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LAGRANGIAN PHASE TRANSITIONS IN NON EQUILIBRIUM THERMODYNAMIC SYSTEMS

D. Gabrielli
(University of L'Aquila)

Join work with: L. Bertini
A. De Sole
G. Jona Lasinio
C. Landim

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Keywords

interacting particle systems,
scaling limits,

large number of degrees of freedom

$\Updownarrow$

Thermodynamic limit

Large deviations $\Leftrightarrow$ free energies

Variational principles, Hamiltonian structure

Phase Transitions

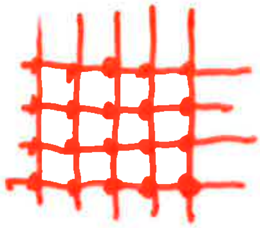
$\Updownarrow$

Singularities of rate functionals

Configurations of particles

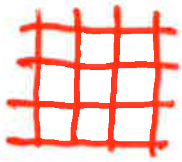
$$\eta \in \{0,1\}^{\Lambda_N} \quad \text{or} \quad \eta \in \{-1,+1\}^{\Lambda_N}$$

$\Lambda_N \subseteq \mathbb{Z}^d$ lattice



$$\eta \to \pi_N(\eta) = \frac{1}{N^d} \sum_{x \in \Lambda_N} \eta_x \, \delta_{x/N} \qquad \left(\text{Coarse Graining}\right)$$

$\pi_N(\eta)$ = Empirical measure



$\}\ 1/N$

Equilibrium models

Energy $\quad H_N(\eta) = \sum_{\substack{x \sim y \\ \in \Lambda_N}} J \eta_x \eta_y$

Gibbs measures

$$\mu_N(\eta) = \frac{1}{Z_N} e^{-H_N(\eta)}$$

Large Deviations

$$P\left(\pi_N(n) \sim \rho(x)\,dx\right) \approx e^{-N^d I(\rho)}$$

$I \geq 0$ rate functional

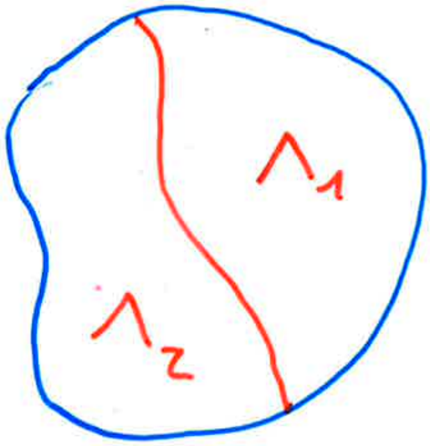
Equilibrium models

"pressure" $p(\lambda) = \lim_{N\to+\infty} \frac{1}{N^d} \log \sum_{n} \frac{e^{-H_N(n)+\lambda\sum_x n_x}}{Z_N}$

$$f(\alpha) = \sup_{\lambda}\left\{\lambda\alpha - p(\lambda)\right\}$$ convex

$$I_\Lambda(\rho) = \int_\Lambda f(\rho(x))\,dx$$

$\Lambda \subset \mathbb{R}^d$



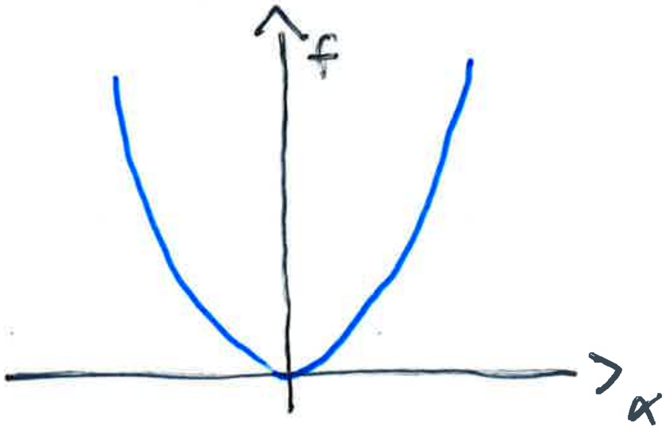
$$I_\Lambda(\rho) = I_{\Lambda_1}(\rho) + I_{\Lambda_2}(\rho)$$

