Phase transitions and symmetry breaking in current distributions of diffusive systems

Vivien Lecomte

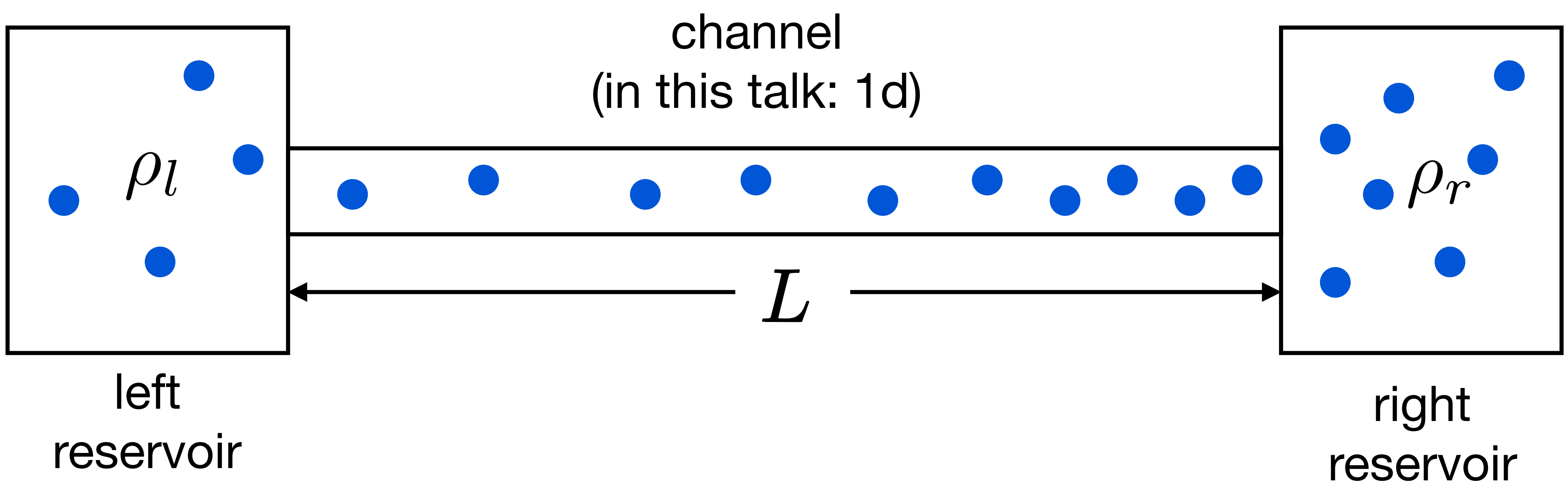
LIPhy, Grenoble-Alpes University, France

Yongjoo Baek (Technion -> Cambridge), Yariv Kafri (Technion)

PRL **118**, 030604 (2017)
arxiv: 1710.07139

Settings: **boundary**-driven diffusive systems

- Diffusive *interacting+conserving* channel (`**disordered**' phase - think gas)
- Channel connected to two reservoirs at given densities



Question: Consider current probability distribution

$P(J) \sim \exp[-TL\underline{\Phi(J)}]$ for large T and L

Large deviation function (LDF)

Here J is the time-averaged current

T the window of time over which we average

Are there cases where $\Phi(J)$ is singular?

[Dynamical Phase Transition (DPT)]

- Know to occur for driven-diffusive-systems with periodic boundary conditions

  WASEP 1D - Bodineau, Derrida, PRE **72**, 066110 (2005) Espigares et al., PRE **87**, 032115 (2013)
  WASEP 2D - Tizón-Escamilla *et al.*, arXiv:1606.07507
  KMP 1D - Bertini *et al.*, JSP **123**, 237 (2006), Hurtado, Garrido, PRL **107**, 180601 (2011)

- Suggested to be possible in boundary driven in Bertini *et al.*, PRL **94**, 030601 (2005)

  no microscopic model, scenario actually different

Answer: yes

- Two types of possible phase transitions:
  1. symmetry breaking (continuous)
  2. first-order

- Mechanism different from periodic boundary conditions

- Give general conditions for which models exhibit phase transitions

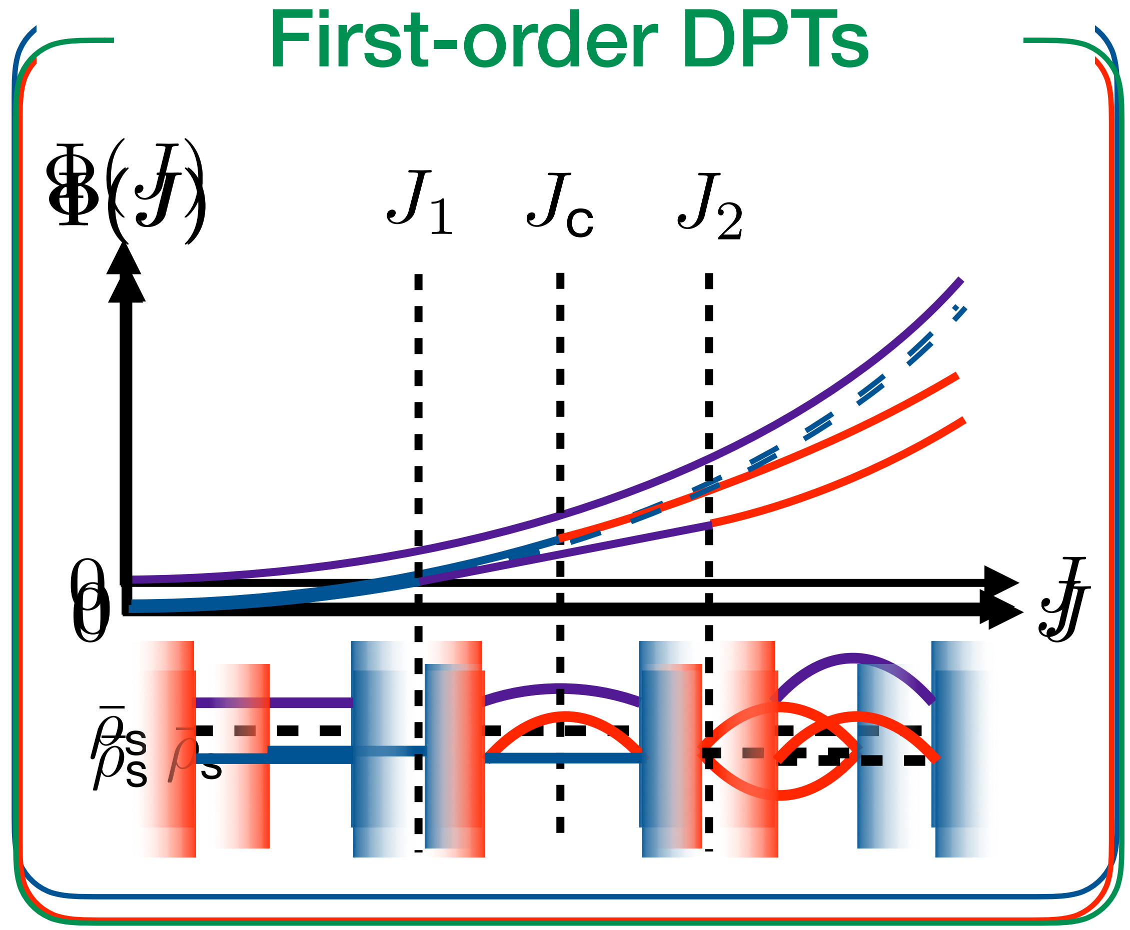
- Identify microscopic models

- Transitions occur even when system is in equilibrium
  (equal reservoir density, no bulk field - reversible dynamics)

Comment:

another mechanism identified in Shpielberg, Don, Akkermans, PRE **95**, 032137 (2017)

Cartoon of transition scenarios



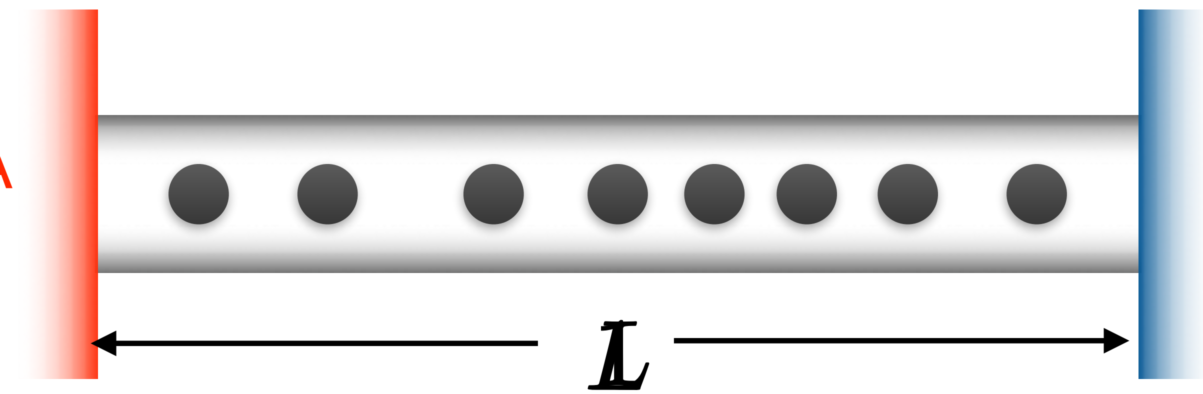
Outline

- Quick recap - formalism, some models, macroscopic fluctuation theory, ensembles, additivity principle.

