Singular Large Deviation Functionals

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with

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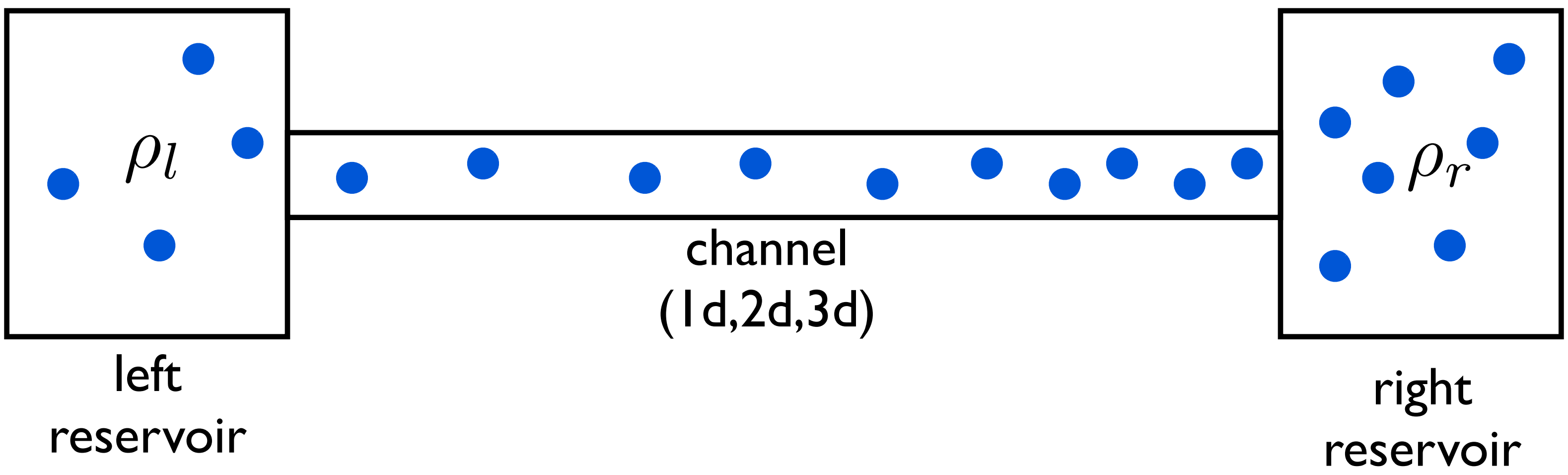
Boundary Driven Diffusive System

- Diffusive *interacting+conserving* channel (`**disordered**' phase - think gas)

- Channel connected to two reservoirs at different densities

- Steady-state



1. What is the average density profile $\overline{\rho}(x) \quad (0 \leq x \leq 1)$?

2. Fluctuations - for example, two point correlations $\langle \rho(x) \rho(y) \rangle$?
   Probability of any configuration $P\left[\rho(x)\right]$?
   How is a fluctuation generated dynamically?

Outline

- Approaches

- Brief recall of equilibrium results

- Out of equilibrium basics - *average density*
  correlations (simple picture for
  positive vs. negative)

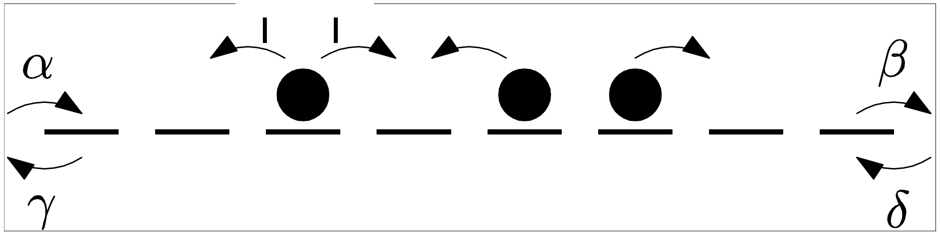
- Probability of arbitrary profile -
  Calculating the large deviation functional
  General properties - nonlocal
  non-differentiable functional
  structure of singularities

- Fluctuation induced forces *(Casimir)*

Approaches

Generally can identify two approaches:

1. **Start from a microscopic model**:
   for example, *simple symmetric exclusion model*



- Evolution of probability $\partial_t |P(t)\rangle = M |P(t)\rangle$

Solve

Fluctuating Hydrodynamics **Phenomenological approach (can also derive in some cases):**

- Density field $\rho(x)$ satisfies

$$\partial_t \rho(x) + \nabla \cdot J = 0$$

- Rescale space $0 \leq x \left(= \frac{x'}{N}\right) \leq 1$ and time $t = \frac{t'}{N^2}$

$$J = \underbrace{-D(\rho)\nabla\rho}_{\text{Fick's law}} + \underbrace{\sqrt{\sigma(\rho)}\eta(x,t)}_{\text{Noise}}$$

- Noise is small due to rescaling (central limit theorem)

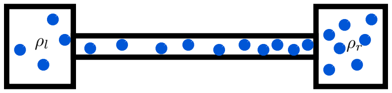
$$\langle \eta(x,t)\eta(x',t')\rangle = \frac{1}{N}\delta(x-x')\delta(t-t')$$

- $D(\rho)$ and $\sigma(\rho)$ connected by fluctuation-dissipation (recall rescaling)

$$\sigma(\rho) = 2k_B T \rho^2 \underbrace{\kappa(\rho)}_{\text{compressibility}} D(\rho)$$

- Boundary conditions $\rho(0) = \rho_l \qquad \rho(1) = \rho_r$

Equations of motion (fluctuating hydrodynamics)



$$\partial_t \rho(x) + \nabla \cdot J = 0$$

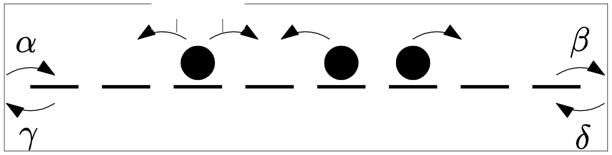
$$J = -D(\rho)\nabla\rho + \sqrt{\sigma(\rho)}\eta(x,t)$$

$$\sigma(\rho) = 2k_B T \rho^2 \kappa(\rho) D(\rho)$$

With boundary conditions $\rho(0) = \rho_l$ and $\rho(1) = \rho_r$

- Phenomenological approach $D(\rho)$ and $\sigma(\rho)$ given/measured*

- Microscopic approach $D(\rho)$ and $\sigma(\rho)$ calculated

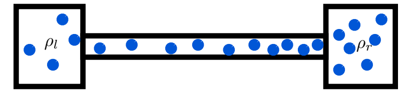


for symmetric exclusion model $D(\rho) = 1$

$$\sigma(\rho) = 2\rho(1-\rho)$$

* Weber et. al. PRB 2001

In Equilibrium $\rho_l = \rho_r = \overline{\rho}$ (on average flat)



Fluctuation dissipation dictates probability of any configuration

$$P\left[\rho(x)\right] e^{-N \int f(\rho(x),\overline{\rho})}$$

with $\quad f\left(\rho\right) \equiv \int_{\overline{\rho}}^{\rho} d\rho_1 \int_{\overline{\rho}}^{\rho_1} d\rho_2 \frac{2D\left(\rho_2\right)}{\sigma\left(\rho_2\right)}$ $\quad$ the *free-energy density*

For example, for symmetric exclusion model

$$\int_0^1 dx \left\{\rho(x)\log\frac{\rho(x)}{\bar{\rho}} + (1-\rho(x))\log\frac{1-\rho(x)}{1-\bar{\rho}}\right\}$$

