Computation of transition trajectories and rare events in nonequilibrium statistical physics

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Universality of large deviations in diffusive systems

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Outline

Diffusive systems, with examples

Questions about rare events

Technical know-how

Message 1 : universality of large deviations

Message 2 : existence of phase transitions

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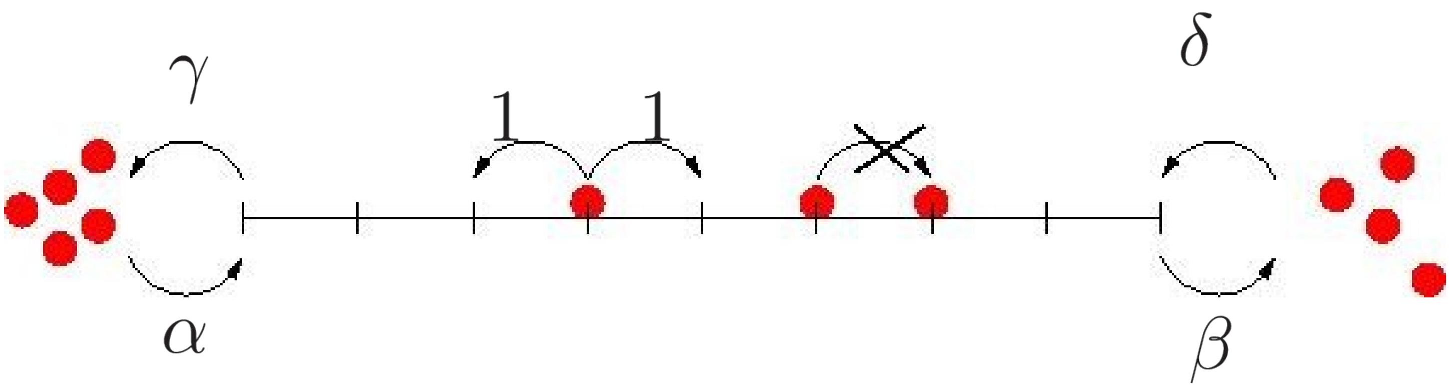
Diffusive systems : example 1

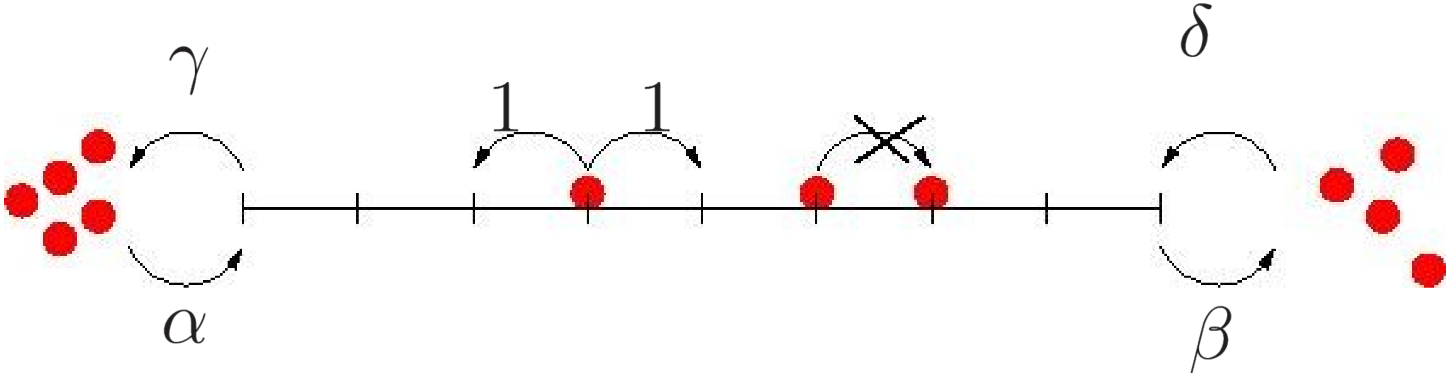
Simple symmetric exclusion process



$$n_j = 0 \text{ or } 1, \quad j = 1, \ldots, L$$

Diffusive systems : example 1

Simple symmetric exclusion process



$$\frac{\alpha}{\gamma} = \text{fugacity}$$

Diffusive systems

Coarse grained description

Space scale of the system size $x = j/L \in [0,1]$
Time scale of the diffusiion time $\tau = t'/L^2 \in [0, t/L^2]$

Make occupation numbers a smoothly varying field :

$$n_j(t') = \rho(x = j/L, \tau = t'/L^2)$$

Diffusive systems : equilibrium statics

In equilibrium, the probability to observe a given profile is

$$P_{\rm eq}[\rho] = e^{-\beta f[\rho]}$$

$$\beta f[\rho] = \int_0^1 dx \left[\rho \ln \frac{\rho}{\rho_0} + (1-\rho) \ln \frac{1-\rho}{1-\rho_0} \right]$$

