Macroscopic versus microscopic approaches to non-equilibrium systems.

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Outline

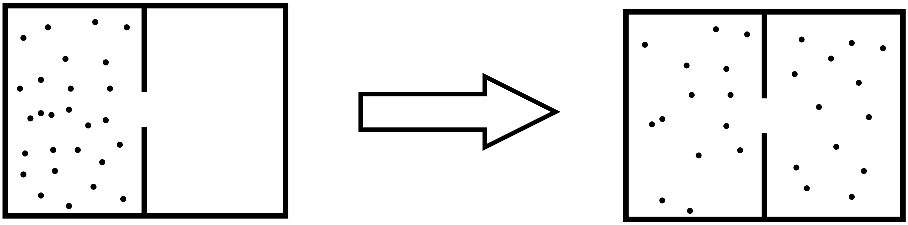
Density fluctuations in non-equilibrium systems

Macroscopic fluctuation theory versus exact solutions

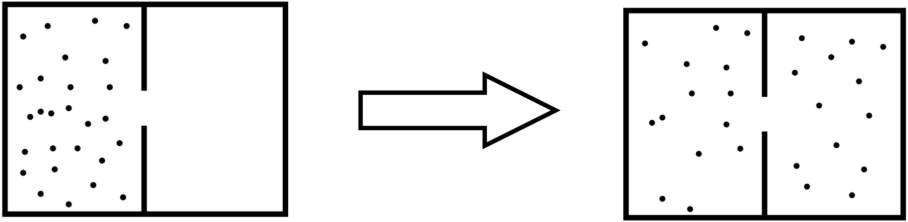
Non steady state situations

Deterministic dynamics

Non equilibrium systems

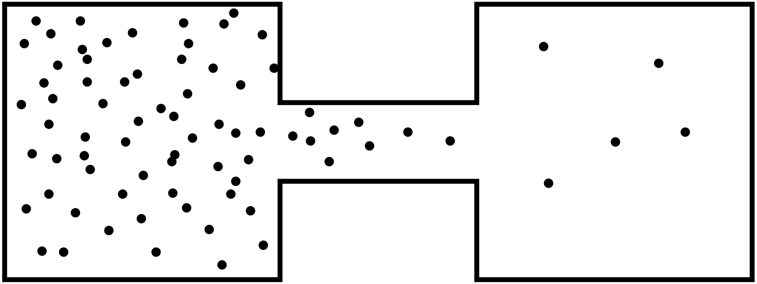


Non equilibrium systems

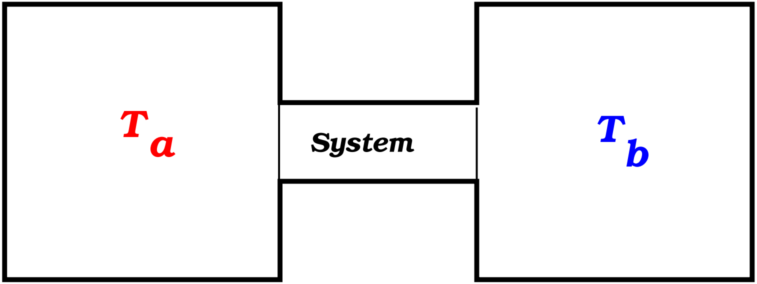


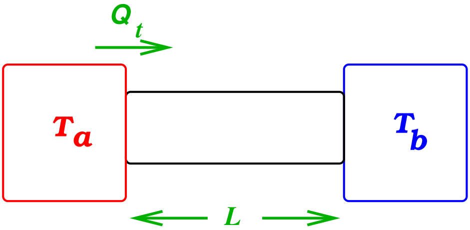
Poincaré: All this Maxwell and Boltzmann have explained ...

Non equilibrium steady states: current of particles

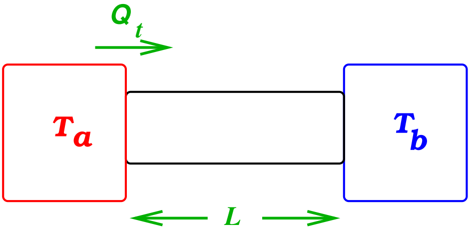


Non equilibrium steady states: current of heat





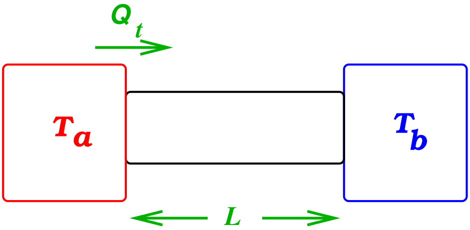
Equilibrium ($T_a = T_b$) Steady state ($T_a \neq T_b$)



Equilibrium ($T_a = T_b$)