Note -

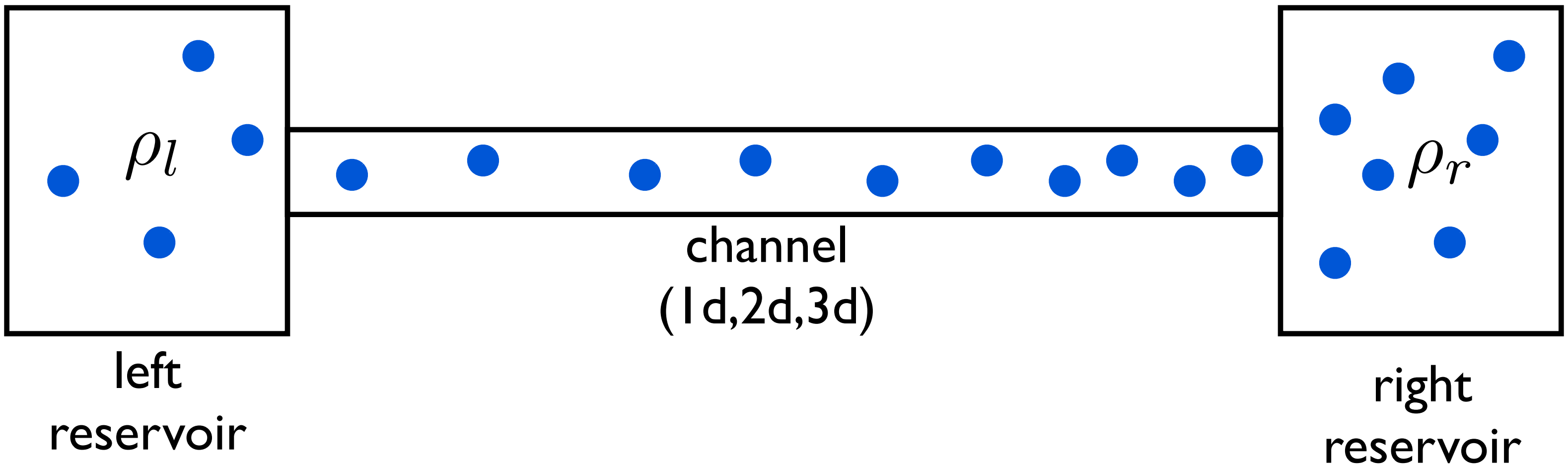
1. Local functional (no correlations)

2. Smooth functional
(result of smooth D and σ)

Out of Equilibrium

(on average non-flat profile)

$$\rho_l \neq \rho_r$$



Question 1 (easy) - The average Density Profile

Average Density Profile

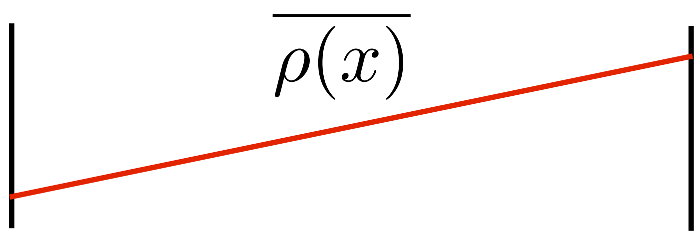
$$\partial_t \rho(x) + \nabla \cdot J = 0$$

$$J = -D(\rho)\nabla\rho + \sqrt{\sigma(\rho)}\,\eta(x,t)$$

Solve $\nabla(D(\overline{\rho})\nabla\overline{\rho}) = 0$ with boundary conditions

$$\overline{\rho(0)} = \rho_l \qquad \overline{\rho(1)} = \rho_r$$

For example, for $D = 1$ get linear profile



Question 11 - Small Fluctuations

Fluctuations

Naive guess - weak drive so locally in equilibrium

Calculate $\overline{\rho(x)}$

And guess

$$P[\rho(x)] \propto e^{-N\int f(\rho(x),\overline{\rho}(x))dx}$$

with

$$f\left(\rho, r\right) \equiv \int_r^{\rho} d\rho_1 \int_r^{\rho_1} d\rho_2 \frac{2D\left(\rho_2\right)}{\sigma\left(\rho_2\right)}$$

How wrong? $\left\langle \left(\int \rho(x) \right)^2 \right\rangle_c$ off by order $\left(\rho_l - \rho_r\right)^2$

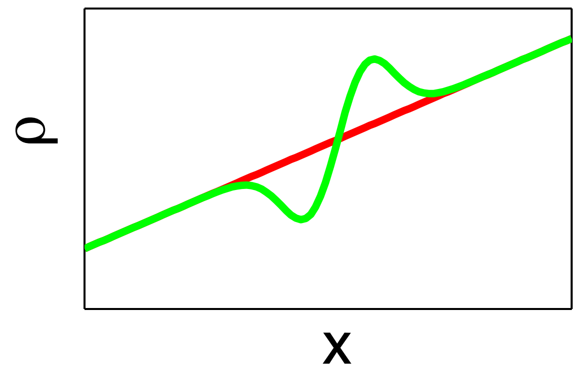
Reason for disagreement is the presence of *generic long range correlations (positive or negative)*

Lattice models - Sphon 1983
Experiments on heat flow - Law et. al. 1988
(review by Dorfman et. al. 1997)

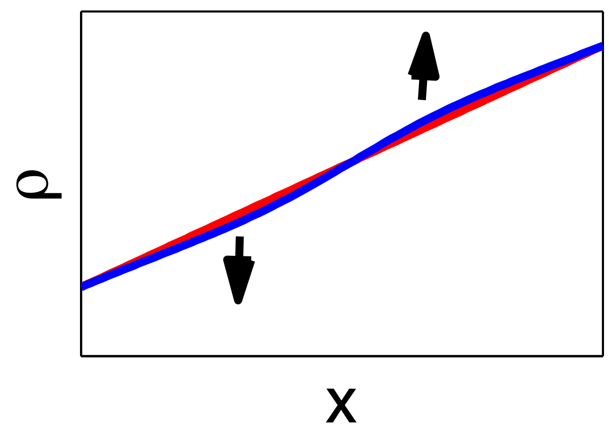
Too see, enough to evaluate two-point correlation for small fluctuations

Simple picture for long range correlations

Look at fluctuation
in bulk of system

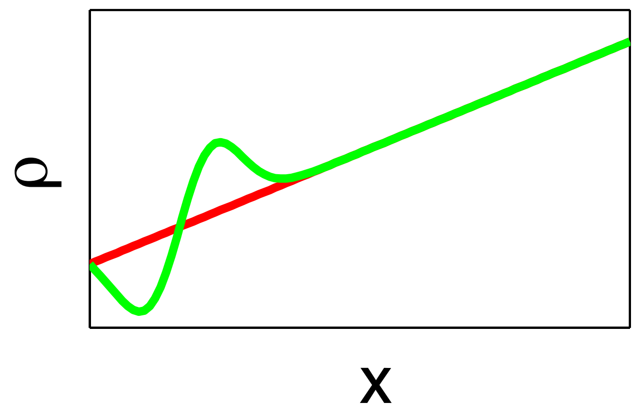


At later times spreads
generating
negative correlations

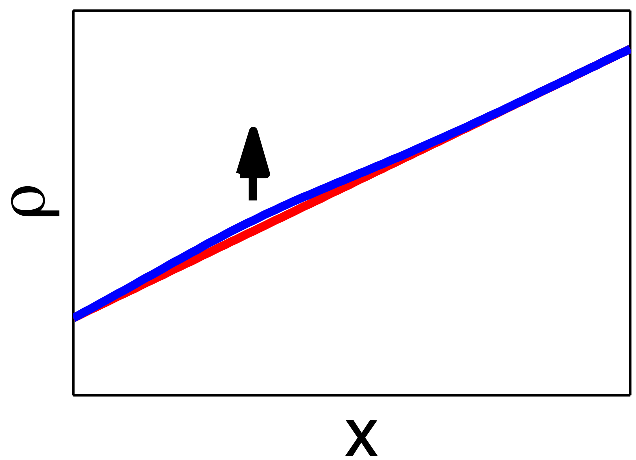


Simple picture for long range correlations

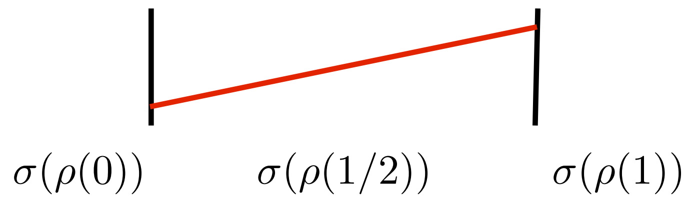
Next, look at fluctuation
near the boundaries
of system