Diffusive systems : dynamics

Continuity equation

$$\partial_\tau \rho + \partial_x j(x,\tau) = 0$$

where, on phenomenological grounds

$$j = -D(\rho)\partial_x \rho + \text{noise}, \quad D(\rho) = 1$$

Diffusive systems : dynamics

Continuity equation

$$\partial_\tau \rho + \partial_x j(x,\tau) = 0$$

where, on phenomenological grounds

$$j = -\frac{\sigma(\rho)}{2}\partial_x \frac{\delta \beta f[\rho]}{\delta \rho} + \text{noise}$$

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

Diffusive systems : dynamics

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$$\partial_\tau \rho + \partial_x j(x,\tau) = 0$$

where, on phenomenological grounds

$$j = -\frac{\sigma(\rho)}{2}\partial_x \frac{\delta \beta f[\rho]}{\delta \rho} + \sqrt{\frac{\sigma}{L}}\xi$$

$$\langle \xi(x,\tau)\xi(x',\tau')\rangle = \delta(x-x')\delta(\tau-\tau')$$

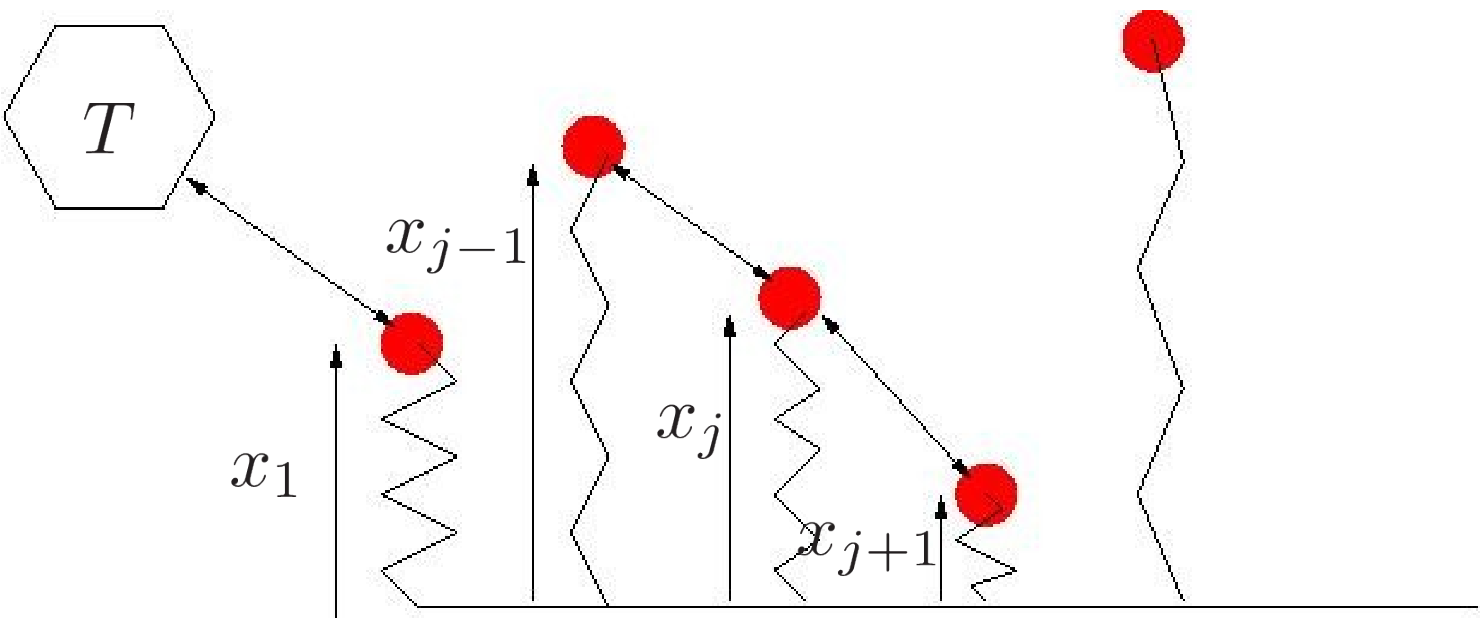
Diffusive systems : dynamics

Green – Kubo relation

$$\frac{D(\rho)}{\sigma(\rho)} = \frac{1}{2}\beta\frac{\delta^2 f}{\delta\rho^2} = \frac{\beta}{2\rho^2\kappa_T}$$