- Perturbative description of transitions - develop a **Landau theory**

Results general for any model

The formalism



On large length scales : one characterizes the system by two linear-response quantities

Diffusivity $D(\rho)$ mobility $\sigma(\rho)$

which obey $\frac{2D(\rho)}{\sigma(\rho)} = f''(\rho)$ $f(\rho)$ - free-energy density

- After diffusive rescaling $i \to Lx, \quad t \to L^2 t$ the density field $\rho(x)$ obeys

$$\partial_t \rho = -\partial_x \left[\underbrace{-D(\rho)\, \partial_x \rho}_{\text{Diffusion}} + \underbrace{\sqrt{\sigma(\rho)}\, \eta}_{\text{Noise}} \right]$$

- The noise is weak in the thermodynamic limit $L \to \infty$

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

The generating function

- Instead of calculating $P(J) \sim \exp[-TL\Phi(J)]$ calculate the generating function

$$\langle e^{TL\lambda J} \rangle \sim \exp[TL\Psi(\lambda)]$$

where as usual $\Psi(\lambda) = \sup_J \left[\lambda J - \Phi(J)\right]$

- Using Martin-Siggia-Rose

$$\langle e^{TL\lambda J} \rangle \sim \int \mathcal{D}\rho\, \mathcal{D}\hat{\rho}_\lambda \, \exp\left\{ -L \int_0^T \mathrm{d}t \int_0^1 \mathrm{d}x \left[\hat{\rho}_\lambda \dot{\rho} - H(\rho, \hat{\rho}_\lambda)\right] \right\}$$

with

$$\rho(0,t) = \rho(1,t) = \bar{\rho}$$
$$\hat{\rho}_\lambda(0,t) = 0, \quad \hat{\rho}_\lambda(1,t) = \lambda$$

and the Hamiltonian $H(\rho, \hat{\rho}_\lambda) = -D(\rho)(\partial_x \rho)(\partial_x \hat{\rho}_\lambda) + \dfrac{\sigma(\rho)}{2}(\partial_x \hat{\rho}_\lambda)^2$

Large L so calculate saddle point:

$$\Psi(\lambda) = -\lim_{T\to\infty} \frac{1}{T} \inf_{\rho(t),\hat{\rho}_\lambda(t)} \int_0^T \mathrm{d}t \int_0^1 \mathrm{d}x \left[\hat{\rho}_\lambda \dot{\rho} - H(\rho,\hat{\rho}_\lambda)\right]$$

or solve (with boundary conditions) - note momentum related to noise

$$\partial_t \rho = \frac{\delta}{\delta \hat{\rho}_\lambda} \int_0^1 \mathrm{d}x\, H(\rho,\hat{\rho}_\lambda) = \partial_x \left[D(\rho)\partial_x \rho - \sigma(\rho)\partial_x \hat{\rho}_\lambda\right]$$

$$\partial_t \hat{\rho}_\lambda = -\frac{\delta}{\delta \rho} \int_0^1 \mathrm{d}x\, H(\rho,\hat{\rho}_\lambda) = -\partial_x \left[D(\rho)\partial_x \hat{\rho}_\lambda\right] - \frac{\sigma'(\rho)}{2} \left(\partial_x \hat{\rho}_\lambda\right)^2$$

Simplification - the solutions which minimize action are *time-independent*

= **additivity principle**

Bodineau, Derrida, PRL **92**, 180601 (2004)

$$\Psi(\lambda) = -\lim_{T\to\infty} \frac{1}{T} \inf_{\rho(t),\hat{\rho}_\lambda(t)} \int_0^T \mathrm{d}t \int_0^1 \mathrm{d}x \left[\hat{\rho}_\lambda \dot{\rho} - H(\rho,\hat{\rho}_\lambda)\right]$$

$$= \sup_{\rho,\hat{\rho}_\lambda} \int_0^1 \mathrm{d}x\, H(\rho,\hat{\rho}_\lambda)$$

Maximize energy

In sum -

To calculate the generating function

$$\langle e^{TL\lambda J}\rangle \sim \exp[TL\Psi(\lambda)]$$

Look for *time-independent solutions (with bc) of*

$$\partial_t \rho = \frac{\delta}{\delta \hat{\rho}_\lambda}\int_0^1 \mathrm{d}x\, H(\rho,\hat{\rho}_\lambda) = \partial_x\left[D(\rho)\partial_x\rho - \sigma(\rho)\partial_x\hat{\rho}_\lambda\right] \qquad = 0$$

$$\partial_t \hat{\rho}_\lambda = -\frac{\delta}{\delta \rho}\int_0^1 \mathrm{d}x\, H(\rho,\hat{\rho}_\lambda) = -\partial_x\left[D(\rho)\partial_x\hat{\rho}_\lambda\right] - \frac{\sigma'(\rho)}{2}\left(\partial_x\hat{\rho}_\lambda\right)^2 \qquad = 0$$

Result -

Typical density and noise profile which realize the fluctuations

We are focused on *looking for singularities* (when? where?)

Comments:

1. Prior to this work phase transitions in current large deviations were constrained to cases where the *additivity principle is broken*.
   (**non-stationary** optimal profile)

2. For continuous transition: one proves that the additivity principle holds

3. Condition for applicability of additivity principle to hold
   Shpielberg & Akkermans, PRL **116**, 240603 (2016)

Next - *Show that transitions can occur*

—> derive Landau theory for transitions

To make discussion easier break into different types:

- Symmetry breaking transitions (continuous)
- First order phase transitions
- For each case identify microscopic model

DERIVATION IN EQUILIBRIUM
THEN OUT OF EQUILIBRIUM

Note, transitions occur even in equilibrium
where, say, density large-deviation is smooth

Symmetry breaking phase transitions

To observe symmetry breaking transition need an underlying symmetry

Particle-Hole symmetry (about, say, $\rho = \bar{\rho} = 1/2$)

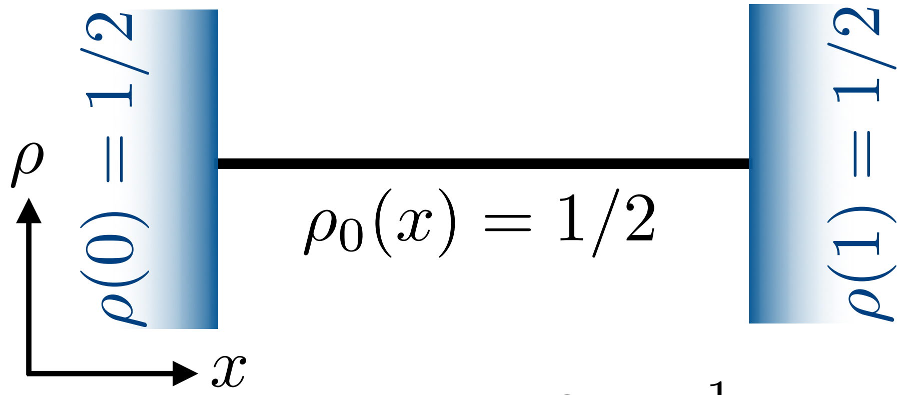
$$D(1/2 - \delta\rho) = D(1/2 + \delta\rho)$$

$$\sigma(1/2 - \delta\rho) = \sigma(1/2 + \delta\rho)$$

recall: consider boundary conditions
at equilibrium point

Consider possible solutions

One solution - symmetric profile (bc obey symmetry)