(5)

Ising

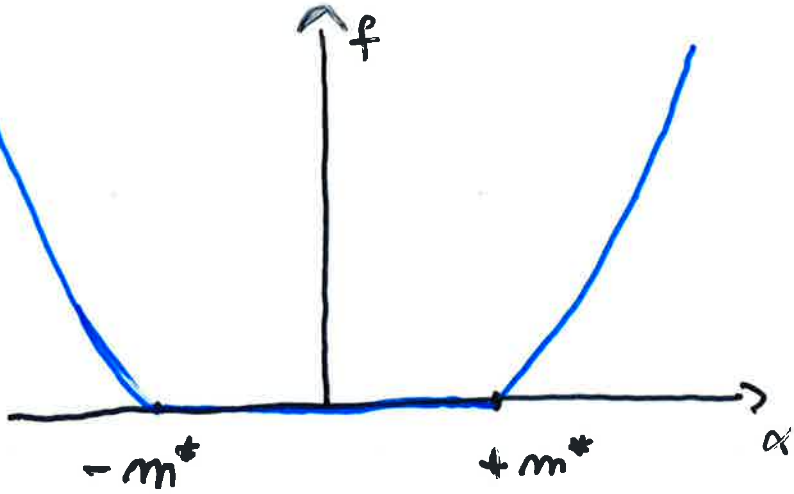
$f(\alpha)$ convex

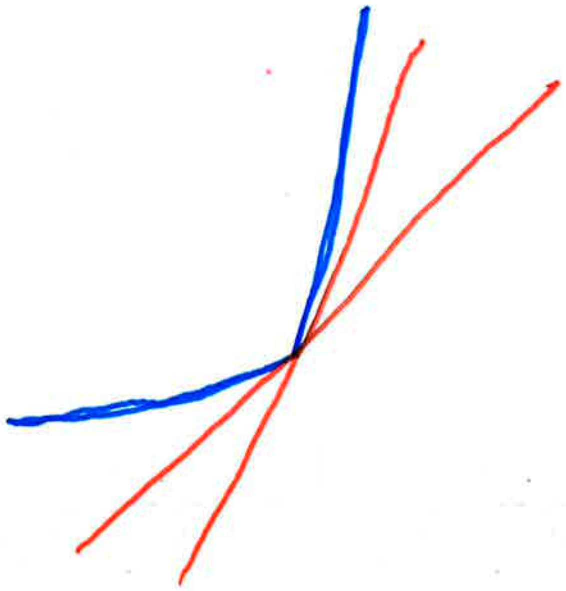
$B < B_c$



$B > B_c$

Singularities
Phase
Transitions





Subdifferential
not empty

Non Equilibrium

No Gibbs formalism

(A) Combinatorial representations of measures

(B) Dynamic variational approach

Freidlin - Wentzell Theory

(finite dimensional)

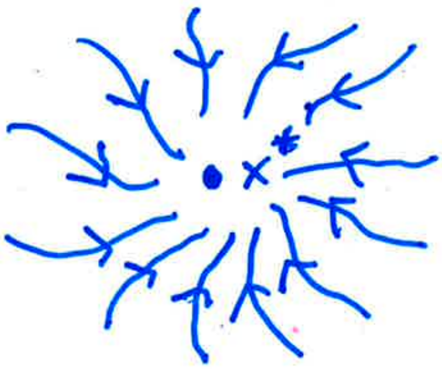
$$dx = b(x)\,dt + \sqrt{\varepsilon}\,dW$$