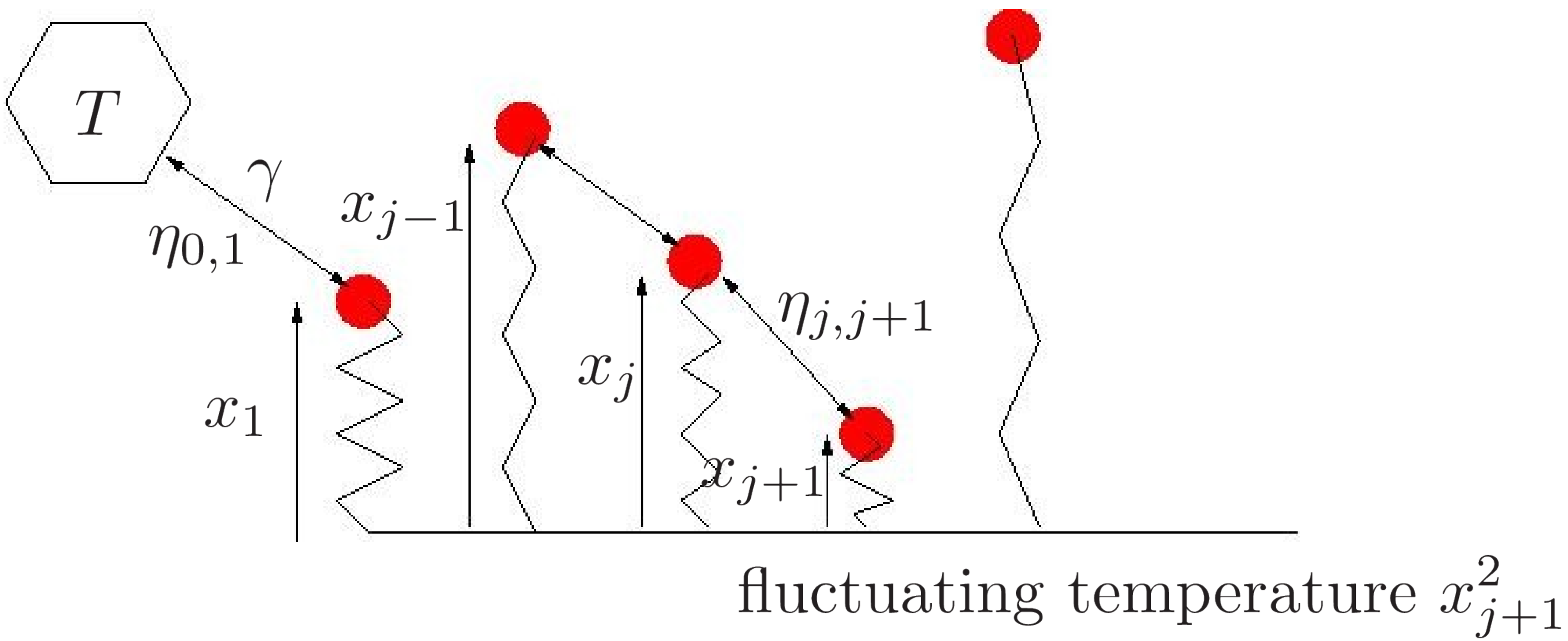
Diffusive systems : example 2

Independent oscillators (Giardiná, Kurchan, Redig version of the Kipnis-Marchioro-Presutti model)



Diffusive systems : example 2

Independent oscillators



Diffusive systems : example 2

Independent oscillators

$$\frac{dx_j}{dt} = -x_j + \sqrt{x_{j+1}^2}\eta_{j,j+1} - \sqrt{x_{j-1}^2}\eta_{j-1,j}$$

with a local conservation law for the energy

$$\varepsilon_j = \frac{x_j^2}{2} = \frac{1}{2}\text{fluct. temperature}$$

Diffusive systems : example 2

Connection to a thermostat

$$\frac{dx_1}{dt} = -x_j + \sqrt{x_2^2}\eta_{1,2} - \sqrt{T}\eta_{0,1}$$

Diffusive systems : example 2

Local energy conservation

$$\frac{d\varepsilon_j}{dt} = J_j - J_{j+1}$$

$$\varepsilon_j(t') = \frac{x_j^2(t')}{2}$$

$$J_{j+1} = \varepsilon_j - \varepsilon_{j+1} + 2\sqrt{\varepsilon_j \varepsilon_{j+1}}\,\eta_{j,j+1}$$

Diffusive systems : example 2

Working at macroscopic scales

$$\rho(x,\tau)=\varepsilon_j(t')$$

$$\tau=t'/L^2,\ x=j/L$$

Diffusive systems : example 2

Equilibrium

$$P_{\rm eq}[\rho] = e^{-\beta f[\rho]}$$

$$\beta f[\rho] = -\frac{1}{2}\ln\rho + \rho$$

Consistent with naive continuum limit from the dynamics

$$j = -\frac{\sigma}{2}\partial_x\frac{\delta\beta f}{\delta\rho} + \sqrt{\frac{\sigma}{L}}\xi = -\partial_x\rho + \sqrt{\frac{\sigma}{L}}\xi,\ \sigma = 4\rho^2$$