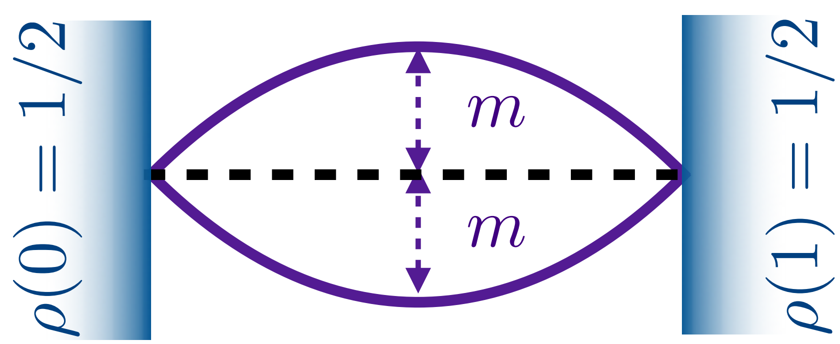
denote this solution

$$\rho_0(x), \hat{\rho}_{\lambda,0}(x)$$

$$\partial_t \rho = \frac{\delta}{\delta \hat{\rho}_\lambda} \int_0^1 \mathrm{d}x \, H(\rho, \hat{\rho}_\lambda) = \partial_x \left[D(\rho) \partial_x \rho - \sigma(\rho) \partial_x \hat{\rho}_\lambda \right]$$

$$\partial_t \hat{\rho}_\lambda = -\frac{\delta}{\delta \rho} \int_0^1 \mathrm{d}x \, H(\rho, \hat{\rho}_\lambda) = -\partial_x \left[D(\rho) \partial_x \hat{\rho}_\lambda \right] - \frac{\sigma'(\rho)}{2} \left(\partial_x \hat{\rho}_\lambda \right)^2$$

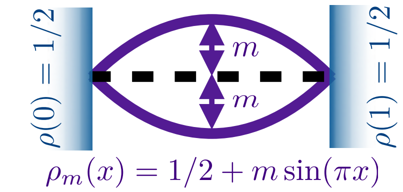
Near transition (if one occurs)
can imagine a deviation whose longest wave length component is



$$\rho_m(x) = 1/2 + m \sin(\pi x)$$

If they occur must be in pairs - *symmetry-breaking profiles*

denote this solution $\rho_m(x), \hat{\rho}_{\lambda,m}(x)$



With this in mind calculate

Landau theory (expansion in m, skipping details)

$$\mathcal{L}_\lambda(m) = \int_0^1 \mathrm{d}x\,[H(\rho_0, \hat{\rho}_{\lambda,0}) - H(\rho_m, \hat{\rho}_{\lambda,m})]$$

Then the scaled CGF

$$\Psi(\lambda) = \sup_{\rho,\hat{\rho}_\lambda} \int_0^1 \mathrm{d}x\, H(\rho, \hat{\rho}_\lambda) = \int_0^1 \mathrm{d}x\, H(\rho_0, \hat{\rho}_{\lambda,0}) - \inf_m \mathcal{L}_\lambda(m)$$

FIND TO LEADING ORDER

$$\mathcal{L}_\lambda(m) = -\frac{\lambda_c \bar{\sigma}''}{4}\,\delta\lambda\, m^2 + \frac{\pi^2 \bar{D}(4\bar{D}''\bar{\sigma}'' - \bar{D}\bar{\sigma}^{(4)})}{64\bar{\sigma}\bar{\sigma}''} m^4$$

$\delta\lambda = \lambda - \lambda_c$ and $\lambda_c = \pm\sqrt{\dfrac{2\pi^2 \bar{D}}{\bar{\sigma}\bar{\sigma}''}}$

To have transition

Condition 1 $\bar{\sigma}'' > 0$

Condition 2 $4\bar{D}''\bar{\sigma}'' > \bar{D}\bar{\sigma}^{(4)}$

TO HAVE A TRANSITION NEED A MODEL WITH A LOCAL MINIMUM IN σ

Recap -

Landau theory shows a symmetry-breaking transitions when

1. Particle-hold symmetry (in b.c. and model)

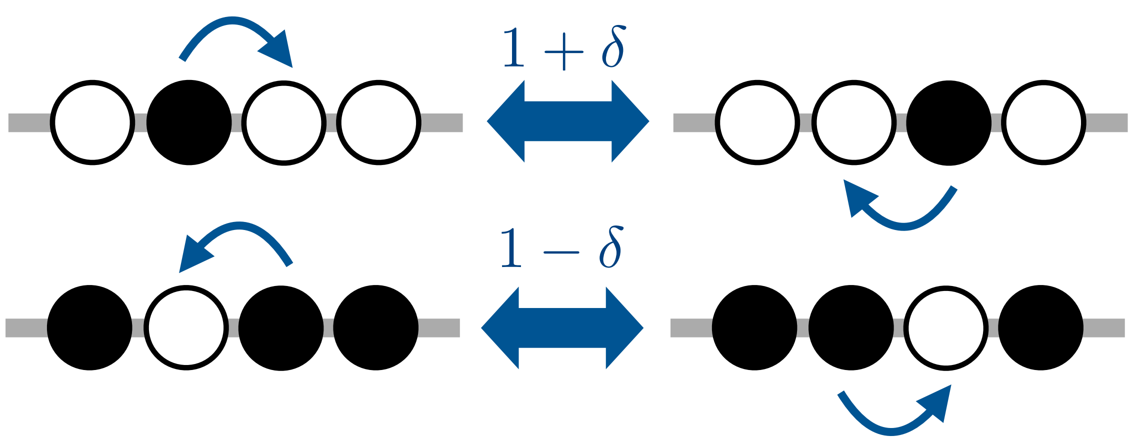
2. mobility σ at this point has a local minimum

Microscopic model

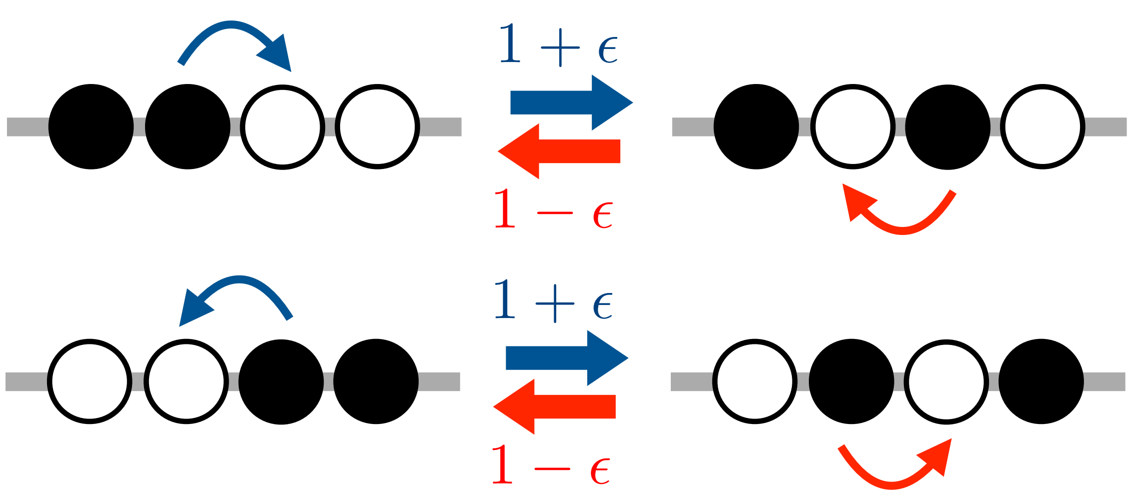
KLS model

Katz, Lebowitz, Spohn, JSP (1984)