$x \in \mathbb{R}^N$

W = Brownian motion

b = globally attractive vector field

x^* = equilibrium



dynamic large deviations

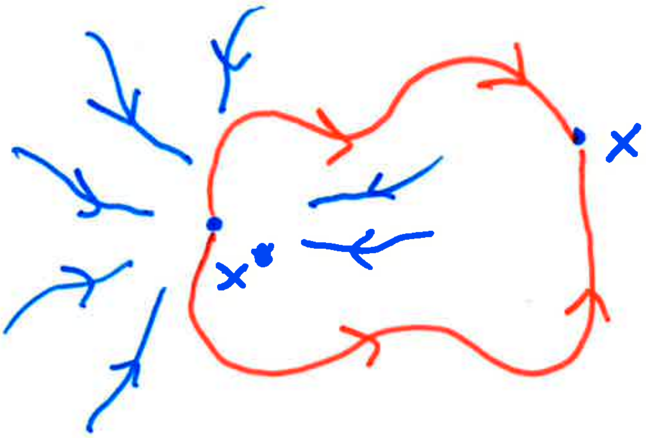
$$P\left(\{x(t)\}_{t\in[0,T]} \approx \{\hat{x}(t)\}_{t\in[0,T]} \right) \sim e^{-\varepsilon^{-1} I_{[0,T]}(\hat{x})}$$

$$I_{[0,T]}(x) = \frac{1}{2}\int_0^T |\dot{x}(s) - b(x(s))|^2\,ds = \int_0^T \mathcal{L}(\dot{x}(s), x(s))\,ds$$

Quasi potential

$$V(x) = \inf_{\left\{\begin{array}{l}\hat{x}(t): \\ \lim_{t \to -\infty} \hat{x}(t) = x^* \\ \hat{x}(0) = x\end{array}\right\}} I_{[-\infty, 0]}(\hat{x})$$

$x \in \mathbb{R}^N$



$\boxed{V(x) = \text{rate functional of the stationary state (invariant measure)}}$

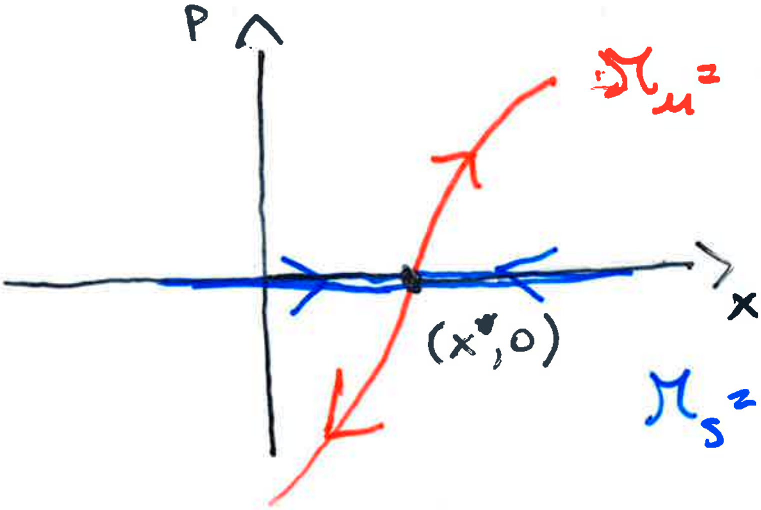
not differentiable

Critical Trajectories for computing

V = quasipotential

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{x}}\right)=\frac{\partial \mathcal{L}}{\partial x}$$ Euler - Lagrange equations

$$x(t)\,,\ p(t)=\frac{\partial \mathcal{L}}{\partial \dot{x}}(\dot{x}(s),x(s)) \Rightarrow$$ Hamilton Equations