Steady state ($T_a \neq T_b$)

$$P(Q) = P(-Q)$$



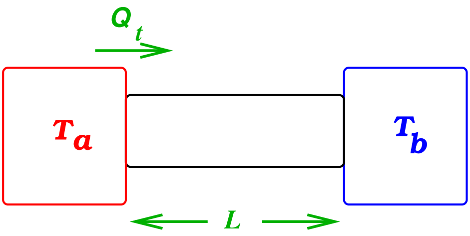
Equilibrium ($T_a = T_b$)

$$P(Q) = P(-Q)$$

Steady state ($T_a \neq T_b$)

$$P(Q) \sim P(-Q)\exp\left[Q\left(\frac{1}{kT_b} - \frac{1}{kT_a}\right)\right]$$

Fluctuation Theorem



Equilibrium ($T_a = T_b$)

$$P(Q) = P(-Q)$$

$$\frac{\langle Q^2 \rangle}{t} \sim \frac{1}{L}$$

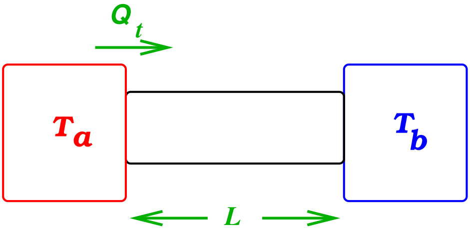
Steady state ($T_a \neq T_b$)

$$P(Q) \sim P(-Q) \exp\left[Q\left(\frac{1}{kT_b} - \frac{1}{kT_a}\right)\right]$$

Fluctuation Theorem

$$\frac{\langle Q \rangle}{t} \sim \frac{A(T_a, T_b)}{L}$$

Fourier's law



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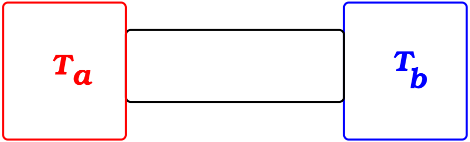
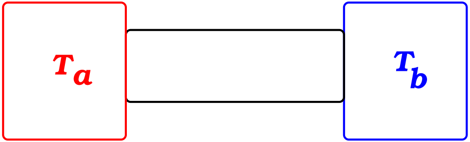
Fourier's law

$P(Q)$?



Equilibrium ($T_a = T_b$)

Non-equilibrium steady state ($T_a \neq T_b$)

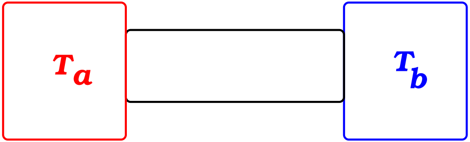


Equilibrium ($T_a = T_b$)

$$P(\mathcal{C}) \sim \exp\left[-\frac{E(\mathcal{C})}{kT}\right]$$

Non-equilibrium steady state ($T_a \neq T_b$)

$$\boxed{P(\mathcal{C}) = ?}$$



Equilibrium ($T_a = T_b$)

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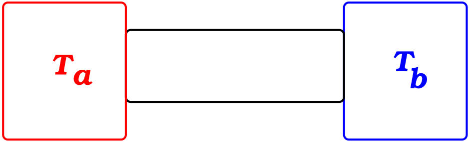
Short range correlations

Non-equilibrium steady state ($T_a \neq T_b$)

$$\boxed{P(\mathcal{C}) = ?}$$

Long range correlations



Equilibrium ($T_a = T_b$)

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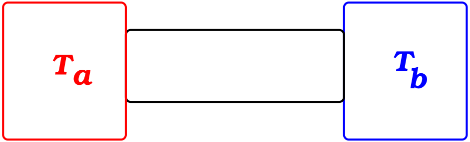
Short range correlations
Local free energy

Non-equilibrium steady state ($T_a \neq T_b$)

$$\boxed{P(\mathcal{C}) = ?}$$

Long range correlations
Non local free energy



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Short range correlations
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Time symmetry of fluctuations

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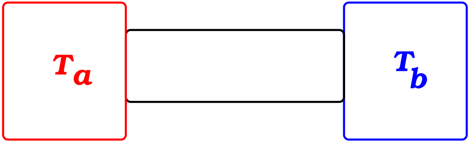


Equilibrium ($T_a = T_b$)

$$P(\mathcal{C}) \sim \exp\left[-\frac{E(\mathcal{C})}{kT}\right]$$

Short range correlations
Local free energy
Time symmetry of fluctuations
No phase transition in 1 d

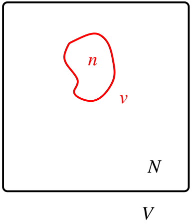
Non-equilibrium steady state ($T_a \neq T_b$)

$$\boxed{P(\mathcal{C}) = ?}$$

Long range correlations
Non local free energy
Time asymmetry of fluctuations
Phase transitions in 1 d

Density fluctuations at equilibrium

Starting from $S = k \log \Omega$ Einstein



N *particles*

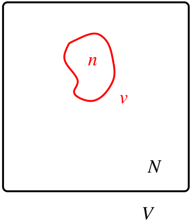
$N = V\rho$

n *particles in* v

n particles in volume v

Density fluctuations at equilibrium

Starting from $S = k \log \Omega$ Einstein



N particles

$N = V\rho$

n particles in v

n particles in volume v

$$\langle n^2 \rangle - \langle n \rangle^2 = kT \; v\rho \; \kappa$$

κ is the compressibility,
ρ the density in the reservoir
and T the temperature.