Microscopic dynamics

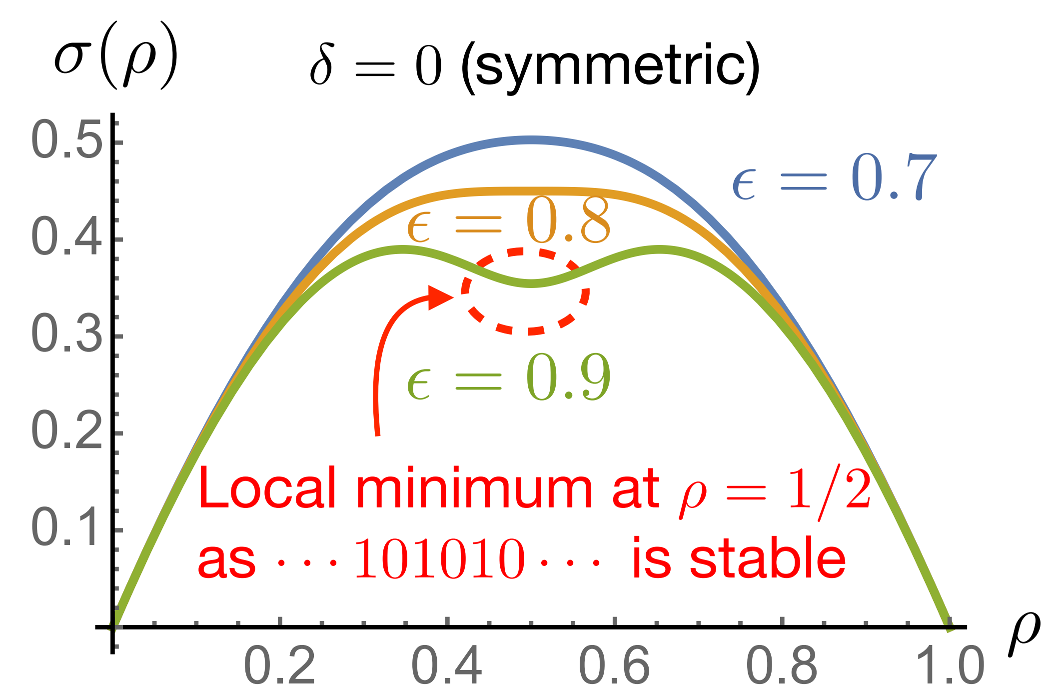


$\delta > 0:$ Particles faster than holes



$\epsilon > 0:$ Short-range repulsion

Transport coefficients

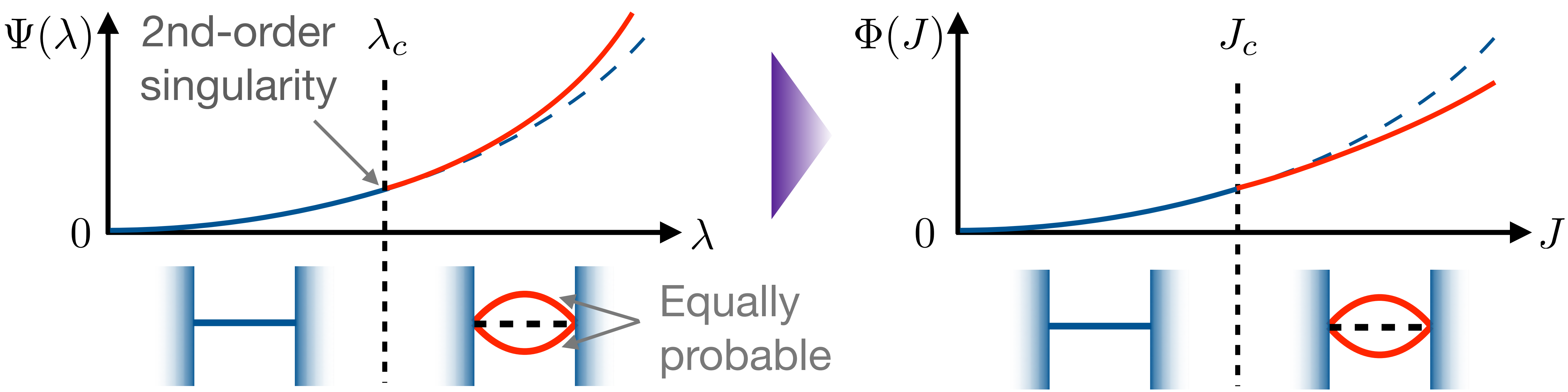


Hager et al., PRE **63**, 056110 (2001); Krapivsky (unpublished)

SUMMARY OF SYMMETRY BREAKING TRANSITION

- System with local minimum of σ at `symmetric' point $\bar{\rho}$
- Up to now in equilibrium
- Results unchanged to leading order for boundary conditions

$$\rho(0) = 1/2 + \delta\rho \qquad \rho(1) = 1/2 - \delta\rho$$



First order phase transitions

Now - models with **no particle-hole symmetry**
again **in equilibrium at minimum of σ**

Landau theory (exactly along the lines outlined before)

$$\mathcal{L}_\lambda(m) = -\frac{\lambda_c \bar{\sigma}''}{4}\,\delta\lambda\, m^2 - \frac{2\pi \bar{D}(\bar{D}\bar{\sigma}^{(3)} - 3\bar{D}'\bar{\sigma}'')}{9\bar{\sigma}\bar{\sigma}''} m^3 + \frac{\pi^2 \bar{D}(4\bar{D}''\bar{\sigma}'' - \bar{D}\bar{\sigma}^{(4)})}{64\bar{\sigma}\bar{\sigma}''} m^4$$

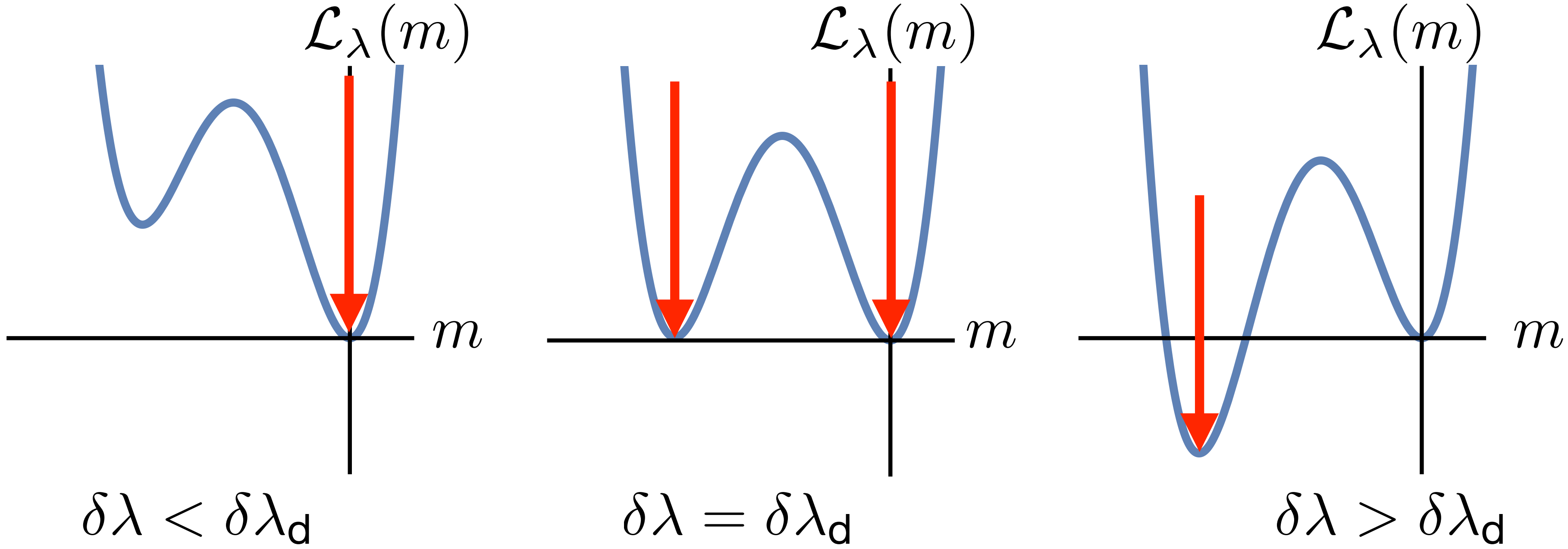
To have transition

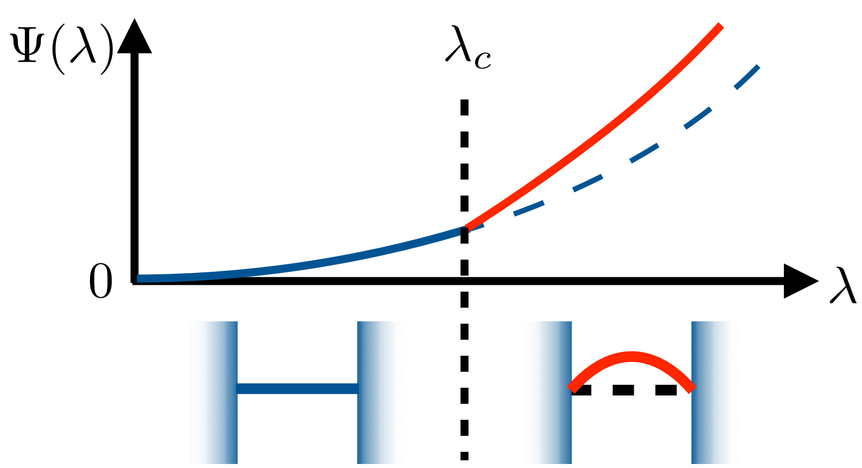
Condition 1 $\bar{\sigma}'' > 0$

Condition 2 $\bar{D}\bar{\sigma}^{(3)} \neq 3\bar{D}'\bar{\sigma}''$

Condition 3 $4\bar{D}''\bar{\sigma}'' > \bar{D}\bar{\sigma}^{(4)}$

$$\mathcal{L}_\lambda(m) = -\frac{\lambda_c \bar{\sigma}''}{4}\,\delta\lambda\, m^2 - \frac{2\pi \bar{D}(\bar{D}\bar{\sigma}^{(3)} - 3\bar{D}'\bar{\sigma}'')}{9\bar{\sigma}\bar{\sigma}''} m^3 + \frac{\pi^2 \bar{D}(4\bar{D}''\bar{\sigma}'' - \bar{D}\bar{\sigma}^{(4)})}{64\bar{\sigma}\bar{\sigma}''} m^4$$