M_u = unstable manifold

$$\boxed{\subseteq \{H(x,p)=0\}}$$

M_s = stable manifold

M_u and M_s are Lagrangian manifolds

$$\oint_\gamma p\,dq=0 \qquad \gamma \subseteq M_u \text{ or } M_s$$

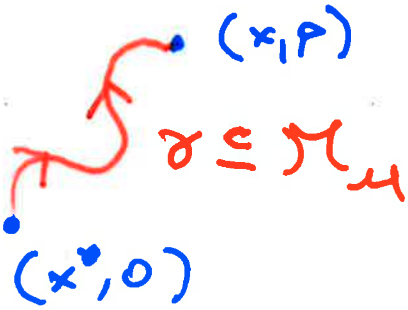
D. Day

$(x,p) \in M_\mu$

$\Downarrow$

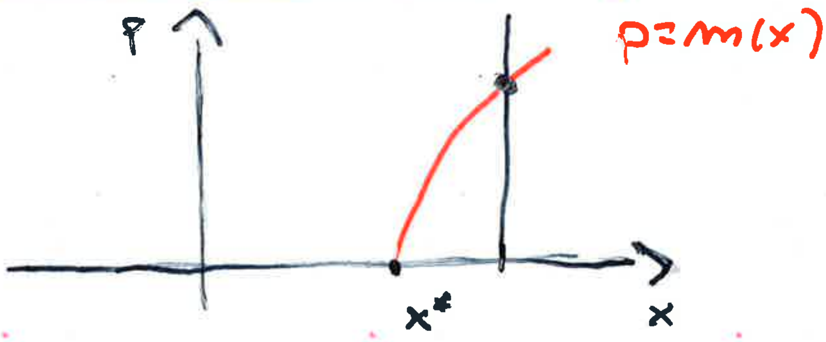
$W(x,p) = $ prepotential

$$W(x,p) = \int_\gamma p\,dq$$

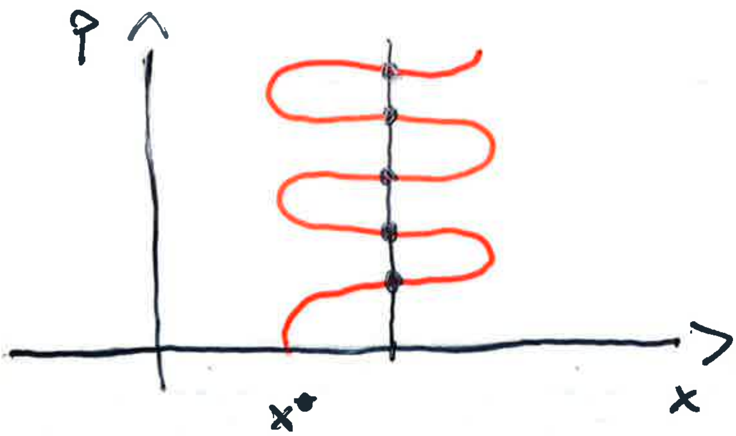


$$\boxed{V(x) = \inf_{\{p\,:\,(x,p)\in M_\mu\}} W(x,p)}$$

$M_\mu =$ graph

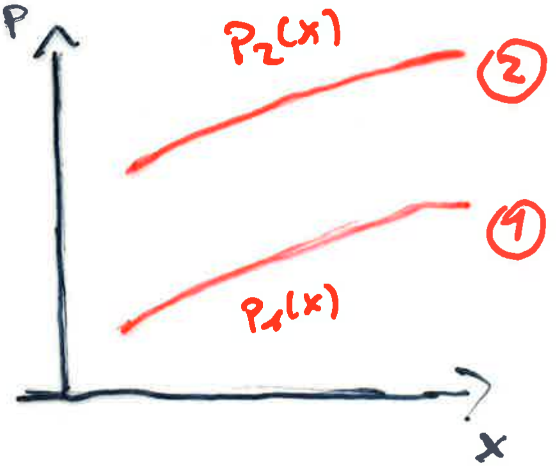


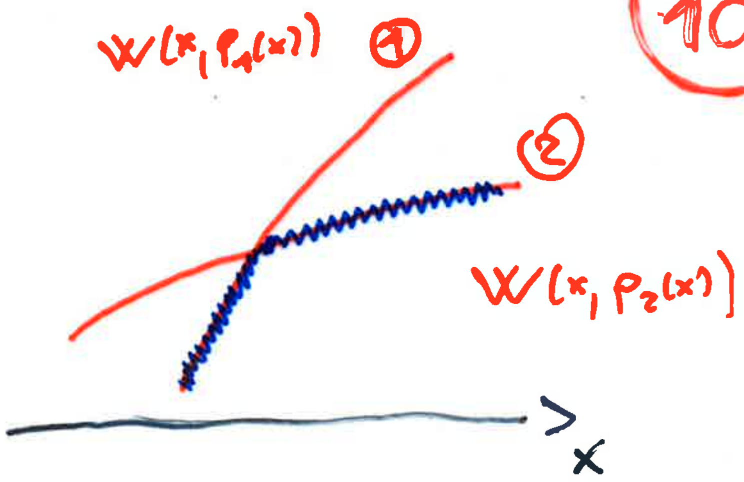
$M_\mu =$ not a graph



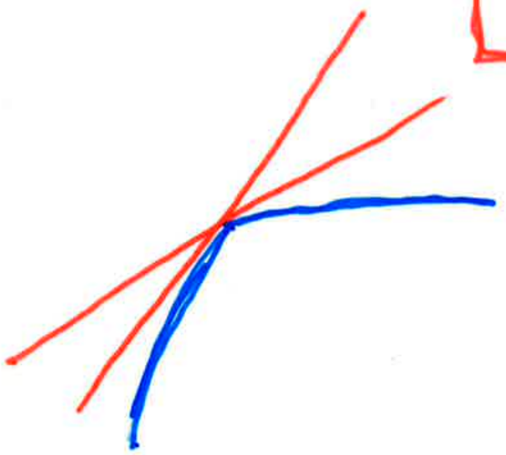
Weak solutions
Hamilton-Jacobi eq.