Density fluctuations at equilibrium

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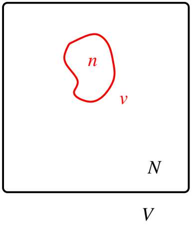

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$$\langle n^2 \rangle - \langle n \rangle^2 = kT \; v \rho \; \kappa$$

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Variance of the fluctuation $=$ $k \times$ Response coefficient

Boltzmann Constant $k \sim 10^{-23} J/K$

Time reversal symmetry of fluctuations at equilibrium

Probability of time dependent fluctuations

Onsager Machlup 1953

Time reversal symmetry of fluctuations at equilibrium

Probability of time dependent fluctuations

Onsager Machlup 1953

Given a fluctuation at $t = 0$

$$\rho(x, 0) = \rho_{\text{equilibrium}}(x) + \phi(x, 0)$$

Time reversal symmetry of fluctuations at equilibrium

Probability of time dependent fluctuations

Onsager Machlup 1953

Given a fluctuation at $t = 0$

$$\rho(x,0) = \rho_{\mathrm{equilibrium}}(x) + \phi(x,0)$$

How does it relax?

$t > 0$ $$\rho(x,t) = \rho_{\mathrm{equilibrium}}(x) + \phi(x,t)$$

How is it produced?

$t < 0$ $$\rho(x,t) = \rho_{\mathrm{equilibrium}}(x) + \phi(x,t)$$

Time reversal symmetry of fluctuations at equilibrium

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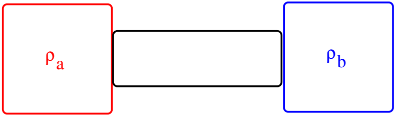
$t < 0$ $$\rho(x, t) = \rho_{\text{equilibrium}}(x) + \phi(x, t)$$

$$\text{Equilibrium} \Rightarrow \boxed{\phi(x, t) = \phi(x, -t)}$$

Non equilibrium steady state ≡ NESS



$$\rho(x,0) = \rho_{\text{steady state}}(x) + \phi(x,0)$$

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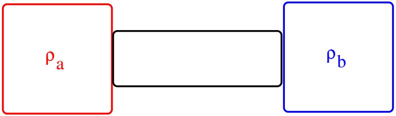
Non equilibrium steady state $\equiv$ NESS



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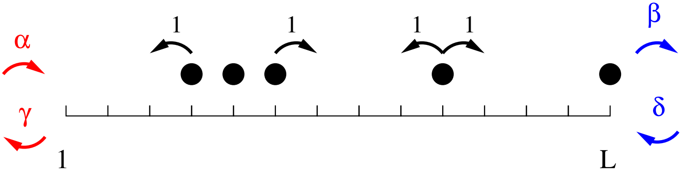
How is it produced?

$t < 0$ $$\rho(x,t) = \rho_{\text{steady state}}(x) + \phi(x,t)$$

$$\text{NESS} \Rightarrow \boxed{\phi(x,t) \neq \phi(x,-t)}$$

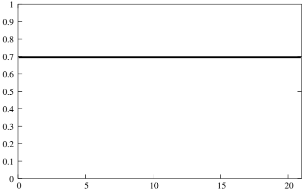
Exclusion processes

SSEP (Symmetric simple exclusion process)

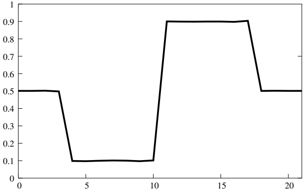


$$\rho_a = \frac{\alpha}{\alpha + \gamma}\ , \qquad \rho_b = \frac{\delta}{\beta + \delta}$$

Density profiles $\rho_a = \rho_b$

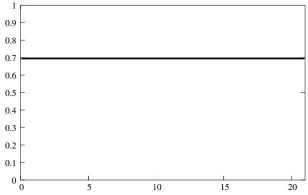


Steady state



Fluctuation

Density profiles $\rho_a = \rho_b$



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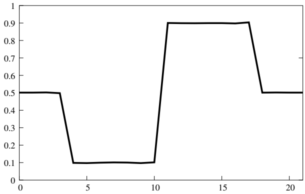
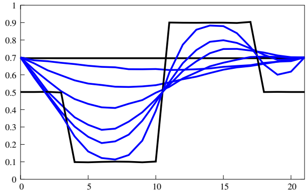


Fluctuation

How does a fluctuation relax?