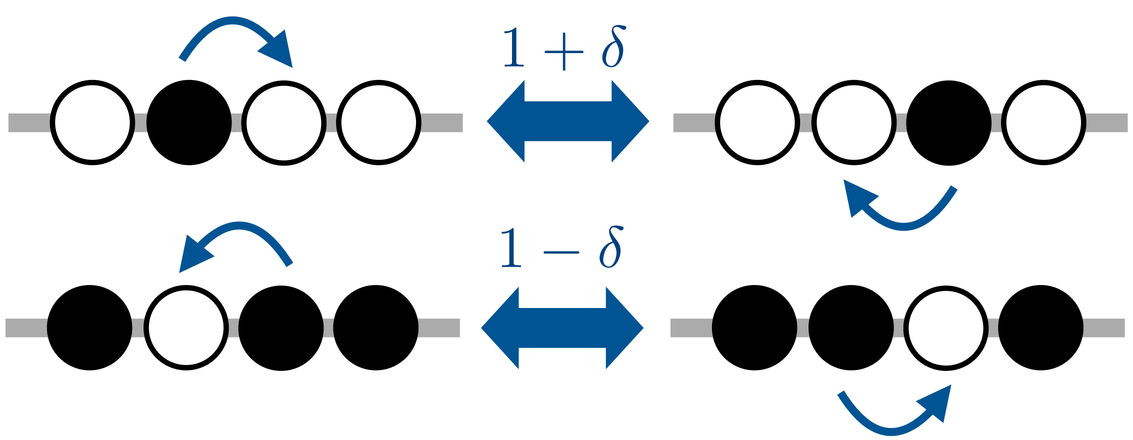


Microscopic model

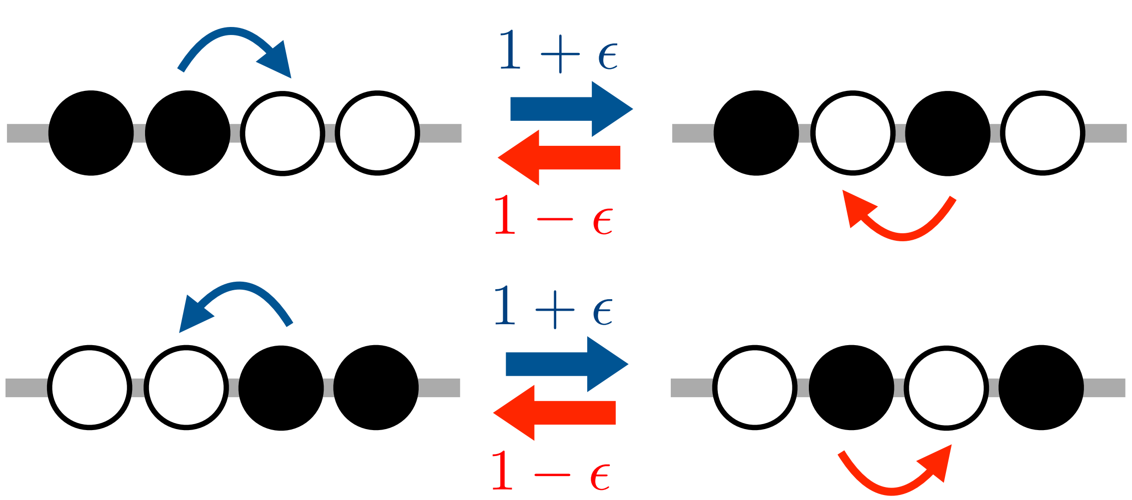
KLS model

Katz, Lebowitz, Spohn, JSP (1984)

