Metastability of the contact process in high dimension

Christophe Deroulers

LPTENS Paris

and

Rémi Monasson

LPTENS Paris & LPT Strasbourg

Villasimius, September, 20th 2003

Thanks to the organizers!

Overview

Motivations

The model...

...translates into a field theory

Intermezzo

The mean field case

Beyond mean field

Conclusion

Motivations

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Metastability...

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Metastability...

is well understood in mean field:

energy barriers $\propto$ volume

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Metastability...

is well understood in mean field:
energy barriers $\propto$ volume

less well understood in finite dimensions

- when there are many metastable states (glasses)
- when exotic dynamics

Aim

To find a formalism that helps to treat metastability (or more general dynamical) problems

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No miracle: at present we can't do better than a $\frac{1}{D}$ expansion.

The model

The Contact Process

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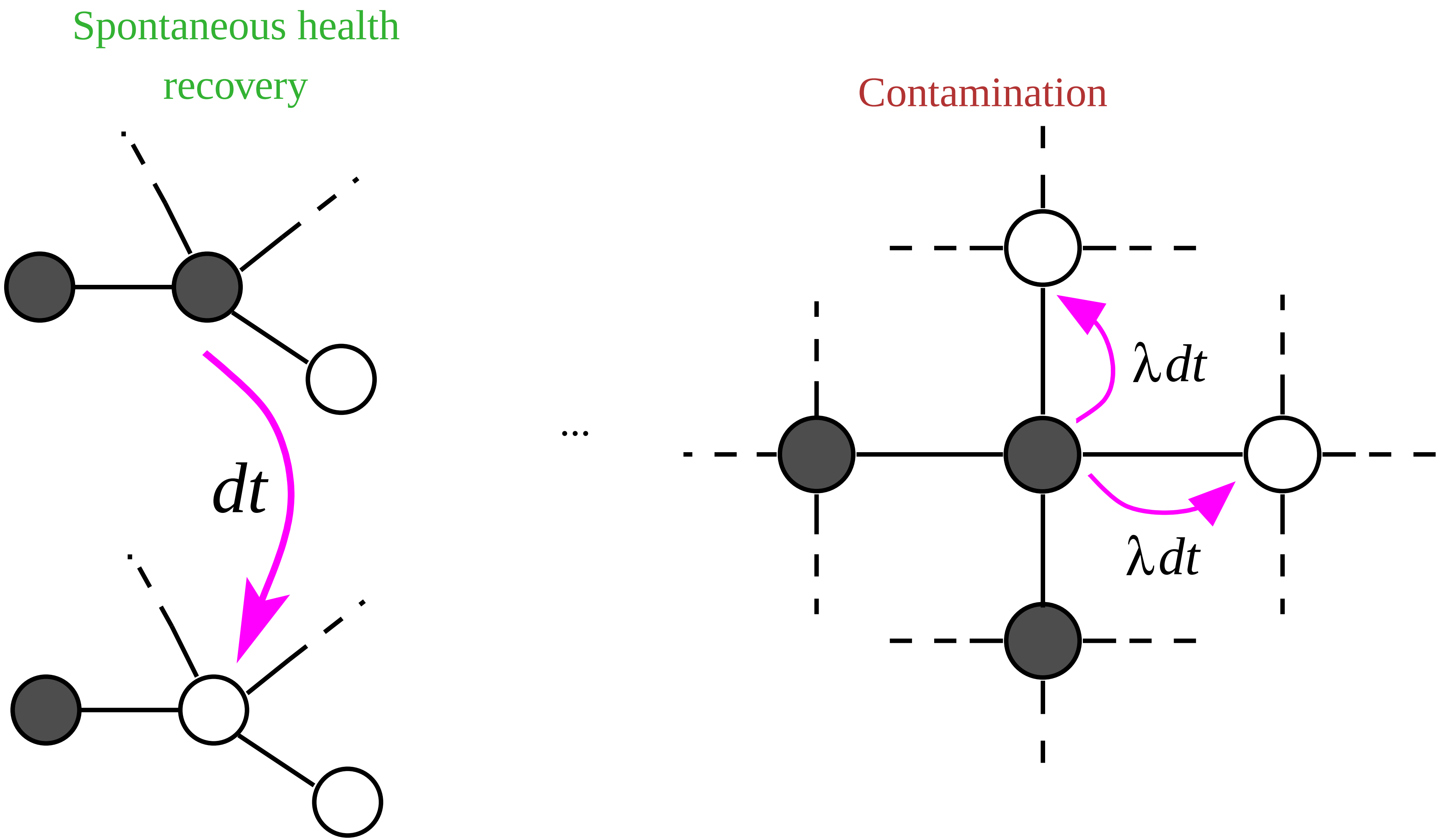
where each site i is either

sick/full/1 or healthy/empty/0

The Contact Process: Dynamical rules



The Contact Process?