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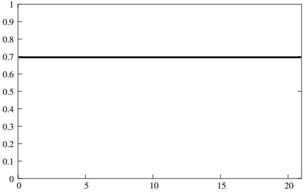

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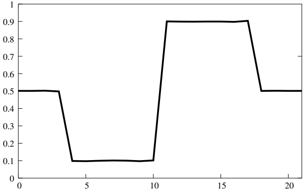

Fluctuation

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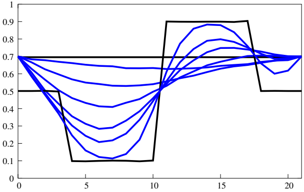

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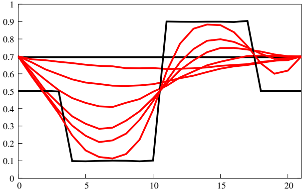

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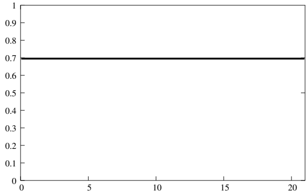

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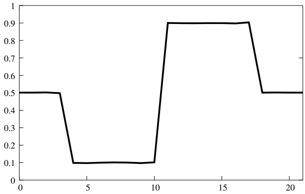

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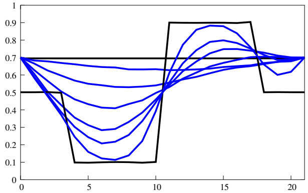
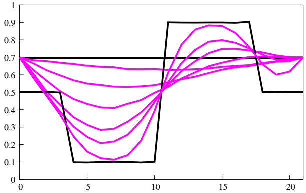
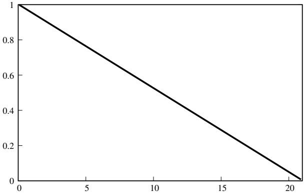


Both



Density profiles $\rho_a = 1, \rho_b = 0$



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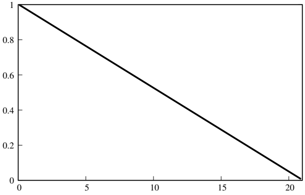

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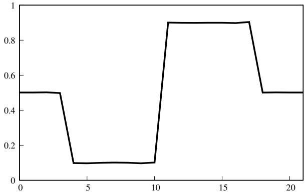

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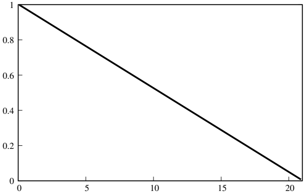

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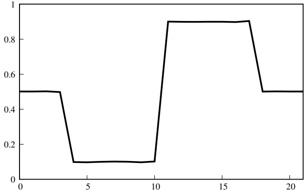
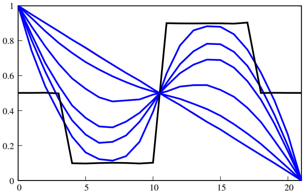


Fluctuation

How does a fluctuation relax?



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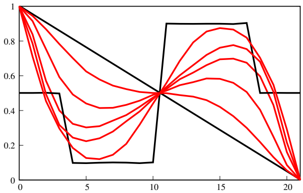

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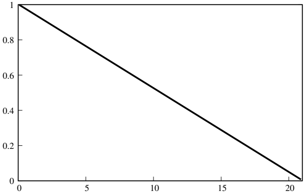

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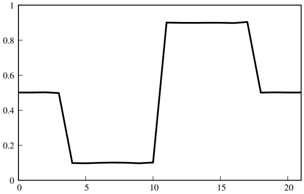
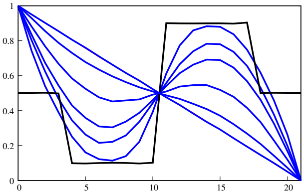


Fluctuation

How does a fluctuation relax?



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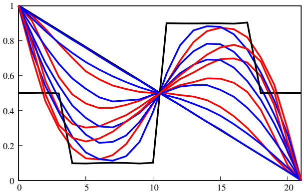
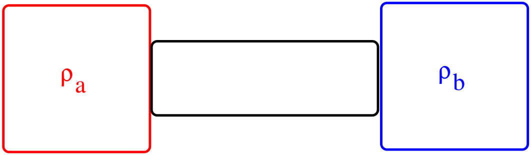


Large diffusive systems

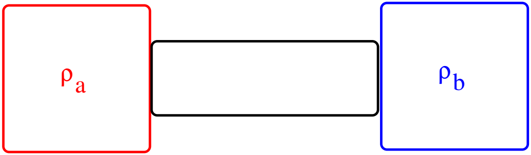


A diffusive system

- For $\rho_a - \rho_b$ small: $$\frac{\langle Q_t \rangle}{t} = \frac{D(\rho)\ (\rho_a - \rho_b)}{L}$$ Fick's law
- $\rho_a = \rho_b = \rho$: $$\frac{\langle Q_t^2 \rangle}{t} = \frac{\sigma(\rho)}{L}$$

One has a theory for $\phi(x,t)$ and $\phi(x,t)$

Large diffusive systems



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One has a theory for $\phi(x,t)$ and $\phi(x,t)$

Note that $\boxed{\sigma(\rho) = 2kT\rho^2\kappa(\rho)D(\rho)}$ where κ is the compressibility

Macroscopic fluctuation theory

Onsager Machlup theory
for non equilibrium diffusive systems

Kipnis Olla Varadhan 89
Spohn 91
⋮
Bertini De Sole Gabrielli
Jona-Lasinio Landim 2001 $\longrightarrow$