Microscopic dynamics

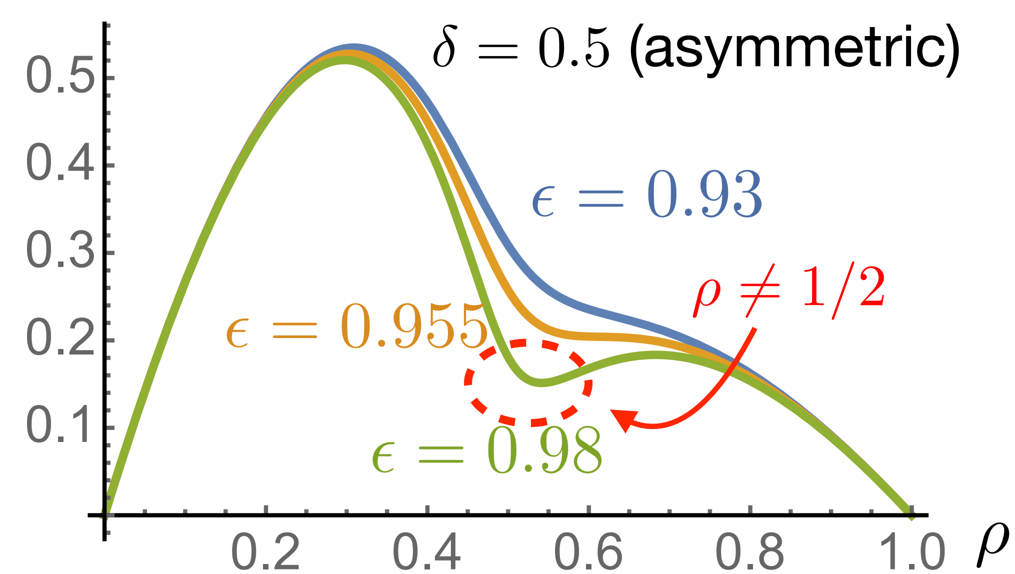


$\delta > 0$: Particles faster than holes



$\epsilon > 0$: Short-range repulsion

Transport coefficients

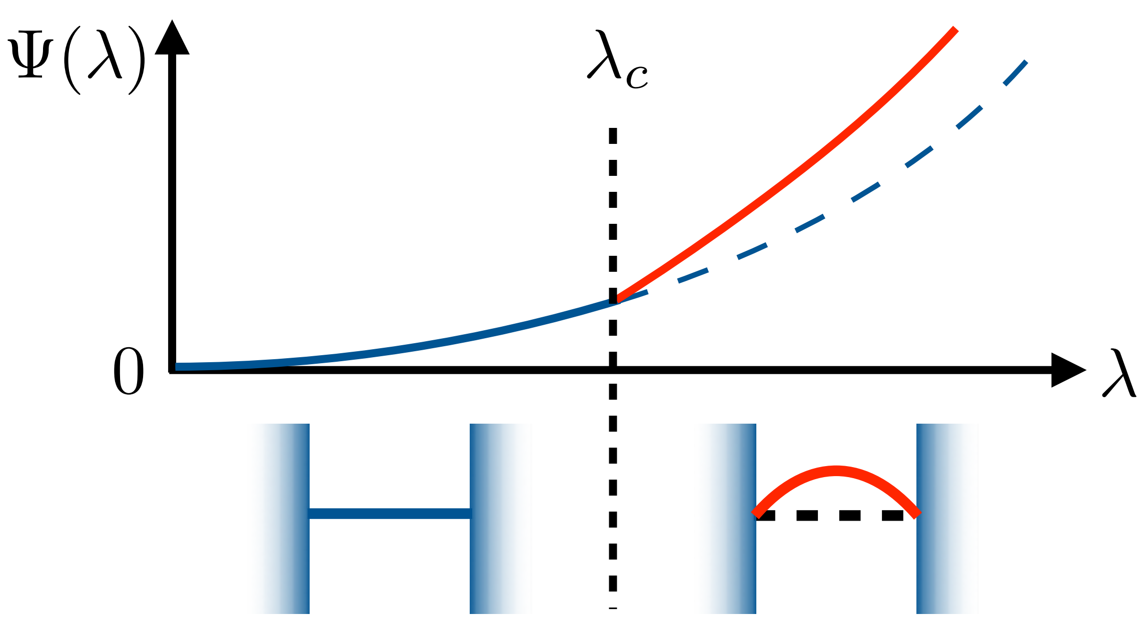


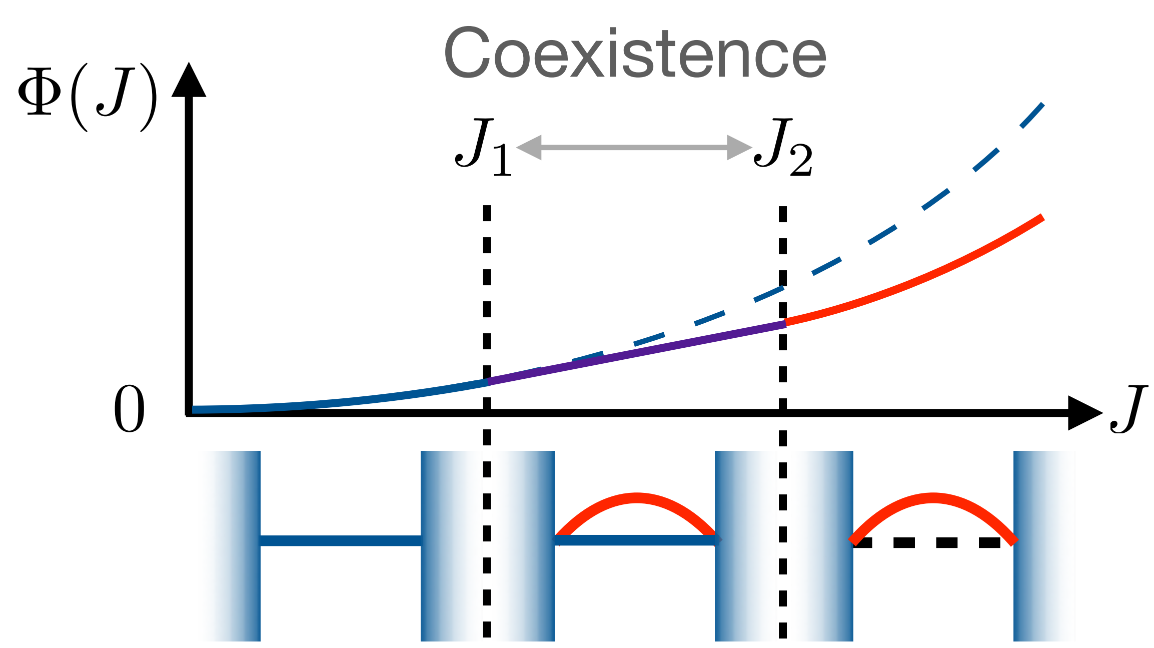
Hager et al., PRE **63**, 056110 (2001); Krapivsky (unpublished)

SUMMARY OF FIRST ORDER TRANSITIONS

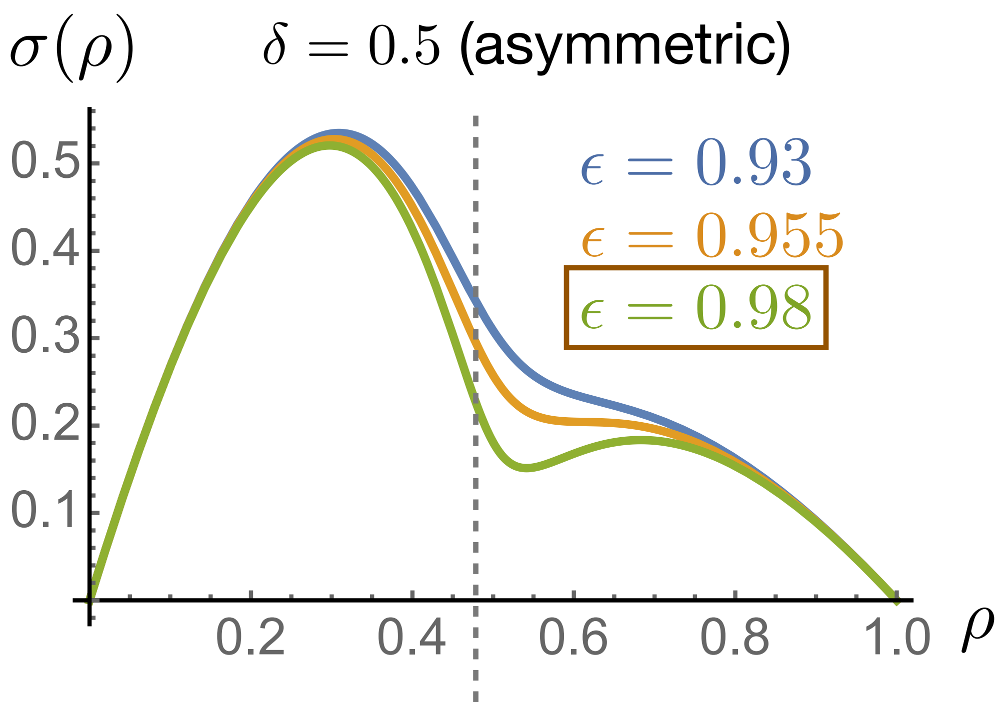
- System with local minima of σ at `symmetric' point $\bar{\rho}$
- Up to now in equilibrium
- Results unchanged to leading order for boundary conditions

$$\rho(0) = 1/2 + \delta\rho \qquad \rho(1) = 1/2 - \delta\rho$$





What happens when not at minima of σ ?



$$\rho(0) = \rho(1) = \bar{\rho} \neq 1/2$$

$$\bar{\sigma}' \neq 0$$

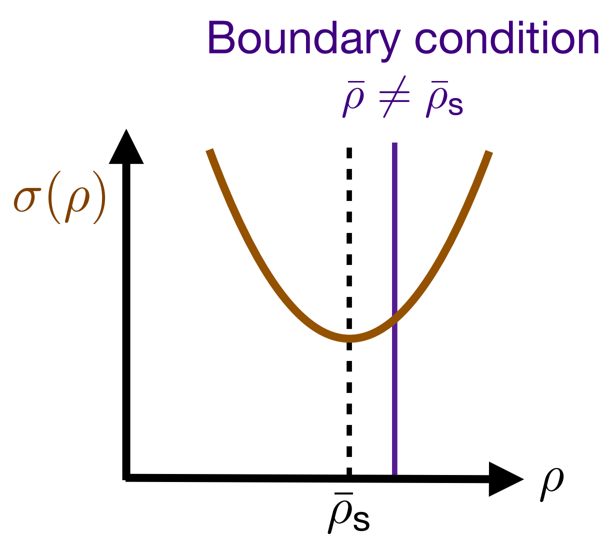
Landau theory

$$\mathcal{L}_\lambda(m) = \boxed{-\frac{2\pi \bar{D}^2}{\bar{\sigma}\bar{\sigma}''}\bar{\sigma}' m} - \frac{\lambda_c \bar{\sigma}''}{4}\,\delta\lambda\, m^2 - \frac{2\pi \bar{D}(\bar{D}\bar{\sigma}^{(3)} - 3\bar{D}'\bar{\sigma}'')}{9\bar{\sigma}\bar{\sigma}''} m^3 + \frac{\pi^2 \bar{D}(4\bar{D}''\bar{\sigma}'' - \bar{D}\bar{\sigma}^{(4)})}{64\bar{\sigma}\bar{\sigma}''} m^4$$

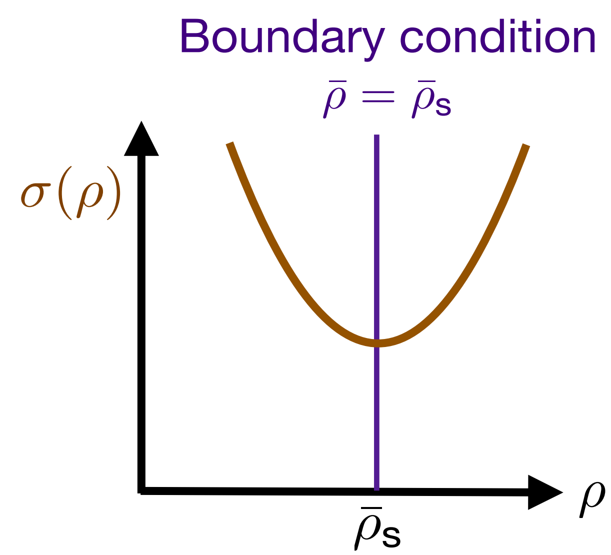
σ' **acts as a `magnetic-field' killing the transitions**