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Because it’s very simple, yet rich.

The contact process is a stochastic process with important sample-to-sample fluctuations

but there is self-averageness (measure concentration) when the number of sites $N \to \infty$.

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Let us precise the typical behaviour: the one that happens almost surely (a.s.).

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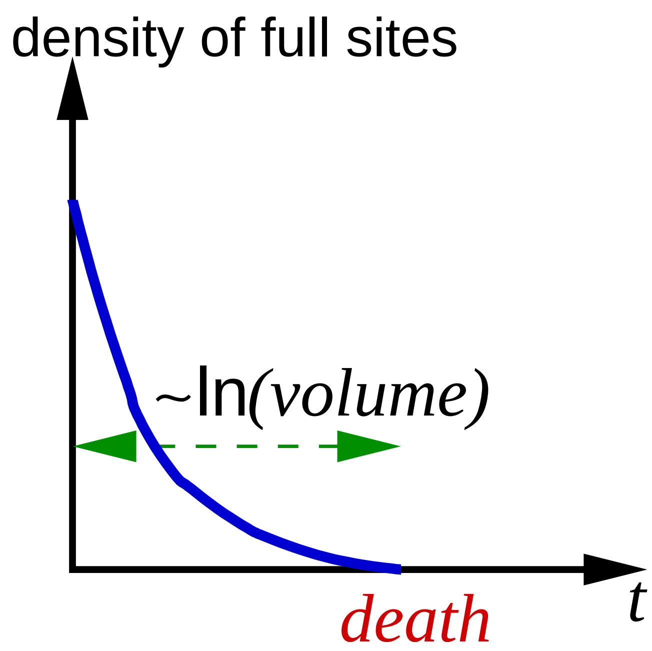

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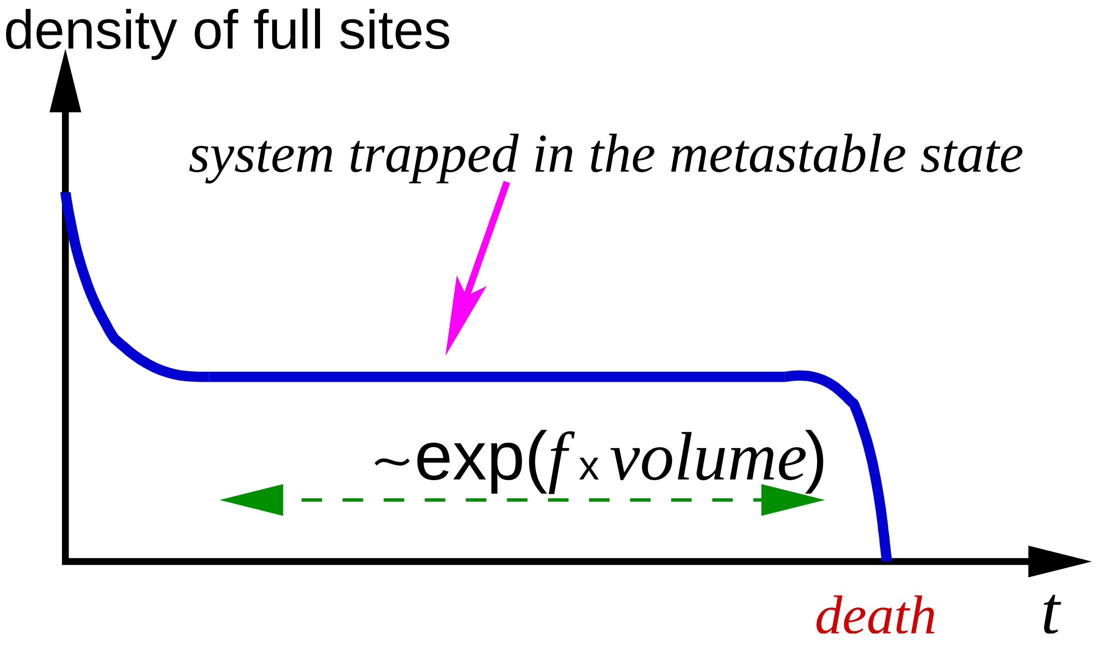