Evolution of a profile $\rho(x,t)$ for $0 \leq t \leq T$

$$\mathrm{Pro}(\{\rho(x,t), j(x,t)\})$$

$$\exp\left[-L\int_0^{T/L^2} dt \int_0^1 dx \; \frac{[j(x,t)+\rho'(x,t)D(\rho(x,t))]^2}{2\sigma(\rho(x,t))}\right]$$

- $\dfrac{d\rho}{dt} = -\dfrac{dj}{dx}$ (conservation law)
- $\rho(0,t) = \rho_a \;\; ; \;\; \rho(1,t) = \rho_b$

Macroscopic fluctuation theory

$$\mathrm{Pro}(\{\rho(x,t), j(x,t)\})$$
$$\exp\left[-L\int_0^{T/L^2} dt \int_0^1 dx\, \frac{[j(x,t)+\rho'(x,t)D(\rho(x,t))]^2}{2\sigma(\rho(x,t))}\right]$$

$$\Updownarrow$$

$$j(x,t) = -\rho'(x,t)D(\rho(x,t)) + \frac{1}{\sqrt{L}}\eta(x,t)$$

Macroscopic fluctuation theory

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$$\exp\left[-L\int_0^{T/L^2} dt \int_0^1 dx \, \frac{[j(x,t)+\rho'(x,t)D(\rho(x,t))]^2}{2\sigma(\rho(x,t))}\right]$$

$$\Updownarrow$$

$$j(x,t) = -\rho'(x,t)D(\rho(x,t)) + \frac{1}{\sqrt{L}}\eta(x,t)$$

with the white noise

$$\langle \eta(x,t)\eta(x',t')\rangle = 2\sigma(\rho(x,t))\delta(x-x')\delta(t-t')$$

$$\frac{d\rho}{dt} = -\frac{dj}{dx} \quad ; \quad \rho(0,t) = \rho_a \;\; ; \;\; \rho(1,t) = \rho_b$$

$$\mathrm{Pro}(\{\rho(x,t), j(x,t)\}) \sim \exp\left[-\mathrm{Action}\right] =$$

$$\exp\left[-L \int_0^{T/L^2} dt \int_0^1 dx \; \frac{[j(x,t) + \rho'(x,t) D(\rho(x,t))]^2}{2\sigma(\rho(x,t))}\right]$$

How does a fluctuation $\rho(x,0)$ relax?

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$$\mathrm{Action} = 0 \quad \Leftrightarrow \quad \frac{d\rho}{dt} = (D(\rho(x,t))\rho(x,t)')'$$

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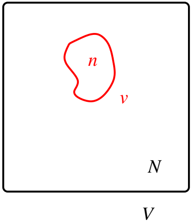
How is a fluctuation $\rho(x,0)$ produced?

Minimize the Action with $\rho(x,-\infty) = \rho_{\text{steady state}}(x)$

Large deviations of the density

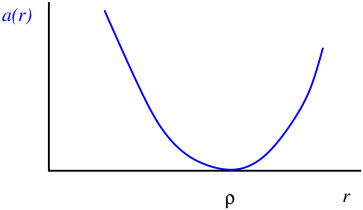


N particles

$N = V\rho$

n particles in v

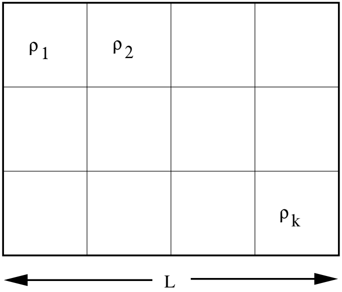
$$\text{Pro}\left(\frac{n}{v} = r\right) \sim \exp[-v\ a(r)]$$



$a(r)$ is the large deviation function

A l'équilibre $a(r)$ est l'énergie libre

Large deviation functional



$$\text{Pro}(\rho_1, ...\rho_k) \sim \exp\left[-L^d \mathcal{F}(\rho_1, ...\rho_k)\right]$$

Large number k of boxes $\vec{r} = L\vec{x}$

$$\text{Pro}(\{\rho(\vec{x})\}) \sim \exp\left[-L^d \mathcal{F}(\{\rho(\vec{x})\})\right]$$

Large deviation functional

$$\mathrm{Pro}(\{\rho(x)\}) \sim \exp[-\mathrm{Action}] = \exp\left[-L\mathcal{F}(\{\rho(x)\})\right]$$

Equilibrium

1. $\mathcal{F}$ local
2. $\mathcal{F} = T^{-1}\int d\vec{x}\, f(\rho(\vec{x}))$ f is the free energy per unit volume
3. No phase transition in one dimension (short range interactions)

Large deviation functional

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Non-equilibrium

1. $\mathcal{F}$ non local
2. Weak long range correlations (SSEP for $x < y$)   Spohn 1982

$$\langle(\rho(x) - \rho^*(x))(\rho(y) - \rho^*(y))\rangle \simeq \frac{1}{L} G(x, y) = \frac{1}{L} x(1 - y)$$