Diffusive systems : summary

Ingredients :

Smooth variations over space and time scales $L, \quad L^2$

Diffusive dynamics characterized by $D(\rho), \; \sigma(\rho)$

Noise is vanishingly small (note the $\frac{1}{\sqrt{L}}$)

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Fluctuations of the current (particles, energy)

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Transport coefficients, linear response
Burnett coefficients, non-linear response

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Asking the question reveals the structure

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Asking the question reveals the structure

Evans-Morris-Cohen-Searles-Gallavotti-Cohen-Kurchan-Lebowitz-Spohn-Maes fluctuation theorem

Deep understanding of the kinetic foundations of the second law

Questions about rare events

Equilibrium statistical mechanics/thermodynamics

Partial view, ignoring dynamics

Nonequilibrium : quest for generic properties

Mimick the approach from the statics (ideas from Ruelle & Bowen, 1970's).

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28e année, 1975/76, n° 480 — Février 1976

FORMALISME THERMODYNAMIQUE

par David RUELLE

Questions about rare events

For a time realization with a prescribed current (or whatever else is of physical interest), what does the system look like ?

In or out of equilibrium

Questions about rare events

Extensive constraints :

Time and space integrated current :

$$Q(t) = L^2 \int_0^{t/L^2} d\tau \int_0^1 dx\ j(x,\tau)$$

Time and space integrated activity (traffic for C. Maes)

$$K(t) = L^3 \int_0^{t/L^2} d\tau \int_0^1 dx\ \sigma(\rho(x,\tau))$$

Questions about rare events

Generating functions (canonical approach) :

$$Z(s,t) = \langle \exp\left[-sQ(t)\right] \rangle$$

$$\psi(s) = \lim_{t\to\infty} \frac{\ln Z}{t}$$

Dynamical versions of a partition function and of an intensive free energy.

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WKB-like technique

Langevin equation for $\rho(x, \tau)$

Equivalent to a path-integral formulation

$$Z(s, t) = \int \mathcal{D}\bar{\rho}\mathcal{D}\rho e^{-LS[\bar{\rho}, \rho]}$$

WKB-like technique

Action encodes dynamics + reweighting.

$$S = \int_0^1 dx \int_0^{t/L^2} d\tau \left[\bar{\rho}\partial_\tau \rho + D\partial_x \bar{\rho}\partial_x \rho - \frac{\sigma}{2}(\partial_x \bar{\rho})^2 \right]$$

$$+ \int (sL^2)\sigma(\rho)$$

WKB-like technique

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$$+ \int (sL) \text{ other } \bar{\rho}, \rho \text{ terms}$$

WKB-like technique

Partition function dominated by the saddle

$$S = \int_0^1 dx \int_0^{t/L^2} d\tau \left[\bar{\rho}\partial_\tau \rho + D\partial_x \bar{\rho}\partial_x \rho - \frac{\sigma}{2}(\partial_x \bar{\rho})^2 \right]$$

$$+ \int (sL) \text{ other } \bar{\rho}, \rho \text{ terms}$$

WKB-like technique : credits

Macroscopic fluctuation theory :

Bertini, De Sole, Gabrielli, Jona-Lasinio, Landim

Lebowitz, Speer, Derrida, Bodineau

See the lecture by Bernard Derrida

WKB-like technique : recipe

Step 1: Find the saddle $\rho_x(x,\tau),\ \bar{\rho}_c(x,\tau)$:

$$\frac{\delta S}{\delta \bar{\rho}} = \partial_\tau \rho - \partial_x(D\partial_x \rho) + \partial_x(\sigma \partial_x \bar{\rho}) + \ldots = 0$$

$$\frac{\delta S}{\delta \bar{\rho}} = 0 = -\partial_\tau \bar{\rho} - \partial_x(D\partial_x \bar{\rho}) + \frac{\sigma'}{2}(\partial_x \bar{\rho})^2 + \ldots$$

$$+ \ldots = +s, L \text{ dependent terms}$$

WKB-like technique : recipe

Step 2: Evaluate action at the saddle

$$\psi(s)|_{\text{saddle}} = -LS[\bar{\rho}_c, \rho_c]$$

Step 3 : Integrate out fluctuations around the saddle

$$S[\bar{\rho}_c + \bar{\phi}, \rho_c + \phi] - S[\bar{\rho}_c, \rho_c] = \frac{1}{2} \int \text{quadratic form in } \bar{\phi}, \phi$$

and get

$$\psi(s)|_{\text{fluct}} = -\frac{1}{2} \ln \det[\text{quadratic form}]$$

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Universality of large deviations