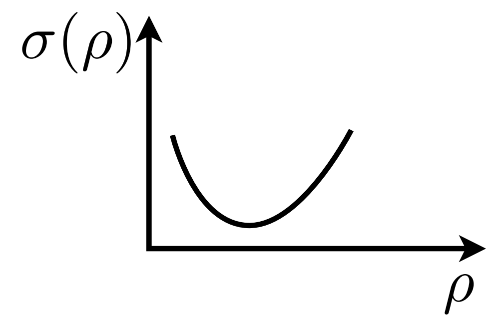
At later times spreads
generating
positive correlations



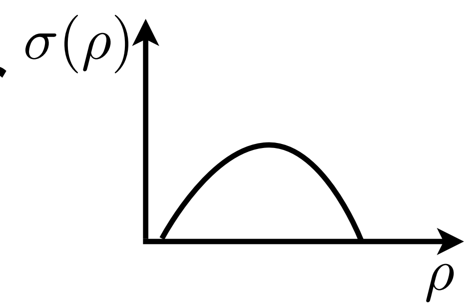
Correlations in system dictated by interplay of two processes:



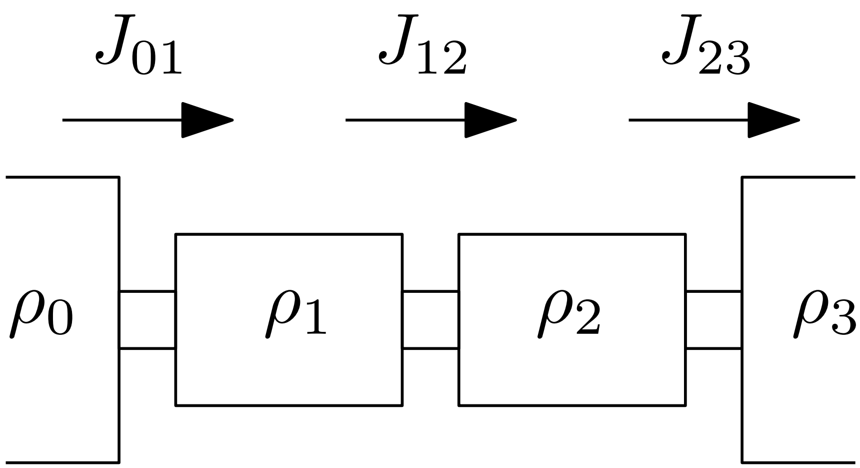
- If noise near the boundaries is stronger
  positive correlations



- If noise near the boundaries in weaker
  negative correlations



Easy to understand within a simple two box system



`Boxed fluctuating hydrodynamics'

Next, large deviation (Question 3):

probability of an arbitrary configuration

- Exact solutions (Derrida, Lebowitz, Speer)

- Macroscopic fluctuation theory (Bertini, Jona-Lasinio, based on large deviations literature Freidlin, Wentzel, Varadhan....)

  (see paper by Tailleur, Kurchan and Lecomte 2008)

Macroscopic fluctuation theory

$$\partial_t \rho(x) + \nabla \cdot J = 0$$

$$J = -D(\rho)\nabla\rho + \sqrt{\sigma(\rho)}\eta(x,t)$$

$$\sigma\left(\rho\right) = 2k_B T \rho^2 \kappa\left(\rho\right) D\left(\rho\right)$$

The probability of a history of noise is

$$P\left[\eta(x,t)\right] \propto e^{-N\int \frac{\eta(x,t)^2}{2} dx dt}$$

or

$$P[\eta(x,t)] \propto e^{-N\int \frac{(J+D(\rho)\nabla\rho)^2}{2\sigma(\rho)} dx dt} \equiv e^{-NS}$$

Large N - use saddle-point/wkb
(hard - nonlinear field equations)

Usually solve Hamiltonian version of saddle-point equations

Introduce Lagrange multiplier to fix current

$$\int dx dt \hat{\rho}(x)(\partial_t \rho + \nabla \cdot J)$$

get

$$\begin{aligned} \partial_t \rho &= \partial_x^2 \rho - 2\partial_x \left(\sigma\left(\rho\right)\partial_x \hat{\rho}\right) \\ \partial_t \hat{\rho} &= -\left(\partial_x \hat{\rho}\right)^2 \cdot \partial_x \sigma\left(\rho\right) - \partial_x^2 \hat{\rho}, \end{aligned}$$

momentum

Non-linear

(Could have got here via Martin-Siggia-Rose and saddle-point)

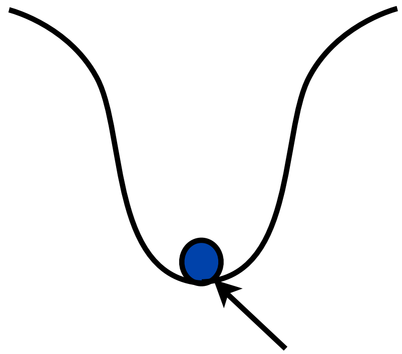
Note, in the large N limit given that a fluctuation occurred its history is deterministic

Illustration of idea

One dimensional brownian particle in periodic potential *(weak noise)*

$$\partial_t x = F(x) + \sqrt{\epsilon/2}\eta(t)$$

$$\langle \eta(t)\eta(t')\rangle = \delta(t-t')$$



Most probable location

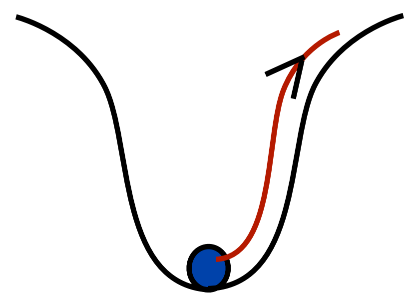
Want probability distribution in steady state $P(x, t = \infty)$

$$P\left[\eta(x,t)\right] \propto e^{-\frac{1}{\epsilon}\int dt(\partial_t x - F(x))^2}$$

$$F(x) = -\partial_x V(x)$$

Look at problem 1. particle starts at $t = -\infty$ in most probably state

2. ends at x at $t = 0$

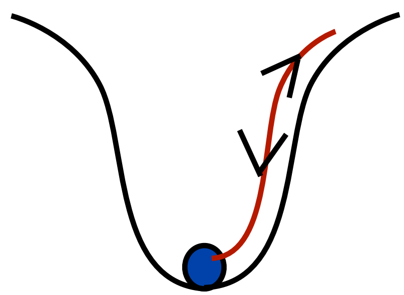


saddle point to find most probably history
(instanton)

(WKB - see Graham, Tel, Dykman, ...)

Comment: Problem above in equilibrium.