3. Phase transitions in one dimension

Large deviation function for the SSEP

$$\text{Pro}(\{\rho(x)\}) \sim \exp[-L\mathcal{F}(\{\rho(x)\})]$$

Equilibrium $\rho_a = \rho_b = F$

$$\mathcal{F}(\{\rho(x)\}) = \int_0^1 dx \left[(1-\rho(x))\log\frac{1-\rho(x)}{1-F} + \rho(x)\log\frac{\rho(x)}{F}\right]$$

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Non-equilibrium $(\rho_a \neq \rho_b)$

D Lebowitz Speer 2001-2002
Bertini De Sole Gabrielli Jona-Lasinio Landim 2002

$$\mathcal{F} = \sup_{F(x)} \int dx \left[(1-\rho(x)) \log \frac{1-\rho(x)}{1-F(x)} + \rho(x) \log \frac{\rho(x)}{F(x)} + \log \frac{F'(x)}{\rho_b - \rho_a} \right]$$

with $F(x)$ monotone, $F(0) = \rho_a$ and $F(1) = \rho_b$

Non-equilibrium $\rho_a \neq \rho_b$

$$\mathcal{F} = \sup_{F(x)} \int dx \left[(1-\rho(x)) \log \frac{1-\rho(x)}{1-F(x)} + \rho(x) \log \frac{\rho(x)}{F(x)} + \log \frac{F'(x)}{\rho_b - \rho_a} \right]$$

$$\Downarrow$$

F is non-local: for example for small $\rho_a - \rho_b$

$$\mathcal{F}(\{\rho(x)\}) = \int_0^1 dx \ (1-\rho(x)) \log \frac{1-\rho(x)}{1-\rho^*(x)} + \rho(x) \log \frac{\rho(x)}{\rho^*(x)}$$
$$+ \frac{(\rho_a-\rho_b)^2}{(\rho_a-\rho_a^2)^2} \int_0^1 dx \int_x^1 dy \ x(1-y)(\rho(x)-\rho^*(x))(\rho(y)-\rho^*(y))$$
$$+ O(\rho_a-\rho_b)^3$$

where $\rho^*(x) = \langle \rho(x) \rangle = (1-x)\rho_a + x\rho_b$

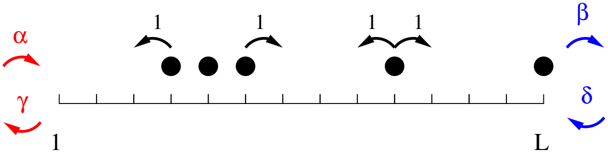
Long-range correlations   Spohn 82

$$\langle \rho(x)\rho(y)\rangle - \langle \rho(x)\rangle\langle \rho(y)\rangle \simeq \frac{1}{L} G(x,y) = -\frac{(\rho_a-\rho_b)^2}{L} x(1-y)$$

Matrix ansatz

Fadeev 1980, ...,
D Evans Hakim Pasquier 1993

Steady state of the SSEP



$$P(\tau_1, \ldots, \tau_L) = \frac{\langle W | X_1 \ldots X_L | V \rangle}{\langle W | (D+E)^L | V \rangle}$$

where $X_i = \begin{cases} D & \text{if site } i \text{ occupied} \\ E & \text{if site } i \text{ empty} \end{cases}$

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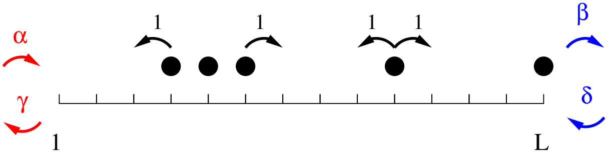

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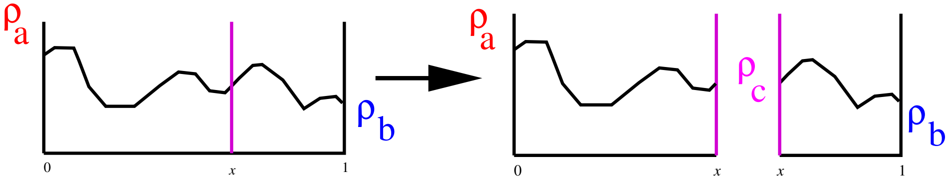
$$\langle W | (\alpha E - \gamma D) = \langle W |$$
$$DE - ED = D + E$$
$$(\beta D - \delta E) | V \rangle = | V \rangle$$

Additivity for the SSEP

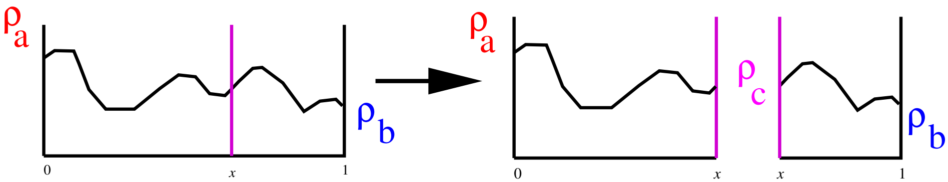


$$P(\tau_1, \ldots, \tau_L) = \frac{\langle W|X_1 \ldots X_L|V\rangle}{\langle W|(D+E)^L|V\rangle}$$