Consider the integrated current large deviations

$$Q(t) = L^2 \int_0^1 dx \int_0^{t/L^2} d\tau j(x,\tau)$$

$$\psi(s) = \lim_{t\to\infty} \frac{\ln\langle e^{-sQ}\rangle}{t}$$

Universality of large deviations : equilibrium

With periodic boundary conditions:

$$\psi(s)|_{\text{saddle}} = \frac{1}{2} L\sigma(\rho_0)s^2$$

Saddle is stationary and homogeneous at ρ_0

Universality of large deviations : equilibrium

With periodic boundary conditions:

$$\psi(s)|_{\text{fluct}} = \frac{D}{L^2}\mathcal{F}\left(\frac{\sigma\sigma''}{16D^2}(sL)^2\right)$$

where the universal scaling function

$$\mathcal{F}(x) = \sum_{k\geq 2} \frac{B_{2k-2}}{(k-1)!k!}(-2x)^k$$

has a branch cut along the real axis for $x > \pi^2/2$

Universality of large deviations : equilibrium

For the SSEP,

$$L \to \infty,\ \frac{\psi(s)}{L} = \frac{1}{2}\sigma s^2 + \frac{\sqrt{2}}{3\pi}\sigma^{3/2}|s|^3$$

hence Burnett coefficients are infinite.

Universality of large deviations : equilibrium

For the KMP, the argument of the scaling function $\mathcal{F}(x)$

$$x = 2\rho^2(sL)^2$$

Can hit the singularity : phase transition.

Universality of large deviations : equilibrium

For the KMP, the argument of the scaling function

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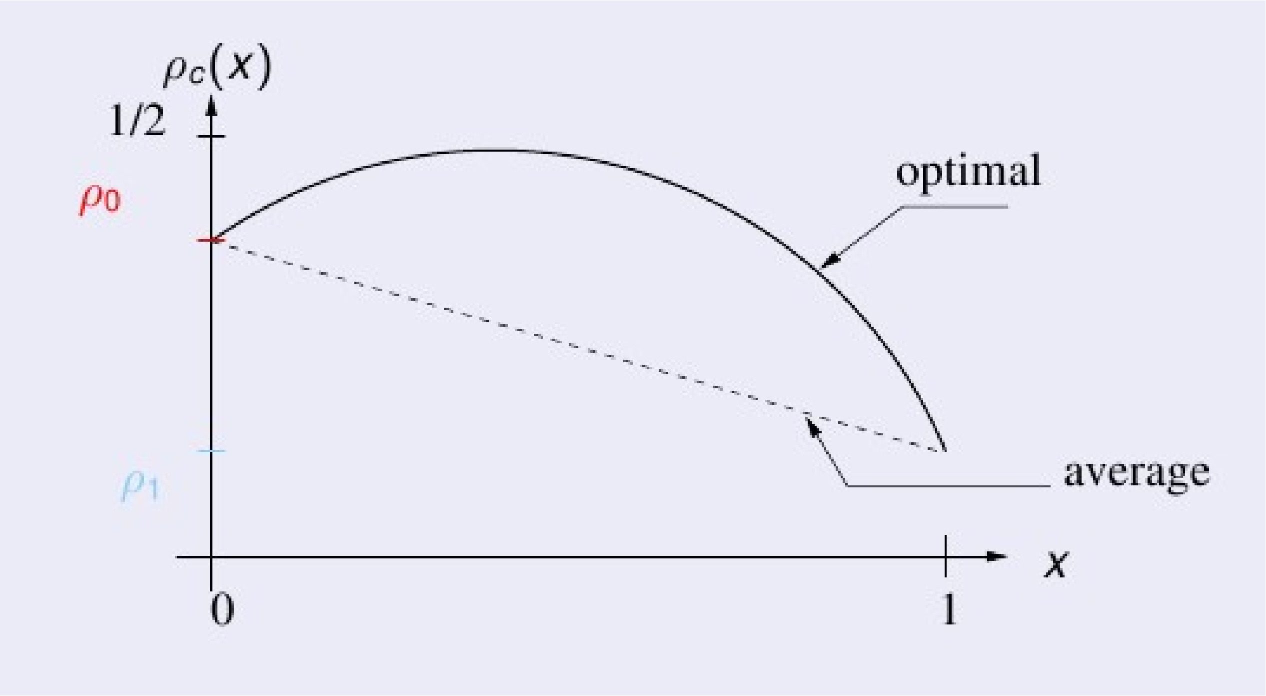
Out of equilibrium

$$\rho_0 \neq \rho_1$$



Out of equilibrium

Boundary-driven diffusive systems $\rho_0 \neq \rho_1$

$$\psi(s)\big|_{\text{saddle}} = L^{-1}\mu(sL)$$

Can be understood in terms of an additivity principle.
For the SSEP (Derrida, Douçot, Roche):

$$\mu(\lambda) = \operatorname{arcsinh}\left[(1-e^{\lambda})(e^{-\lambda}\rho_0 - \rho_1 - (e^{-\lambda}-1)\rho_0\rho_1)\right]$$

