a time



microscopical view: to decrease activity, particles gather in clusters.