SUMMARY UP TO HERE

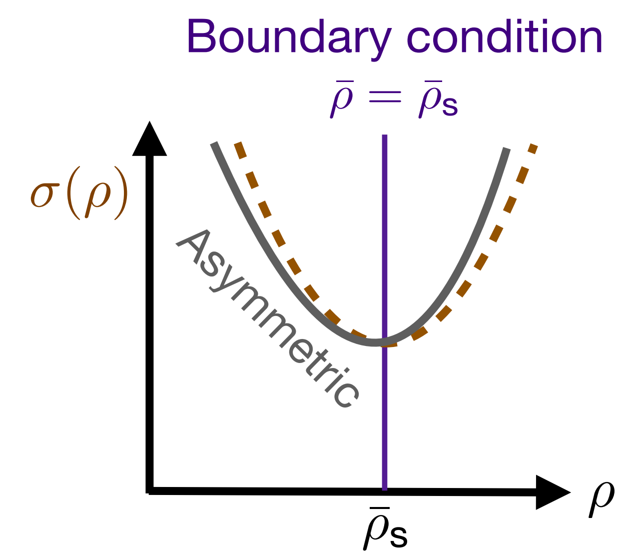
No DPTs



Symmetry breaking



First-order DPTs

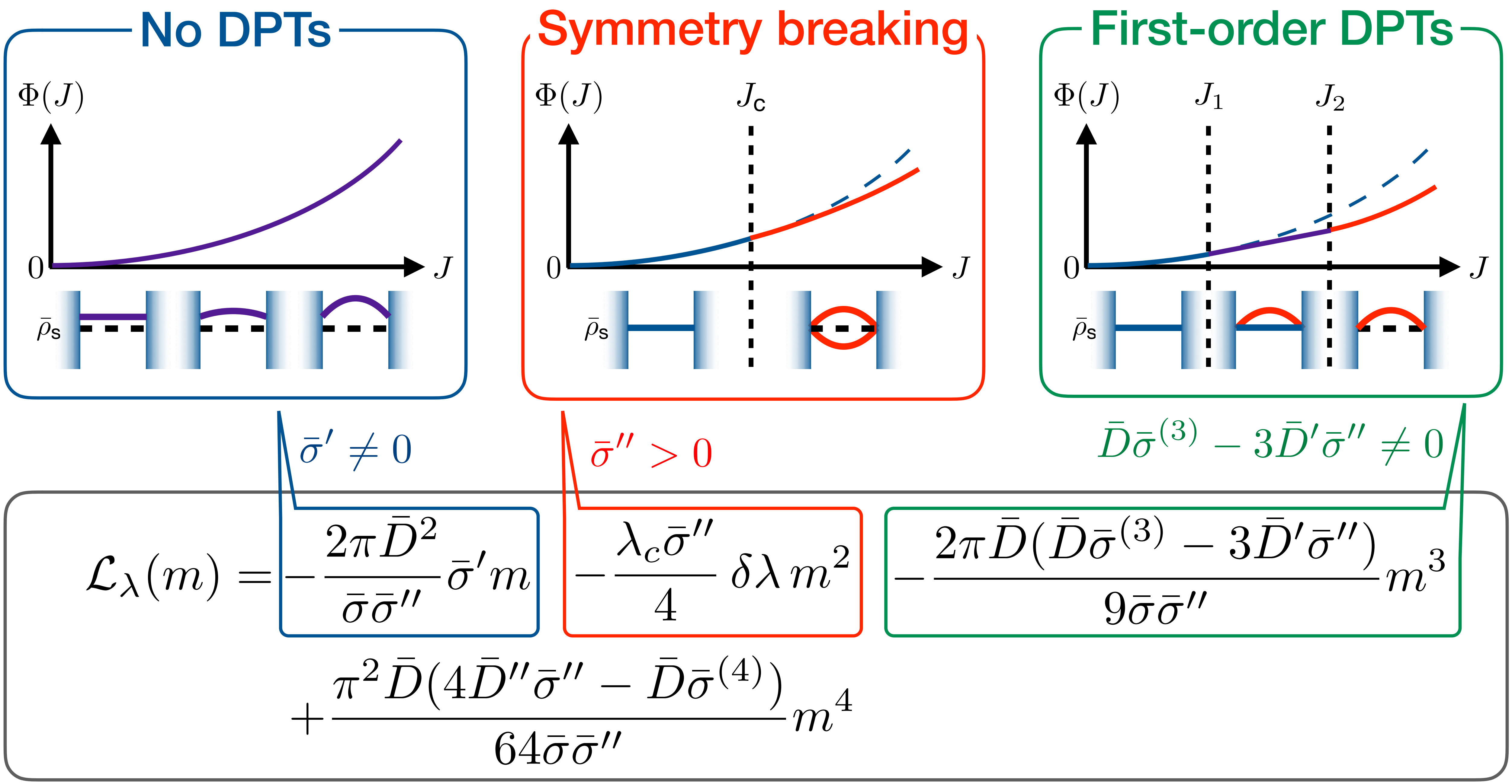


$\bar\sigma' \neq 0$

$\bar\sigma'' > 0$

$\bar D\bar\sigma^{(3)} - 3\bar D'\bar\sigma'' \neq 0$

$$\mathcal{L}_\lambda(m) = -\frac{2\pi\bar D^2}{\bar\sigma\bar\sigma''}\bar\sigma' m - \frac{\lambda_c\bar\sigma''}{4}\delta\lambda\, m^2 - \frac{2\pi\bar D(\bar D\bar\sigma^{(3)} - 3\bar D'\bar\sigma'')}{9\bar\sigma\bar\sigma''}m^3 + \frac{\pi^2\bar D(4\bar D''\bar\sigma'' - \bar D\bar\sigma^{(4)})}{64\bar\sigma\bar\sigma''}m^4$$



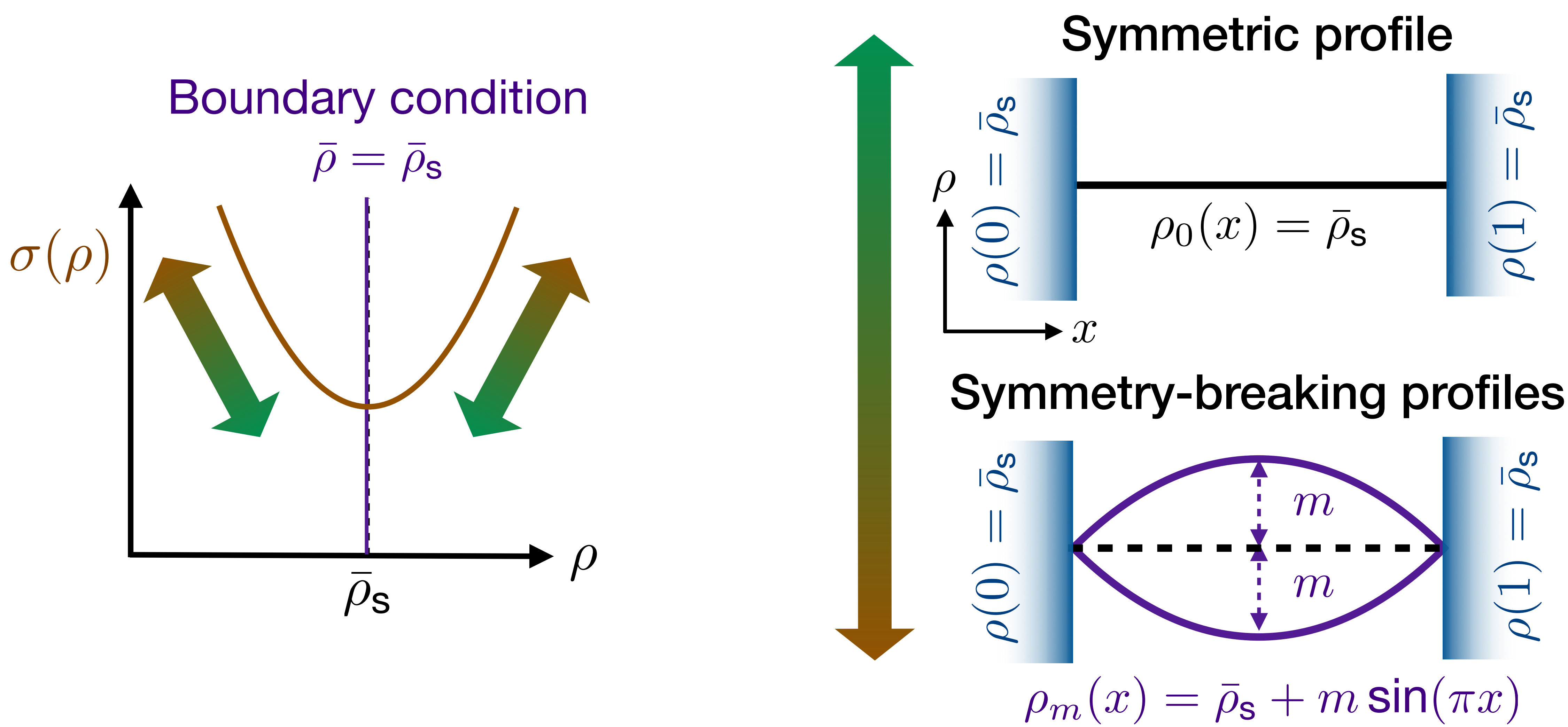
No DPTs
Symmetry breaking
First-order DPTs
$\Phi(J)$
J_c
J_1
J_2
0
J
$\bar{\rho}_s$
$\bar{\sigma}' \neq 0$
$\bar{\sigma}'' > 0$
$\bar{D}\bar{\sigma}^{(3)} - 3\bar{D}'\bar{\sigma}'' \neq 0$
$\mathcal{L}_\lambda(m) = -\frac{2\pi \bar{D}^2}{\bar{\sigma}\bar{\sigma}''}\bar{\sigma}' m - \frac{\lambda_c \bar{\sigma}''}{4}\delta\lambda\, m^2 - \frac{2\pi\bar{D}(\bar{D}\bar{\sigma}^{(3)} - 3\bar{D}'\bar{\sigma}'')}{9\bar{\sigma}\bar{\sigma}''}m^3 + \frac{\pi^2\bar{D}(4\bar{D}''\bar{\sigma}'' - \bar{D}\bar{\sigma}^{(4)})}{64\bar{\sigma}\bar{\sigma}''}m^4$