Out of equilibrium : some universality

For a constant diffusion constant
and a quadratic noise strength

$$\psi(s)|_{\text{fluct}} = \frac{D}{8L^2}\mathcal{F}\left(\frac{\sigma''}{2D^2}\mu(sL)\right)$$

Out of equilibrium : some universality

Same scaling function as in equiibrium

Out of equilibrium=equilibrium in disguise

For the SSEP and KMP, can be proved directly on the lattice models.

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Large deviations of the activity

Focus on the equilibrium SSEP with pbc at ρ_0

Activity = number of hops,

$$K(t) = L^3 \int_0^1 dx \int_0^{t/L^2} d\tau 2\rho(1-\rho)$$

Mott Insulator vs Superfluid in cold atoms

$$\hat{H} = -\frac{e^{-s}}{2}\sum_{i=1}^{L}\left[\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + e^s\sigma_i^z\sigma_{i+1}^z\right]$$

Anisotropy parameter

Mott Insulator vs Superfluid in cold atoms

Phase diagram of two-component bosons on an optical lattice

Ehud Altman, Walter Hofstetter, Eugene Demler and Mikhail D Lukin
Department of Physics, Harvard University, Cambridge, MA 02138, USA
E-mail: altman@fas.harvard.edu

3. Deep Mott phase: effective spin Hamiltonian

Large deviations of the activity

Cumulant generating function of the activity

$$\psi(s) = -L\sigma(\rho_0)s + \frac{D}{L^2}\mathcal{F}\left(-\frac{\sigma\sigma''}{8D}sL^2\right)$$

But the singularity can be hit when

$$x = -\frac{\sigma\sigma''}{8D}sL^2 > \pi^2/2$$

Large deviations of the activity

Rephrase in terms of $\phi(\lambda) = L\psi(\lambda L^{-2})$

In the regime where $\lambda \geq \lambda_c,\ \lambda_c = \dfrac{\pi^2}{\sigma(\rho_0)}$

$$\phi(\lambda) = -\lambda\sigma(\rho_0) + \frac{1}{L}\mathcal{F}\left(\frac{\sigma}{2}\lambda\right)$$

Large deviations of the activity

Saddle point equation, integrated once:

$$\frac{1}{2}(\partial_x\rho)^2 + f(\rho) = 0$$

Large deviations of the activity

Saddle point equation, integrated once:

$$\frac{1}{2}(\partial_x \rho)^2 + E_P(\rho) = 0$$

Use the intuitive correspondence

$$x \to \text{time}, \ \rho \to \text{position}$$

And search for periodic trajectories.