Time reversal symmetry (ala Onsager)
Path to fluctuation *same* as
relaxation to most probably state

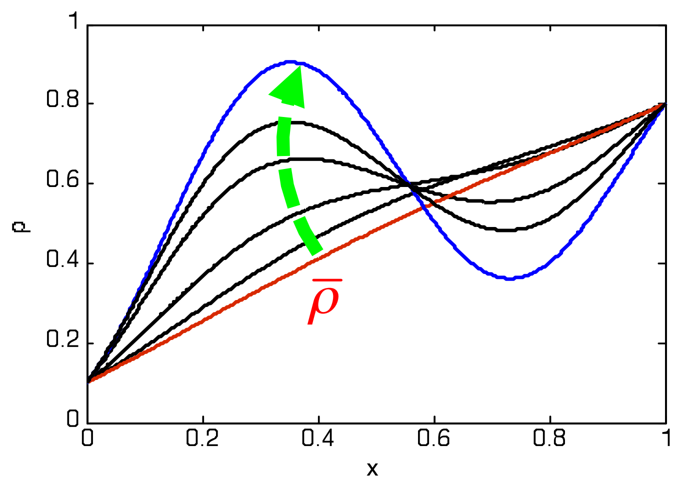


Makes hard problem relatively easy

For diffusive fields - same idea

$$P[\eta(x,t)] \propto e^{-N\int \frac{(J+D(\rho)\nabla\rho)^2}{2\sigma(\rho)}dxdt} \equiv e^{-NS}$$

Look for most probably history that leads to configuration of interest at $t=0$ starting from most probable at $t=-\infty$



Technically minimize over J,ρ subject to constraint $\partial_t\rho + \nabla J = 0$

Result of calculation

$$P[\rho(x)] \propto e^{-N\phi[\rho(x)]}$$

Called **Large Deviation Functional**

It is the direct analog of a free energy away from equilibrium

Recap

systematic way to calculate probability of arbitrary configuration for diffusive systems

Results to date

- Exact solution for $D = 1$ and $\sigma(\rho) = a + b\rho + c\rho^2$ only in 1d
  (obtained first via microscopic path by Derrida et. al. 2002)

For example, $D = 1$, $\sigma(\rho) = 2\rho(1-\rho)$

$$\phi[\rho(x)] = \int_0^1 dx \left[(1-\rho(x))\ln\frac{1-\rho(x)}{1-F(x)} + \rho(x)\ln\frac{\rho(x)}{F(x)} + \ln\frac{\nabla F}{\rho(1)-\rho(0)}\right]$$

where $\rho(x) = F(x) + F(x)(1-F(x))\frac{\nabla^2 F}{(\nabla F)^2}$

Note - nonlocal a direct manifestation of the long range correlations (very different from equilibrium)

Can also show a smooth functional (exception see below)

- Numerical algorithm evaluate probability of a given configurations (Bunin, YK, Podosky 2012)

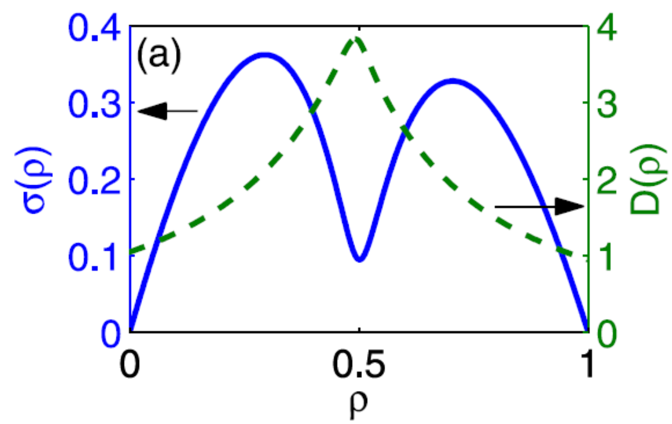
1. Allows one to *explore* ***general models*** *and in* ***any dimension***

2. Gives a hint on how to build *perturbative treatment*

Non-differentiable (non-local) functionals

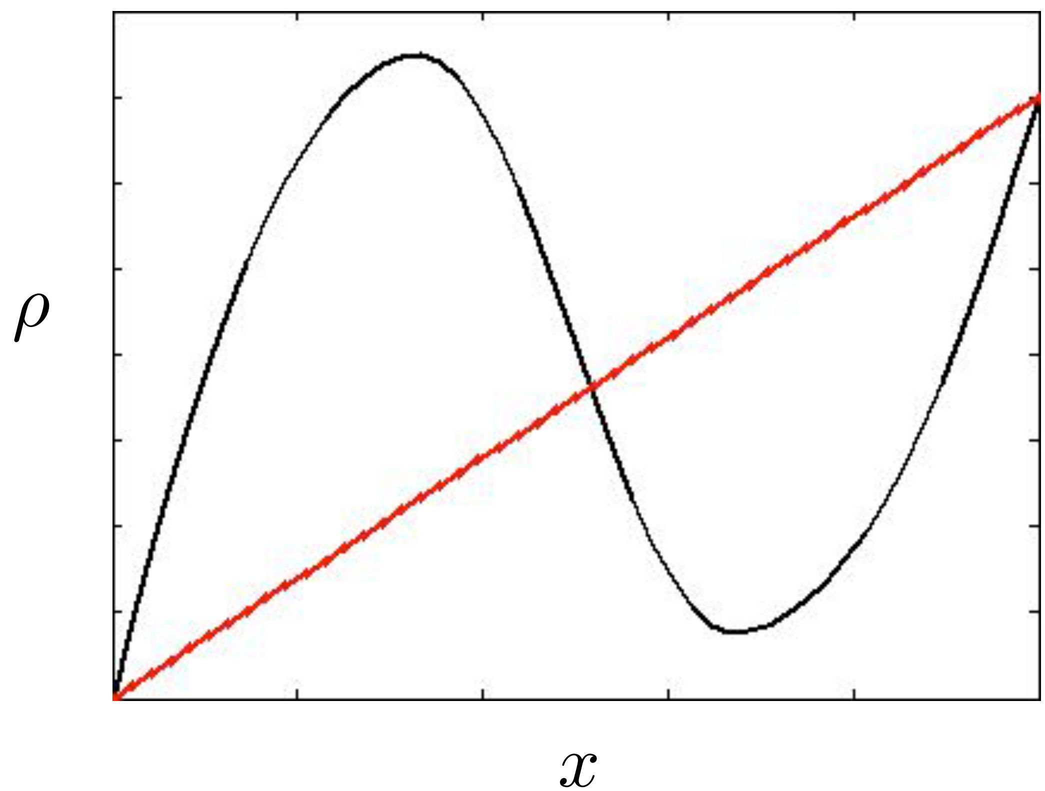
Bertini et. al. 2011 (infinite bulk drive)
Bunin, YK, Podosky 2012 (no bulk drive + rough conditions
+ structure of singularity)

Example:
Boundary Driven
Ising Model



Recall that find path that leads to configuration.

For this model find that sometimes there are
multiple
saddle point solutions



Some intuition why can have singularities in non-equilibrium

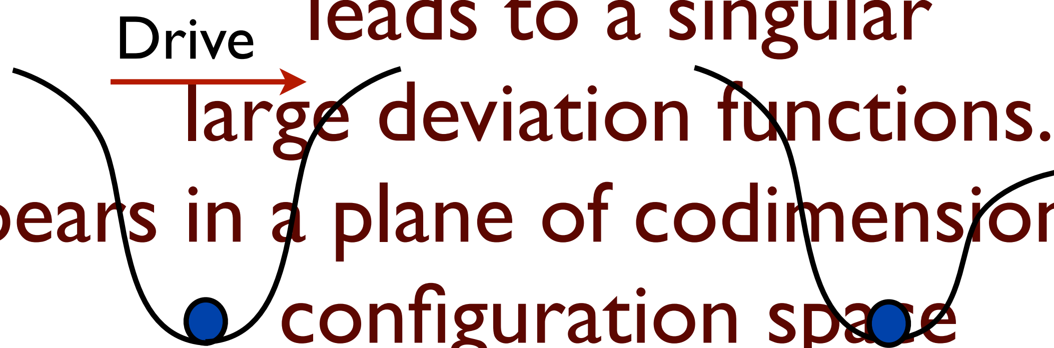
(warning mechanism very different!)