$$\boxed{H(x, \nabla V(x)) = 0}$$



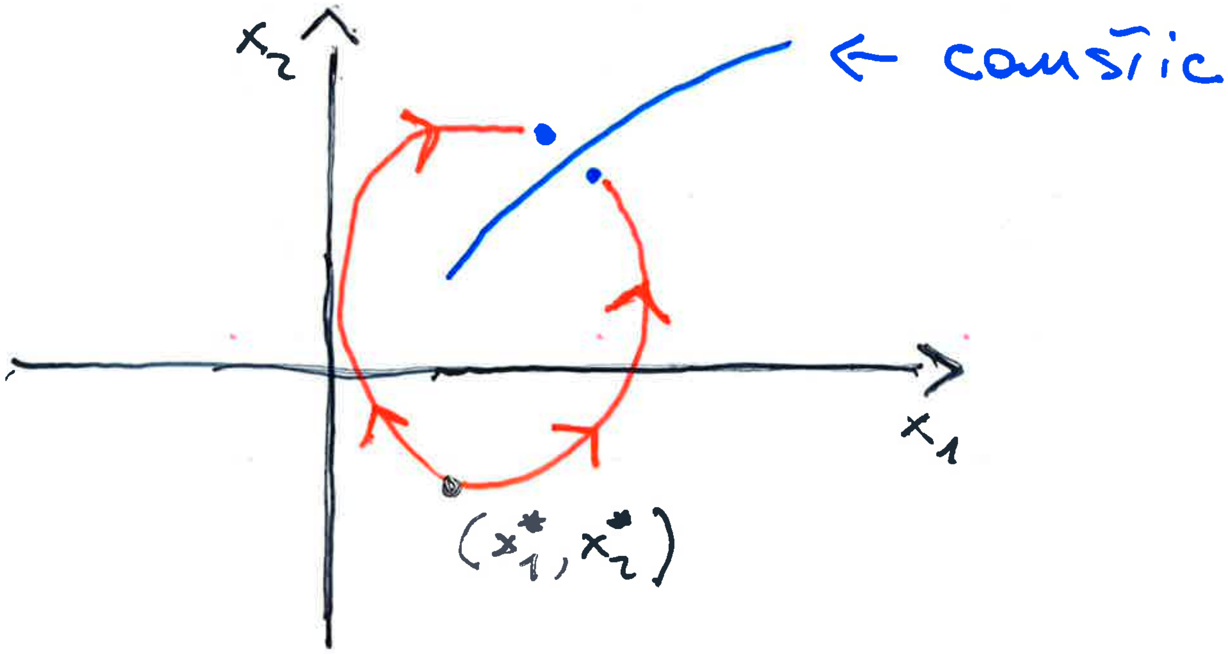


= $V(x)$



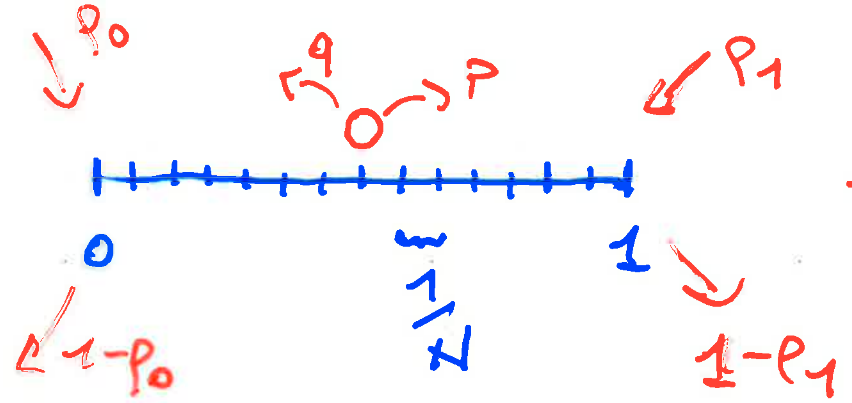
superdifferential
not empty

No convexity
=> instability



Exactly solvable ∞-dimensional case

WASEP 1-d + boundary sources



+ exclusion interaction

$\rho_0 < \rho_1$ ←

$p > q$ →

$p - q \sim \frac{E}{N}$

$E > s'(\rho_1) - s'(\rho_0) > 0$ External field

$$s(x) = x \log x + (1-x) \log (1-x)$$

Hydrodynamic limit

Time accelerated by N^2

$$\pi_N(\eta(t)) \xrightarrow[N \to +\infty]{} \rho(x,t)\,dx$$