Large deviations of the activity

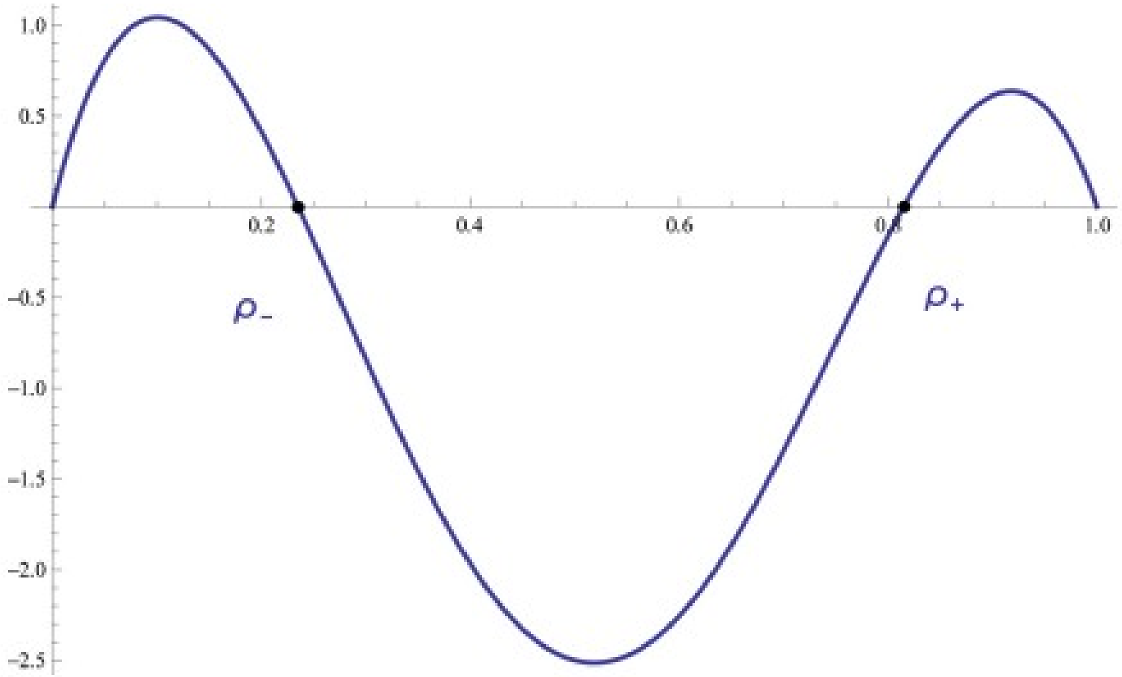

Figure 1. The potential energy profile $E_P(\rho)$ is shown for a set of typical values of the parameters λ, H, μ and ρ_0.

Large deviations of the activity

After a few liters of sweat, at half-filling:

$$\phi(\lambda) = -\sqrt{2}\left[\sqrt{2u+\lambda}+\sqrt{\lambda}\right]\mathrm{E}\left(\frac{2\sqrt{\lambda(2u+\lambda)}}{u+\lambda+\sqrt{\lambda(2u+\lambda)}}\right)$$

where

$$\frac{1}{2} = \frac{\sqrt{2u+\lambda}-\sqrt{\lambda}\mathrm{K}\left(\frac{2\sqrt{\lambda}(2u+\lambda)}{u+\lambda+\sqrt{\lambda(2u+\lambda)}}\right)}{\sqrt{2}u}$$

Physical picture of the phase transition

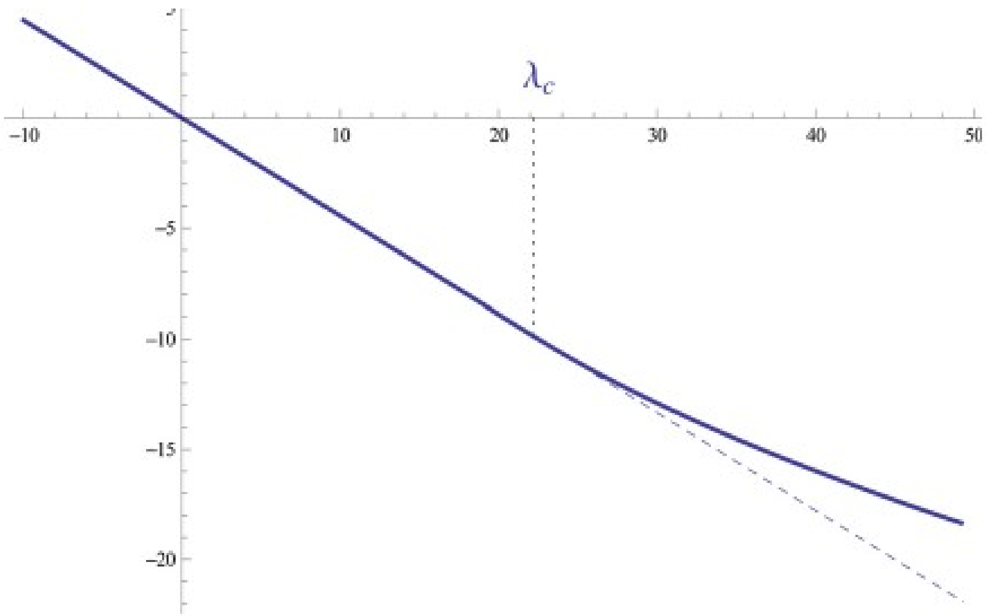

Figure 3. Large deviation function $\phi(\lambda)$ (thick line) as a function of λ, at an average density $\rho_0 = \frac{2}{3}$. The function is singular at $\lambda = \lambda_c = \frac{\pi^2}{\sigma(\rho_0)}$ (the second derivative is discontinuous), marking the entrance in the regime where the density profile is non-uniform ($\lambda > \lambda_c$). The value of the large deviation function for a uniform profile at $\lambda > \lambda_c$ is shown for comparison (dashed line).