Biased Brownian walker periodic boundary conditions

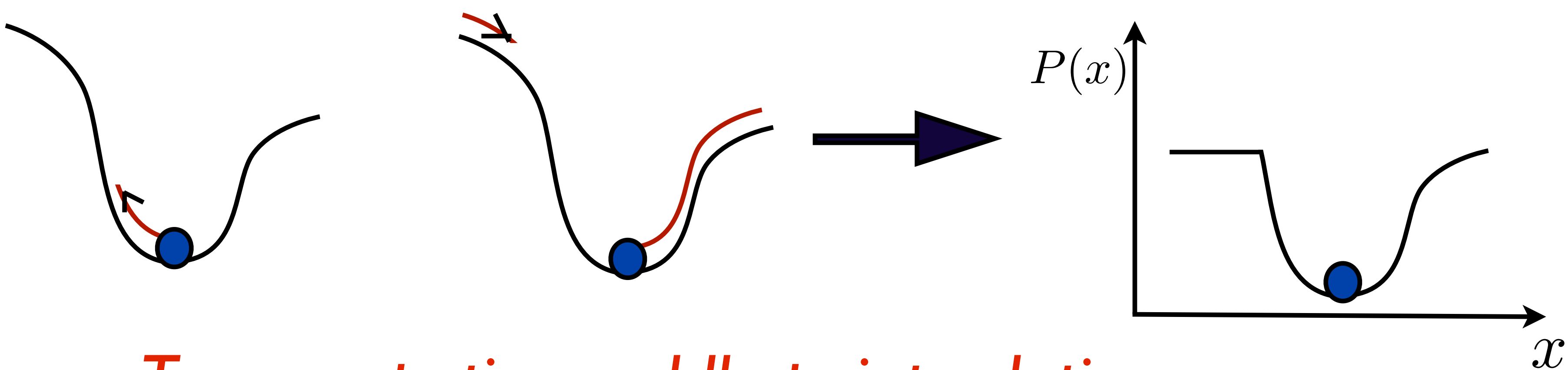
(large literature on low dimensional low noise - Graham, Tel, Dykman)

the occurrence of multiple paths leads to a singular large deviation functions.

Appears in a plane of codimension 1 in the configuration space with smooth equation parameters



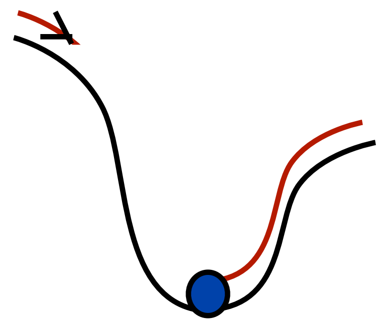
Most probably path



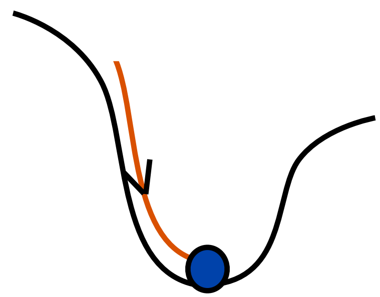
Two competing saddle point solutions

Note breaking of time reversal symmetry

Create fluctuation

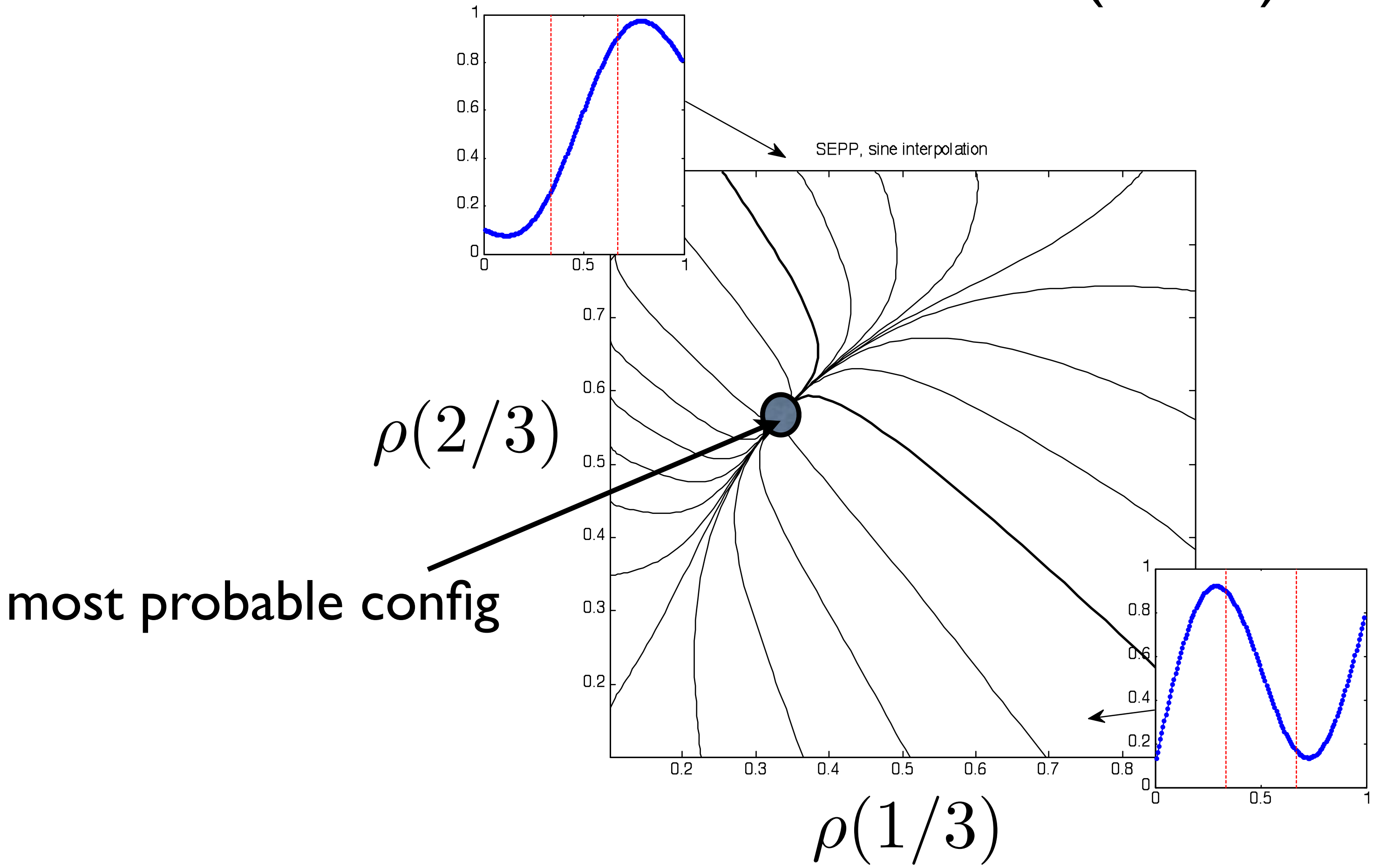


Relax from fluctuation



For diffusive fields this is true for all configurations (not just singular)

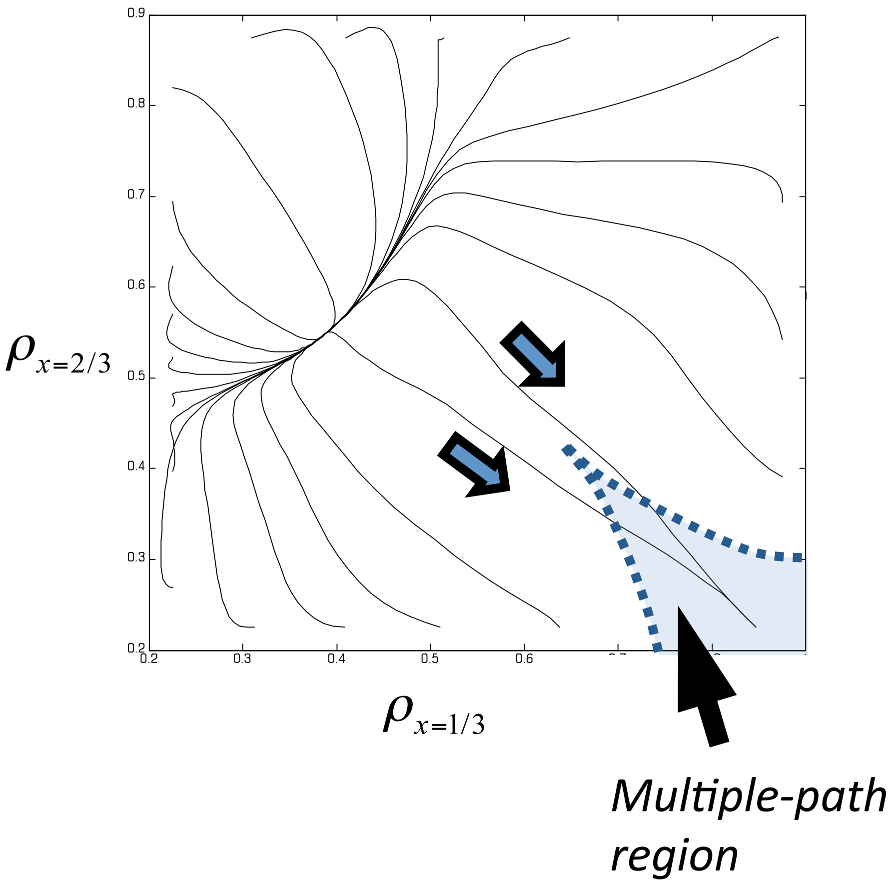
To see singularities look at 2d cross-sections first smooth case (SSEP)