$$\begin{cases} \rho_t = \rho_{xx} - E\left(\rho(1-\rho)\right)_x \\ \rho(0,t) = \rho_0 \,, \quad \rho(1,t) = \rho_1 \end{cases}$$

Globally attractive

$\bar{\rho}$ = unique stationary solution

Dynamic Large Deviations

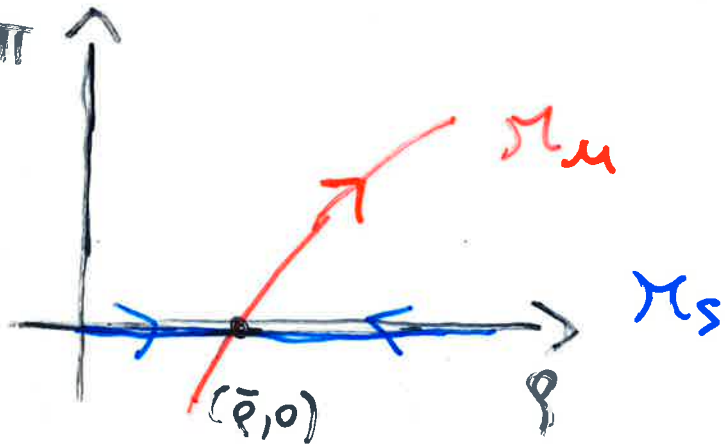
$$I_{[T_1,T_2]}(\rho) = \frac{1}{4}\int_{T_1}^{T_2} dt \int_0^1 dx\, \rho(x,t)\,(1-\rho(x,t))\, F(x,t)^2$$

$$= \int_{T_1}^{T_2} dt\, \mathcal{L}(\rho_t(t), \rho(t))$$

$H(\rho,\pi)$ Hamiltonian

$$\boxed{\begin{aligned} &\rho(0,t)=\rho_0\,,\quad \rho(1,t)=\rho_1 \\ &\pi(0,t)=\pi(1,t)=0 \end{aligned}}$$