Physical picture of the phase transition

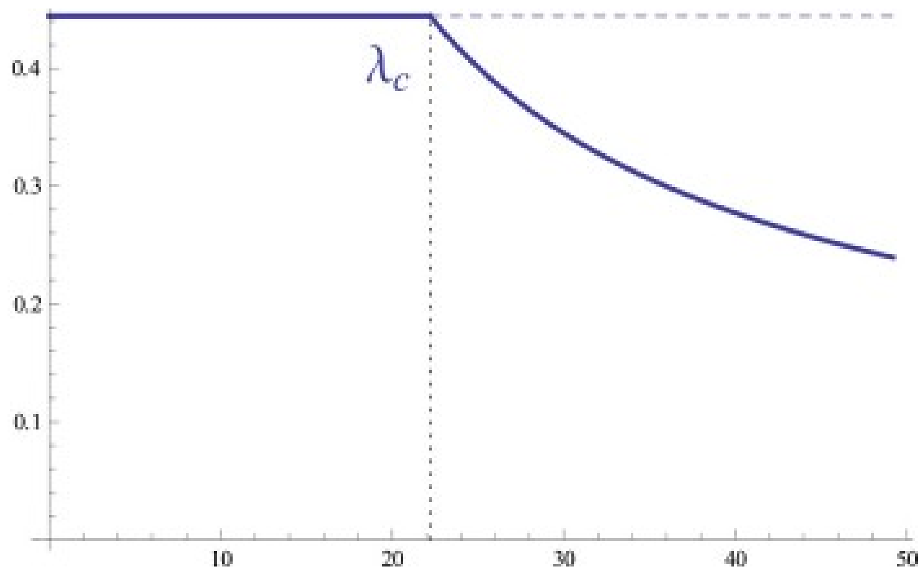

Figure 4. Mean activity $\frac{1}{Lt}\langle K\rangle_\lambda = -\phi'(\lambda)$ (thick blue line) as a function of λ, at an average density $\rho_0 = \frac{2}{3}$. The function is singular at $\lambda = \lambda_c = \frac{\pi^2}{\sigma(\rho_0)}$. The value of $\frac{1}{Lt}\langle K\rangle_s$ is shown for a uniform profile at $\lambda > \lambda_c$ is shown for comparison (dashed line). As expected, above λ_c, the activity for histories with a non-uniform profile is lower than for uniform profiles.

Physical picture of the phase transition

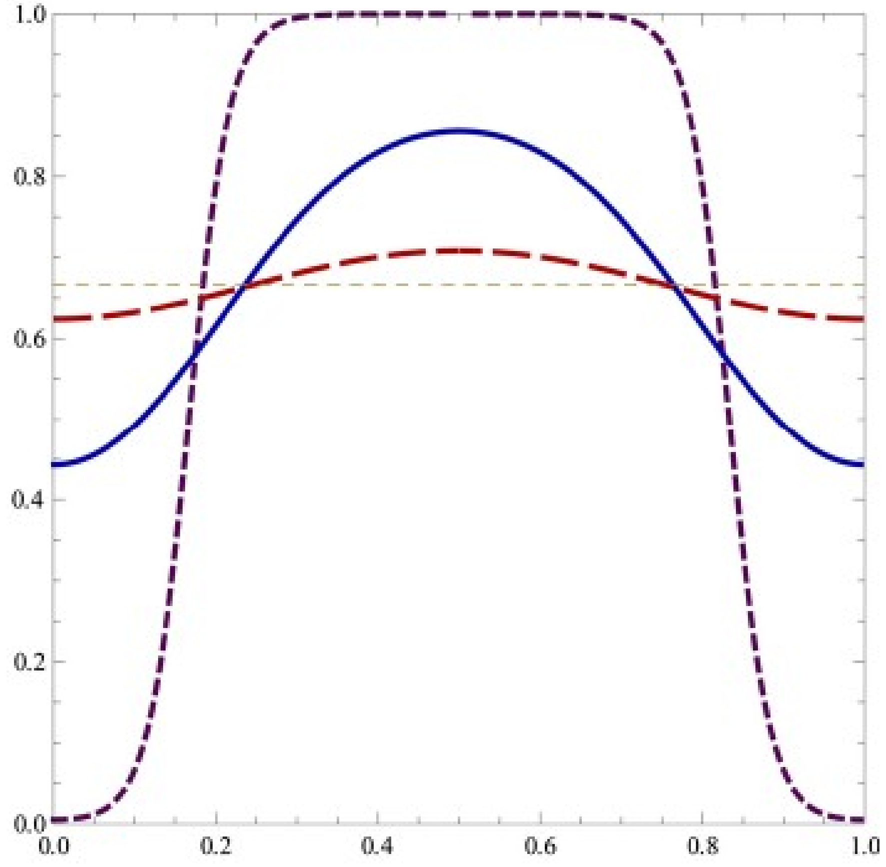

Figure 5. The density profile is shown for $\lambda = \lambda_c + \frac{1}{10}$ (red, large dashes), 25 (blue), 200 (purple, small dashes) at an average density $\rho_0 = \frac{2}{3}$ (thin dashes). The kink becomes steeper as λ is increased.

Final remarks/wishes

Large deviation issues

-can they be measured ? See Nemoto & Sasa.

Universality issues :

- how universal out of equilibrium ?
- how deep is the eq/out of eq connection?

Phase transitions

- can they be observed ?
- can first order transitions be worked out?