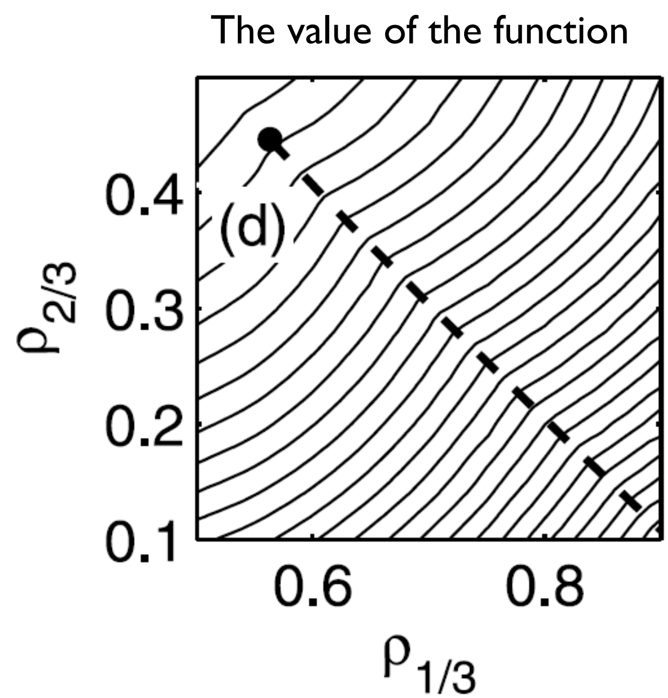


One history leading to every final configuration

$$\rho_f(x) = \bar{\rho}(x) + \alpha_1 \sin \pi x + \alpha_2 \sin 2\pi x$$

For boundary driven Ising model (2d cut)





Similar to first order line ending at ``critical point''

Bunin, YK, Podosky 2013

Motivated by similarities to critical phenomena look at order parameter

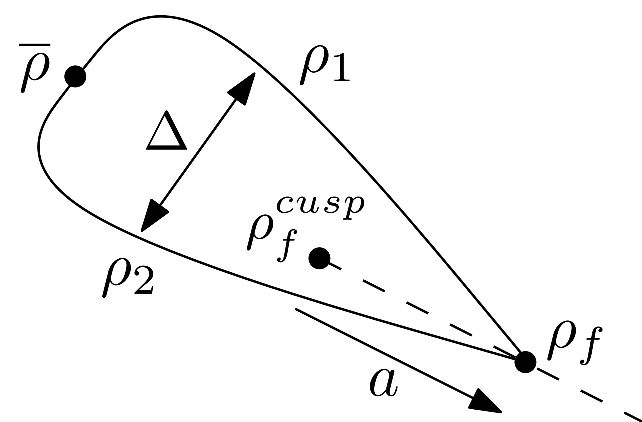
$$\Delta = \|\delta\rho\|$$

$$\|\delta\rho\|^2 = \int dx dt \left[\rho_2(x,t) - \rho_1(x,t)\right]^2$$

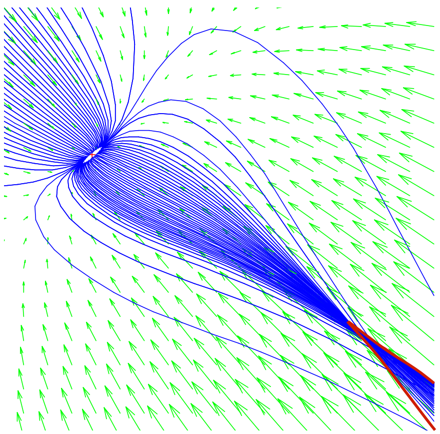
two locally minimizing histories

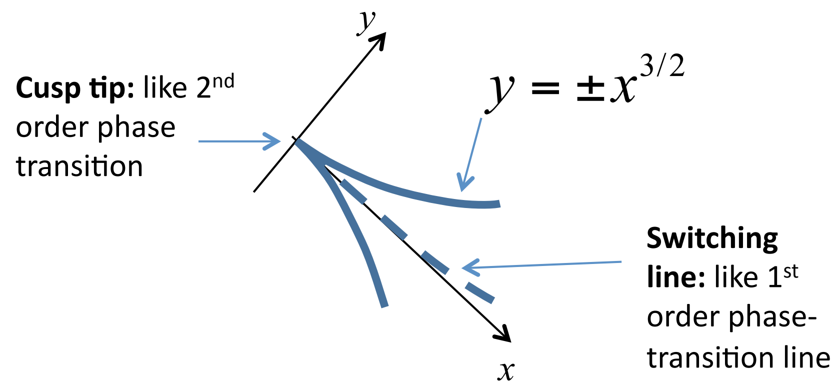
Can construct a Landau theory with \`$(T - T_c)/T_c$‘

$$a = \left(\int dx \left[\rho_f(x) - \rho_{crit}(x)\right]^2 \right)^{1/2}$$



Because have two solutions the structure of singularities given by a simple Ising Landau theory





$$e^{-N\phi(\rho_{cusp})+\frac{1}{4}\ln N}$$

universal model independent
(as long as singularity there)

Comments:

- Can show analytically that occurs also in model with

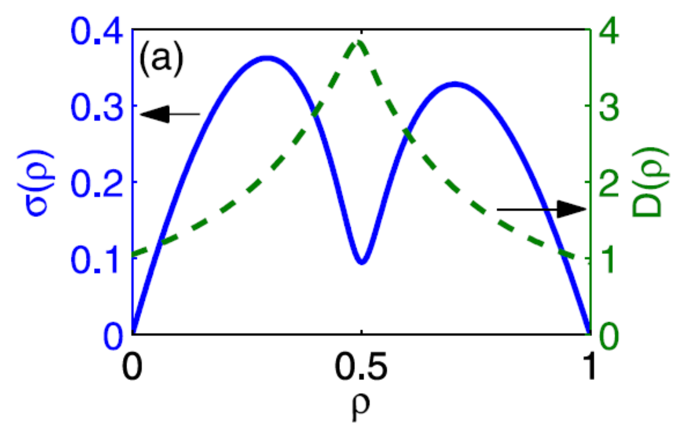
$$D = 1 \qquad\qquad \sigma(\rho) = a + c\rho^2$$

for $c > 0$

- For this model occurs for any non-equilibrium boundary conditions

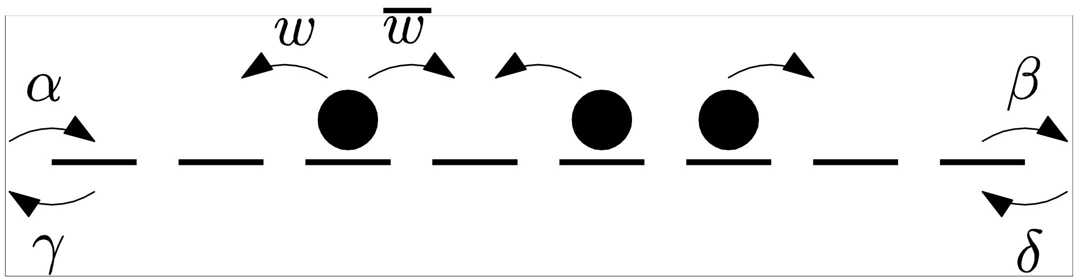
- For Boundary driven Ising model occurs only for large enough boundary drive $|\rho(1) - \rho(0)|$

For boundary driven appear when $\sigma(\rho)$ has a `deep enough' convex region



Natural question: Can you have more than two (locally minimizing) histories?