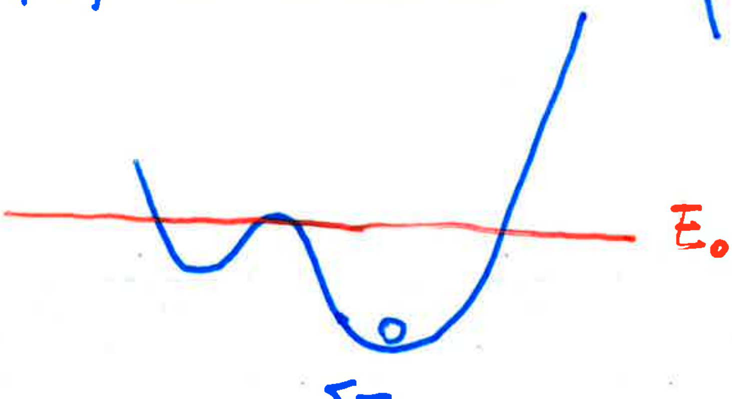
$(\bar{\rho},0)=$ equilibrium of the Hamiltonian flow



Hamilton equations

$(\rho^H,0)$ is solution

$$\begin{cases} \rho_t = \rho_{xx} - \big(\rho(1-\rho)(E+2\pi_x)\big)_x \\ \pi_t = -\pi_{xx} + (2\rho-1)(\pi_x^2 - E\pi_x) \end{cases}$$



Symplectic Transformation

$$\begin{cases} \varphi = s'(\rho) - \pi \\ \psi = \rho \end{cases}$$

Equilibrium point

$$(s'(\bar\rho), \bar\rho)$$

$$\varphi(0,t) = s'(\rho_0), \quad \varphi(1,t) = s'(\rho_1)$$

$$\mathcal{M}_s = \left\{ (\varphi, \rho) : \varphi = s'(\rho) \right\}$$

$$\mathcal{M}_u = \left\{ (\varphi, \rho) : \rho = \underbrace{\frac{1}{1+e^{\varphi}} - \frac{\varphi_{xx}}{\varphi_x (E - \varphi_x)}}_{\frac{\delta W_E}{\delta \varphi} = 0}, \ 0 < \varphi_x < E \right\}$$

$$W_E(\rho, \pi) = \int_\gamma \pi \, d\rho =$$

$$= \int_0^1 \left[s(\rho(x)) + s\left(\frac{\varphi_x(x)}{E}\right) + (1 - \rho(x))\varphi(x) - \log\left(1 + e^{\varphi(x)}\right) \right] dx$$

$$V_E(\rho) = \inf_{\varphi : (\varphi, \rho) \in \mathcal{M}_u} W_E(\rho, \varphi) = \inf_{\varphi} W_E(\rho, \varphi)$$

$$P_{ST}\left(\pi_N(\eta) \sim \rho(x)\,dx \right) \simeq e^{-N V(\rho)}$$

limiting cases

$E \downarrow \quad s'(\rho_1) - s'(\rho_0) = E_0$

$0 < \varphi_x < s'(\rho_1) - s'(\rho_0) \qquad \varphi(0) = s'(\rho_0), \ \varphi(1) = s'(\rho_1)$

$\exists ! \quad \bar{\varphi}(x)$ linear

$M_u = \{(\bar{\varphi}, \rho)\}$ is a graph

$$V_{E_0}(\rho) = W_{E_0}(\bar{\varphi}, \rho)$$

$$= \int_0^1 \left[s(\rho(x)) + (1-\rho(x))\bar{\varphi}(x) - \log\left(1 + e^{\varphi(x)}\right) \right] dx$$

Equilibrium model (additivity)