Idea

$$\langle W|X_1 \ldots X_L|V\rangle = \int dU \ \langle W|X_1 \ldots X_{L'}|U\rangle \ K(U) \ \langle U|X_{L'+1} \ldots X_L|V\rangle$$

Additivity for the SSEP



$$P(\tau_1, \ldots, \tau_L) = \frac{\langle W | X_1 \ldots X_L | V \rangle}{\langle W | (D+E)^L | V \rangle}$$

One can prove that:

$$\mathrm{Pro}_{L+L'}(Y\ ,\ Y' | \rho_a, \rho_b) = \oint_{\rho_b < |\rho_c| < \rho_a} \frac{d\rho_c}{2i\pi}\ \mathrm{Pro}_L(Y|\rho_a, \rho_c) \times \mathrm{Pro}_{L'}(Y'|\rho_c, \rho_b)$$

$$\times \frac{L!\ L'!\ (\rho_a - \rho_b)^{L+L'+1}}{(L+L')!\ (\rho_a - \rho_c)^{L+1}\ (\rho_c - \rho_b)^{L'+1}}$$

Models

1. Stochastic dynamics + Stochastic thermostats
   exclusion processes,
   diffusive systems

2. Deterministic dynamics + Determinstic Thermostats

3. Deterministic dynamics + Stochastic heat baths
   chain of anharmonic oscillators,
   hard particle gas

anomalous Fourier's law

Lepri, Livi, Politi 2003

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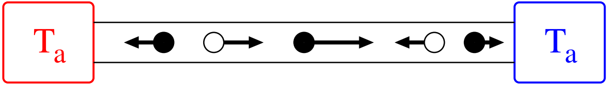
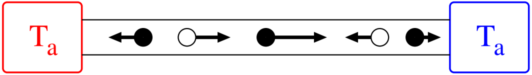
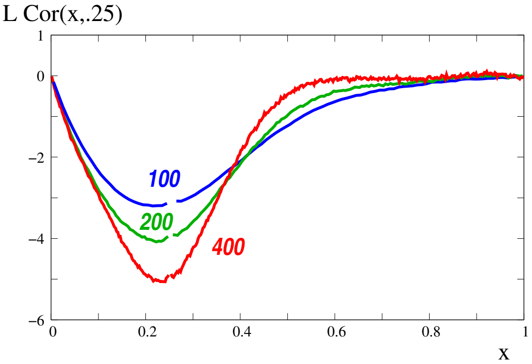


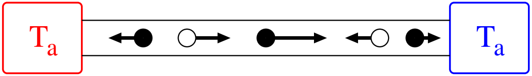
Correlations on a mesoscopic scale

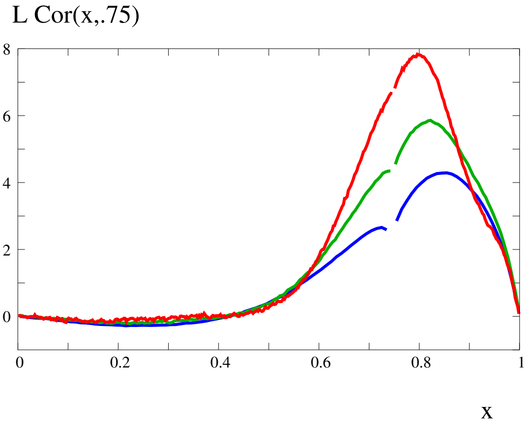




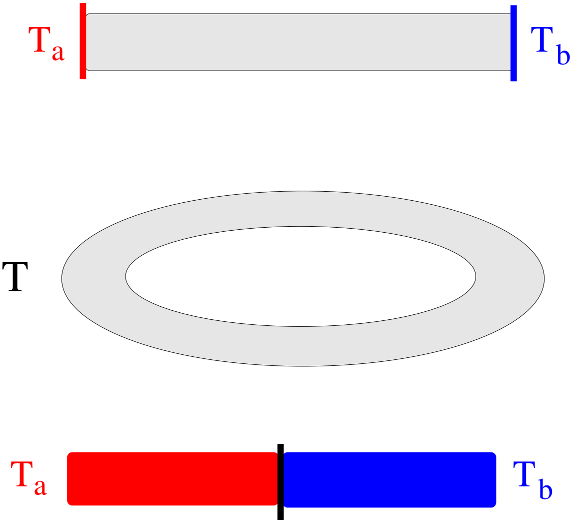
Delfini, Lepri, Livi, Mejia-Monasterio, Politi 2010
Gerschenfeld, D., Lebowitz 2010