Weakly Asymmetric Simple Exclusion Process



same model as before but with non-symmetric rates

$$\overline{w} - w = \frac{E}{N}$$

Equation of motion

$$\partial_t \rho\left(x,t\right) + \partial_x J\left(x,t\right) = 0$$

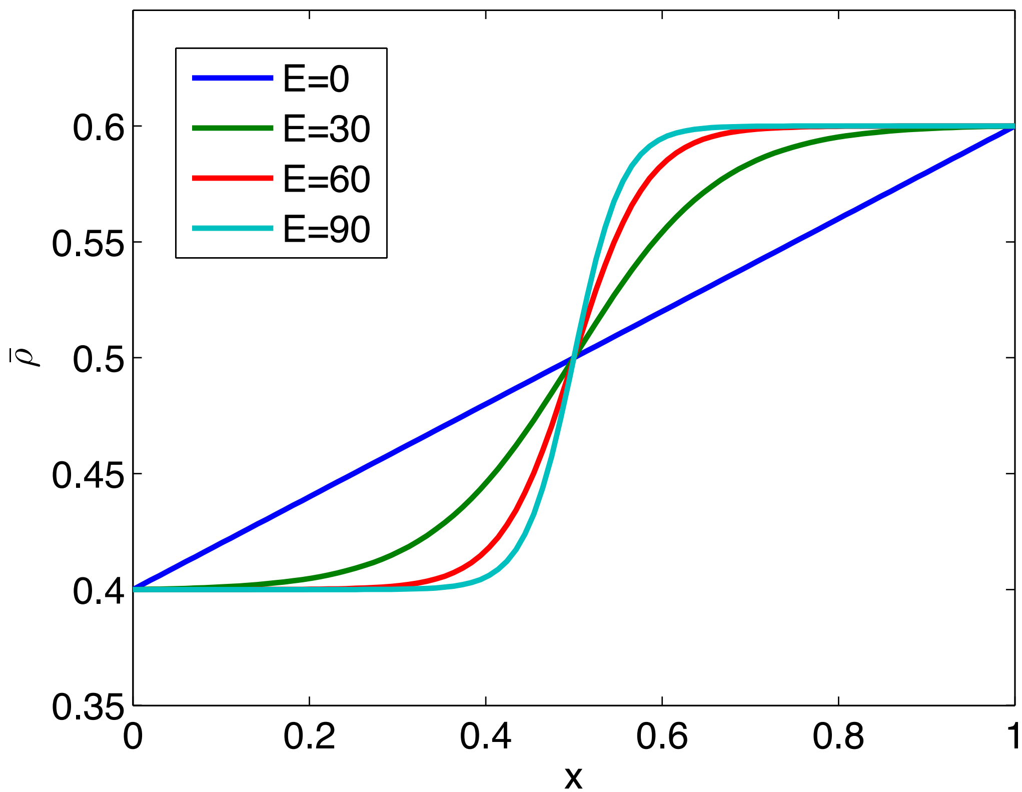
$$J\left(x,t\right) = -\frac{1}{2}\partial_x \rho\left(x,t\right) + \sigma\left(\rho\right)E + \sqrt{\sigma\left(\rho\right)}\eta\left(x,t\right).$$

$$\sigma\left(\rho\right) = \rho\left(1-\rho\right)$$

Bertini et. al. (2011) showed that in the infinite bias case (PASEP) there are singularities with two histories.
Structure was not discussed.

Steady-state Blythe et. al. 2000

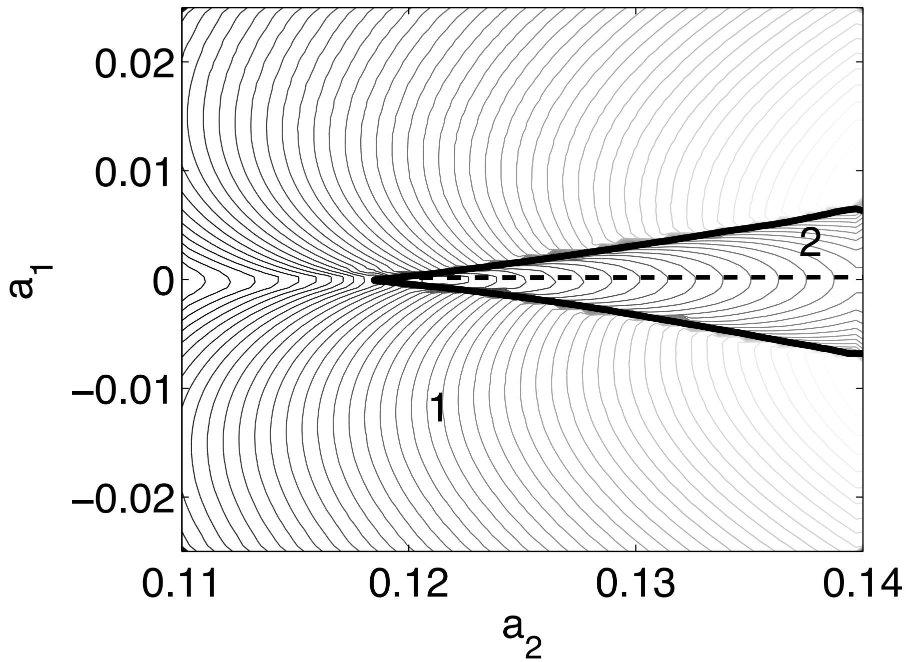
Most probable



Look at large deviations using cuts in configuration space
Take particle hole symmetric boundary conditions
(cleaner)

Small Field (think SSEP) smooth

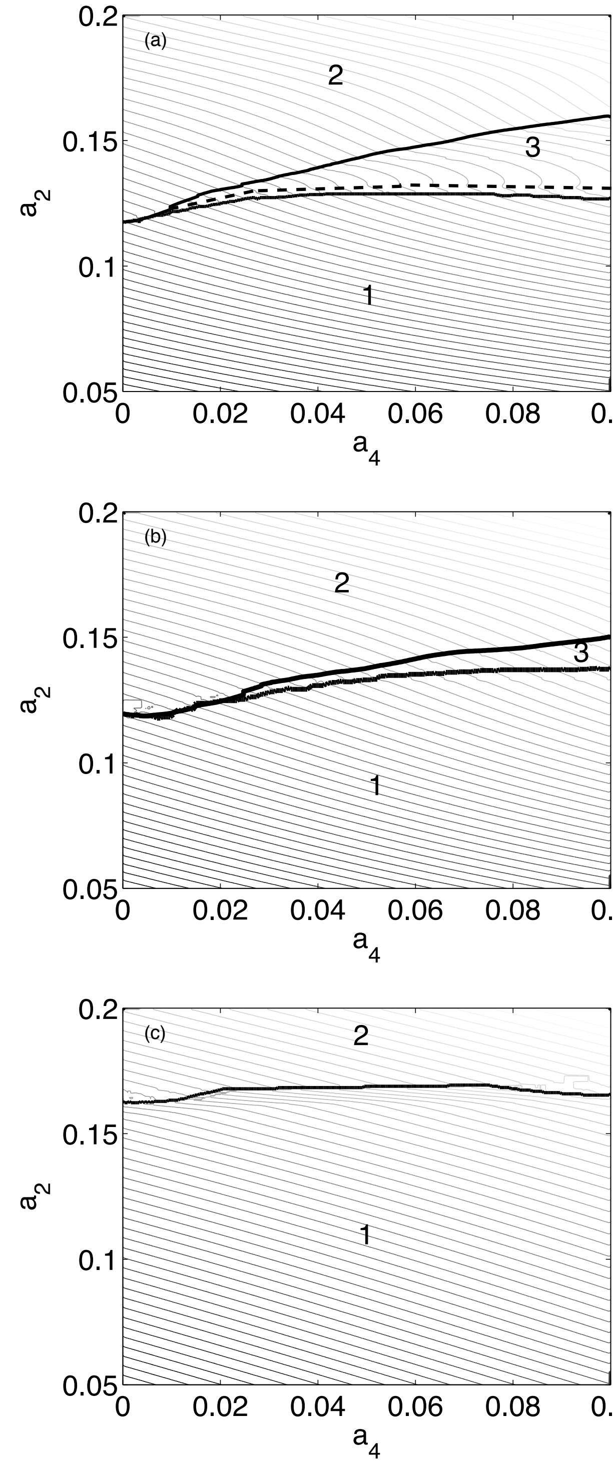
Larger field find cusp



$$\rho_f(x) = \bar{\rho}(x) + a_1 \sin(\pi x) + a_2 \sin(2\pi x) + a_4 \sin(4\pi x)$$