Physical Intuition

$$\partial_t \rho = -\partial_x \left[-D(\rho)\,\partial_x \rho + \sqrt{\sigma(\rho)}\,\eta \right]$$

Diffusion favors flat profile

High J is easier if $\sigma(\rho)$ is high



Lagrangian picture

$$\Phi(J) = \inf_{\rho} \int_0^1 \mathrm{d}x \, \frac{[J + D(\rho)\partial_x \rho - \sigma(\rho)E]^2}{2\sigma(\rho)} \, .$$

Expand in m

$$\Phi(J) \simeq \frac{\delta J^2}{2\bar{\sigma}} + \inf_{m} \left[\left(\frac{\bar{D}^2}{2} - \frac{\bar{\sigma}'' \, \delta J^2}{4\bar{\sigma}} \right) m^2 + O(m^4) \right]$$

numerator **denominator**

With $\delta J \equiv J - \bar{\sigma} E$

DENOMINATOR WINS FOR LARGE ENOUGH δJ

Effect of Bulk Field

So far the possibility of a bulk field (with diffusive scaling) was ignored.

Including a bulk field gives the following dynamical equation for the density

$$\partial_t \rho = -\partial_x \left[-D(\rho)\, \partial_x \rho + \sqrt{\sigma(\rho)}\, \eta + \sigma(\rho) E \right]$$

REPEAT SAME ANALYSIS AS BEFORE

Landau theory

$$\mathcal{L}(m) \simeq -\frac{2\pi \bar{D}^2}{\bar{\sigma}\bar{\sigma}''}\,\bar{\sigma}'\,m - \frac{(\lambda_c + E)\bar{\sigma}''}{4}\,\delta\lambda\,m^2 - \frac{2\pi\bar{D}(\bar{D}\bar{\sigma}^{(3)} - 3\bar{D}'\bar{\sigma}'')}{9\bar{\sigma}\bar{\sigma}''}\,m^3$$
$$+ \left[\frac{\pi^2\,\bar{D}\left(4\bar{D}''\bar{\sigma}'' - \bar{D}\bar{\sigma}^{(4)}\right)}{64\bar{\sigma}\bar{\sigma}''} + \frac{\bar{\sigma}''^2\,E^2}{64\bar{\sigma}}\right] m^4\,.$$

As long as $\bar{\sigma}' = 0$ even if not sitting at minima of σ

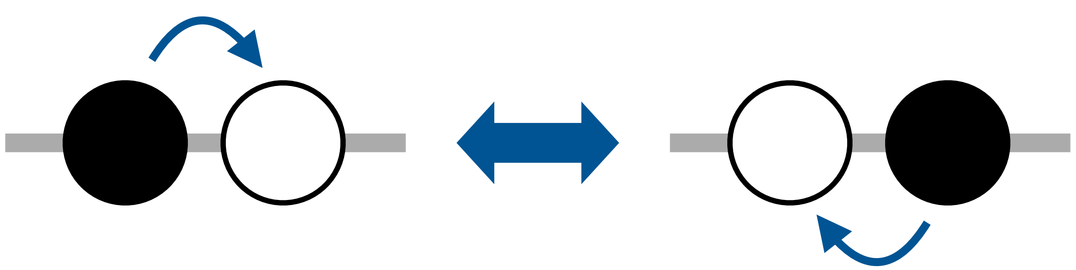
for large enough field E ***have a transition***

Microscopic model

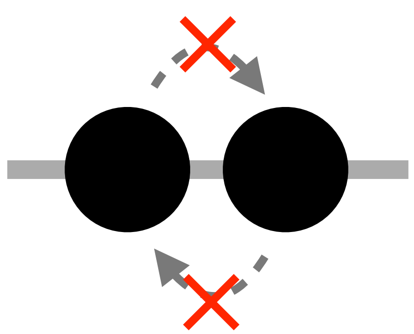
WASEP

Microscopic dynamics

Symmetric random walk



Exclusion

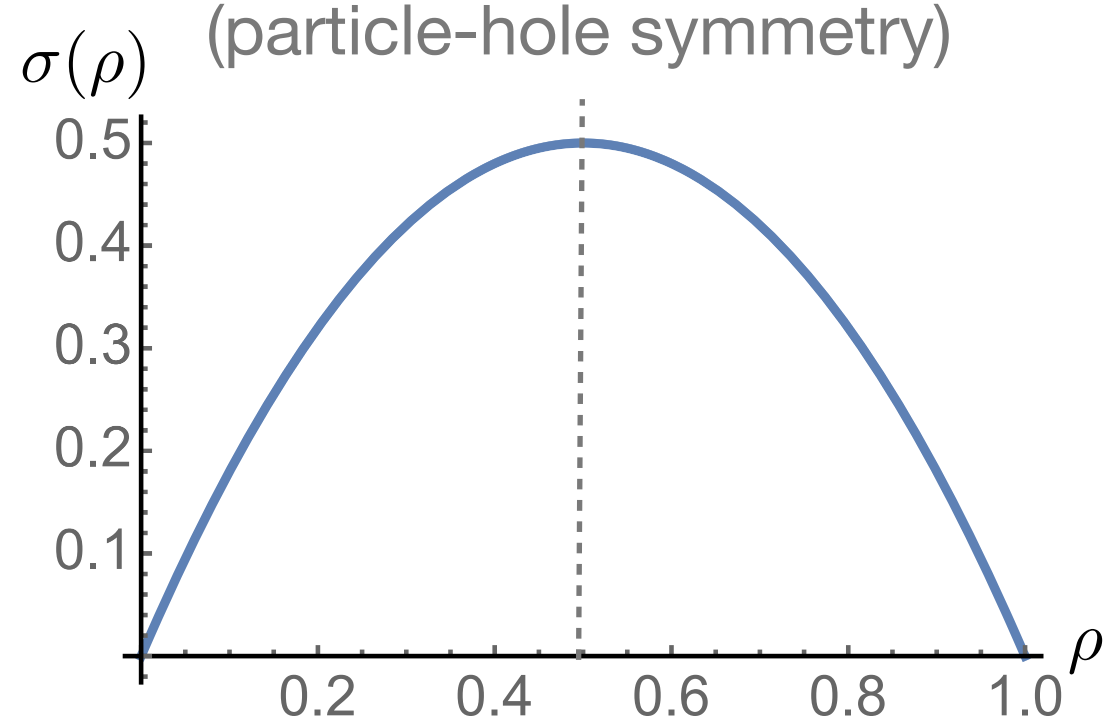


Transport coefficients

$$D(\rho) = 1$$

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

Symmetric w.r.t.
$\rho - 1/2 \to 1/2 - \rho$
(particle-hole symmetry)



SUMMARY

- Current LDF of boundary driven diffusive systems can have singularities
- Identified models for difference scenarios - 1st, 2nd order
- Transitions *not* associated with breaking of additivity principle

QUESTIONS

- Transition in boundary-driven which breaks additivity?
- Finite-size and finite-time behaviour?
  (intermittency between coexisting profiles)
- Spatially discrete systems?