$E \sim E_0$ still a graph

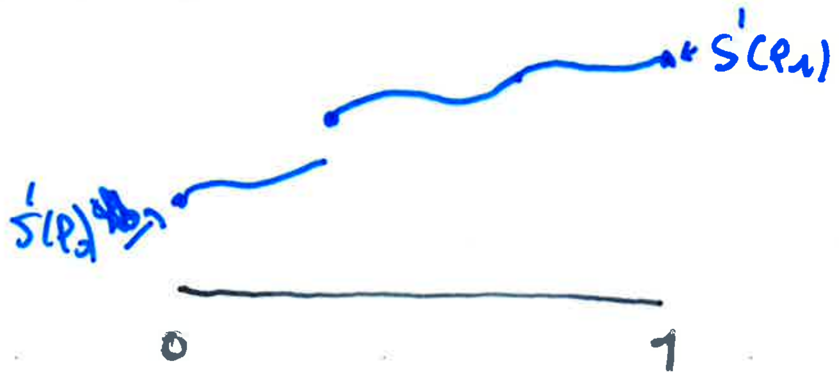
$\Downarrow$

No Lagrangian phase transition

Limiting cases

$E \to +\infty$

φ increasing

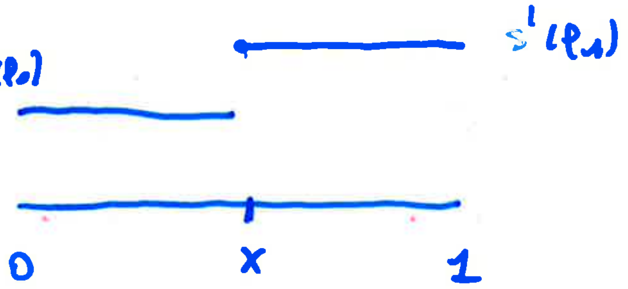


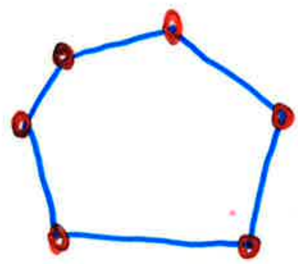
$$W_E(\varphi,\rho) \xrightarrow{E\to+\infty} W_\infty(\varphi,\rho)$$

$$= \int_0^1 \left[s(\rho) + (1-\rho)\varphi - \log\left(1+e^{\varphi}\right) \right] dx$$

Concave in φ $\Rightarrow$ minimum is obtained on extremal points

$\varphi^x =$





$\{\varphi^x\}_{x\in[0,1]}$ extreme points

$$\min_{\varphi} W_\infty(\varphi,\rho) = \min_{x\in[0,1]} W_\infty(\varphi^x,\rho)$$

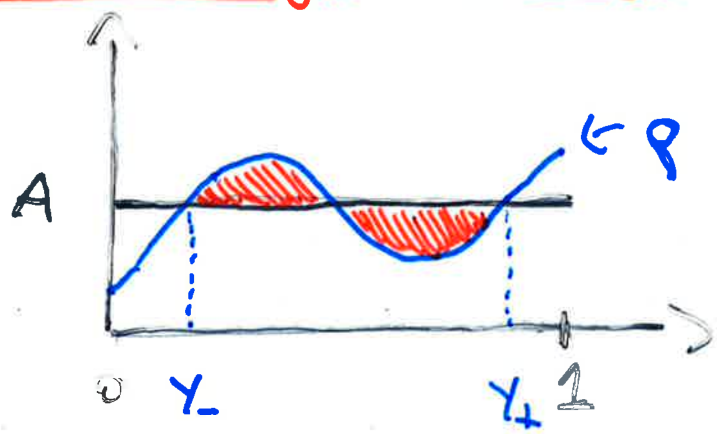
$$= \min_{x\in[0,1]} \int_0^x s(\rho) + s'(\rho_0)(1-\rho) - \log\left(1+e^{s'(\rho_0)}\right)$$

$$+ \int_x^1 s(\rho) + s'(\rho_1)(1-\rho) - \log\left(1+e^{s'(\rho_1)}\right)$$

$$\|$$

LDP for TASEP (Derrida Lebowitz Speer)

$\exists\, A$



$$\min_x W(\varphi^x,\rho) = W(\varphi^{Y_-},\rho) = W(\varphi^{Y_+},\rho)$$

$$\Downarrow$$

By a perturbative argument Lagrangian phase transitions occur for E big enough.

(Thanks!)