$$a_4 = 0$$

Increase field further and find tricritical analogues

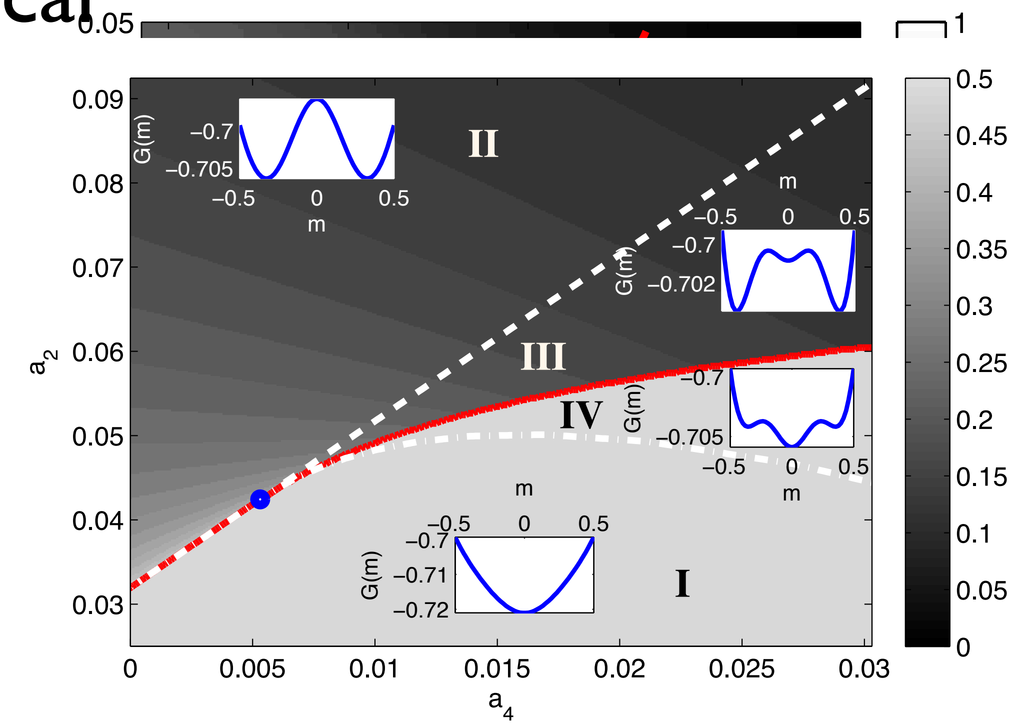


At infinite field (PASEP) can show analytically that there are configurations where s histories lead to the same configuration

MAP EXACTLY TO LANDAU THEORY

Cusp

Tricritical



Slightly different: Casimir Forces in Diffusive Systems

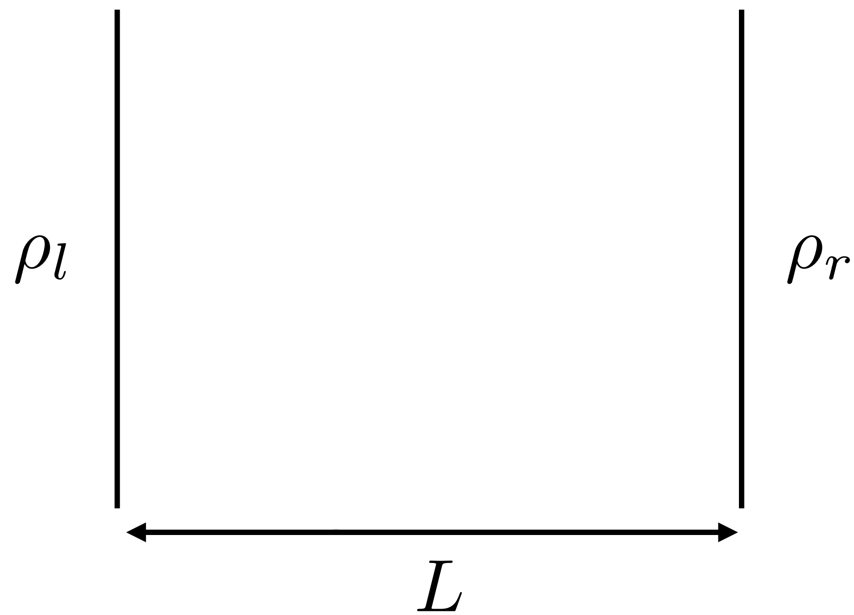
Recall generic long-range correlations

Many times presence of long ranged correlations associated with fluctuation induced forces

Casimir, Critical point (Fisher, de Gennes), Goldstone modes (Kardar et. al.)

Fluid dynamics case

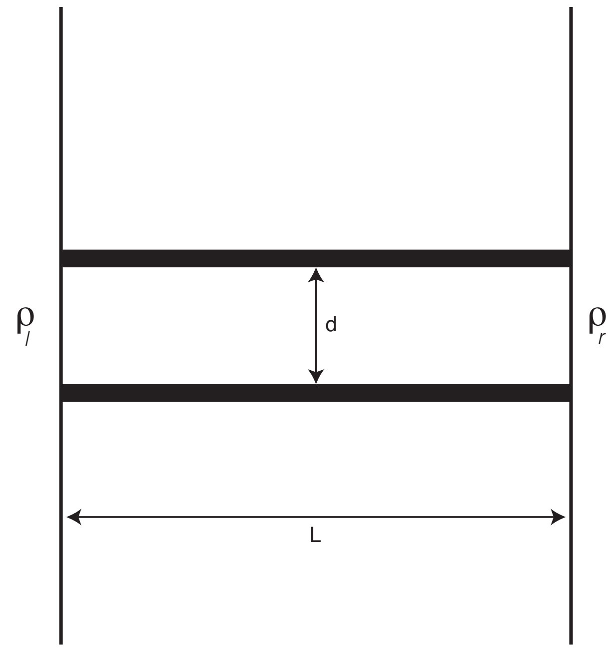
Pressure modification due to fluctuations in fluid dynamics shown by Kirkpatrick et. al, PRL (2013)



$$P \propto -k_B T (\nabla \rho)^2 L \times g(x)$$

vanishes at boundaries

Diffusive systems



Can calculate force between plates for simple models.
For hard core gas attractive (relatively small force)

$$F \propto -\frac{k_B T}{d}(\nabla\rho)^2 L^2$$

(YK, M. Kardar)

For other models can have repulsive

Note, absent at linear response level

Summary

1. Out of equilibrium large deviation functionals are both generically non-local due to long-range correlations and can be **singular**.
2. Well defined method to analyze singular structure, can classify.
3. Can roughly know which models are singular and which are not (no bulk bias)
4. Casimir like forces

1. Higher dimensions?
2. Systematic perturbation theory?
3. Is there an influence of the singularities on small fluctuations?
4. Approach to ordered phases?
5. Simple effective low dimensional models

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