Correlations on a mesoscopic scale

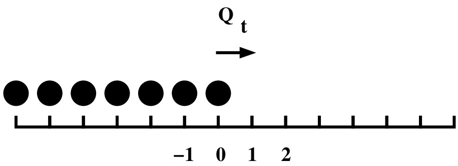




Current fluctuations



Step initial condition



ASEP

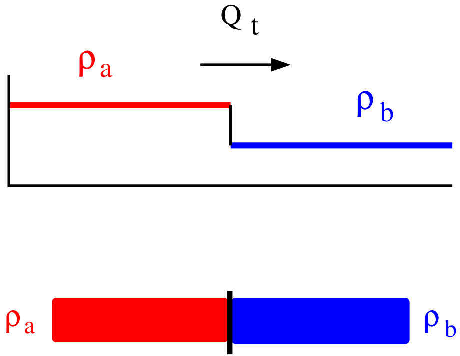
G. Schütz 98

⋮

Prähofer Spohn 2000-2002

⋮

Tracy Widom 2008

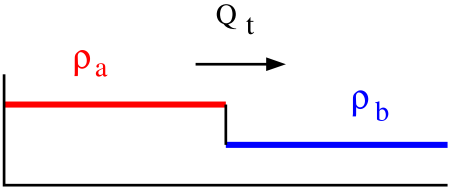


SSEP

D Gerschenfeld 2009

$$\boxed{\left\langle e^{\lambda Q_t} \right\rangle = ?}$$

Step initial condition on the infinite line



SSEP

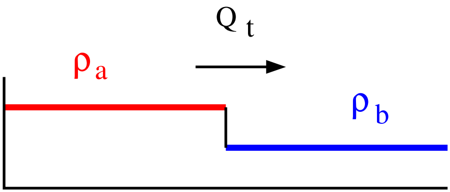
D Gerschenfeld 2009

$$\left\langle e^{\lambda Q_t} \right\rangle \simeq \exp[\sqrt{t}\ H(\omega)]$$

with $H(\omega) = \frac{1}{\pi} \int_{\infty}^{\infty} dk \log \left[1 + \omega e^{-k^2} \right]$

and $\omega = 1 - [1 - (e^{\lambda} - 1)\rho_a][1 - (1 - e^{-\lambda})\rho_b]$

Step initial condition on the infinite line



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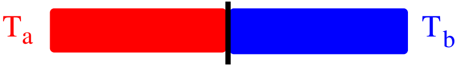
$$\text{For large } Q_t : \boxed{\text{Pro}(Q_t) \sim \exp\left[-\frac{\pi^2}{12}\ Q_t^3/t \right]}$$



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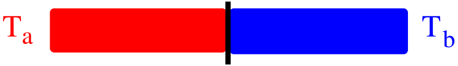

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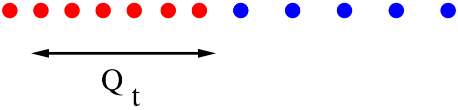
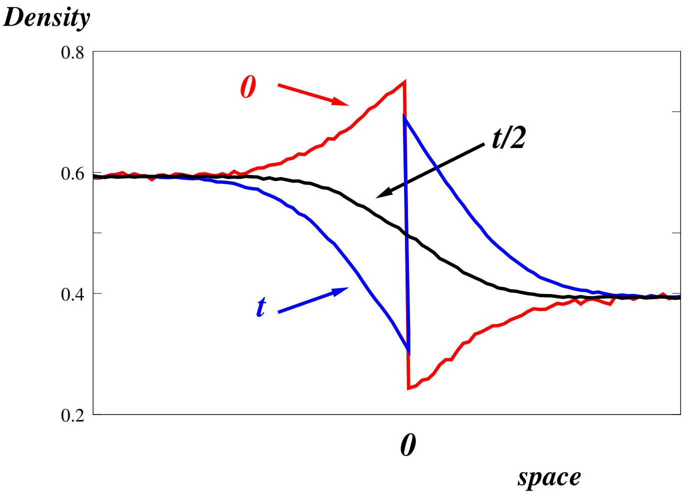


$$\mathrm{Pro}(Q_t) \sim \prod_{x=1}^{Q_t} \exp\left[-\frac{x^2}{t}\right]$$

Density profiles condionned on the current



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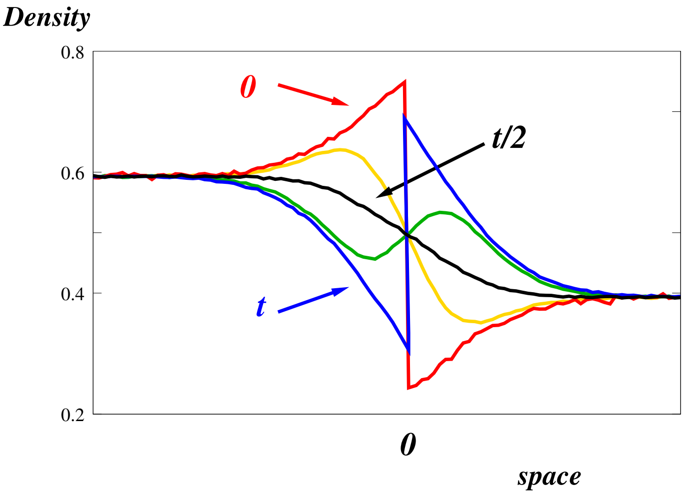

Open questions

General diffusive systems (even close to equilibrium)

Mechanical (non diffusive) systems

Non steady state situations