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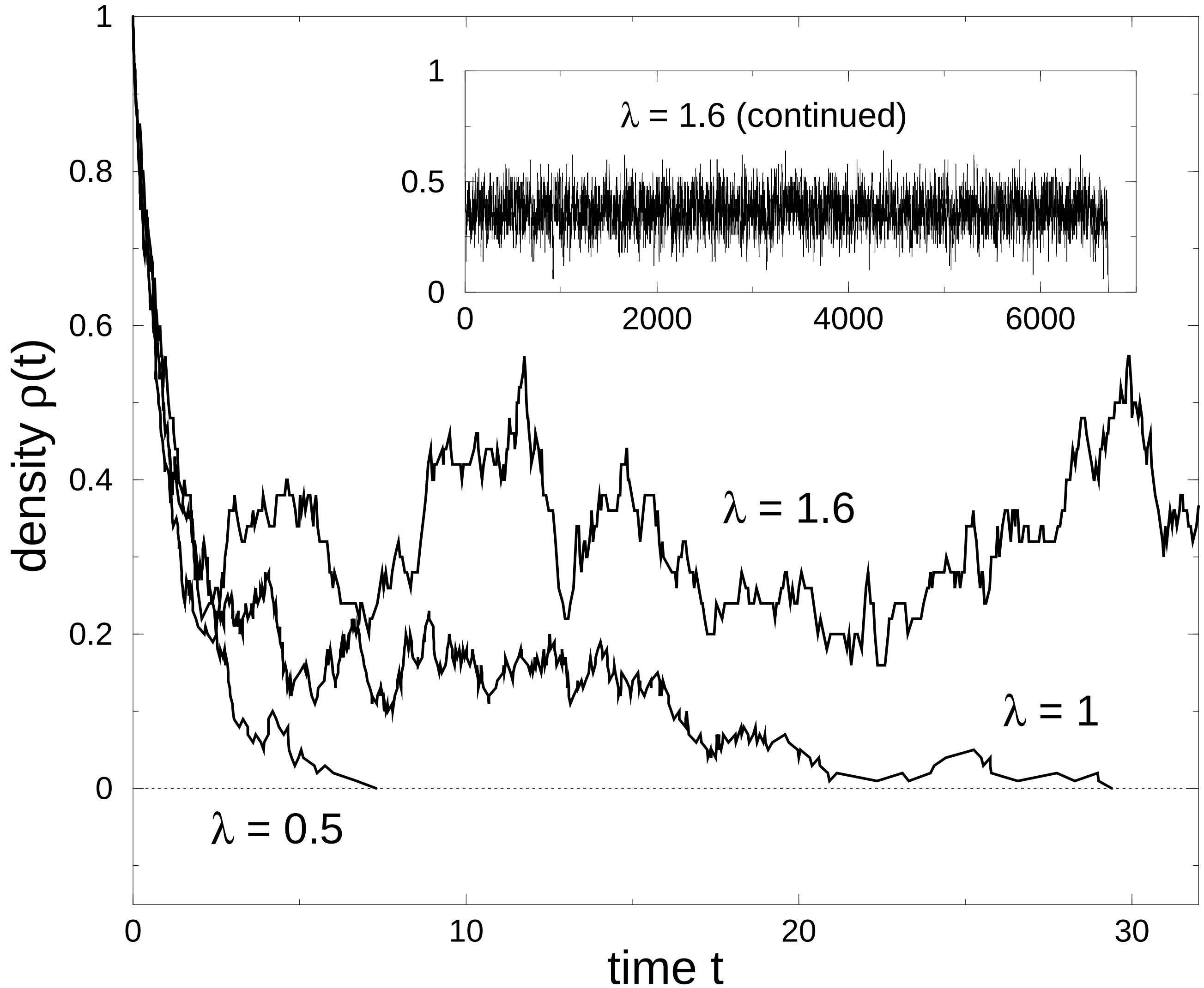
- If $\lambda < \lambda_c$, almost surely the process dies out quickly
- If $\lambda > \lambda_c$, almost surely the process survives for a long time
- If $\lambda = \lambda_c$, polynomial decay with critical exponents.

The Contact Process: Phenomenology

For a (mean field) real system:



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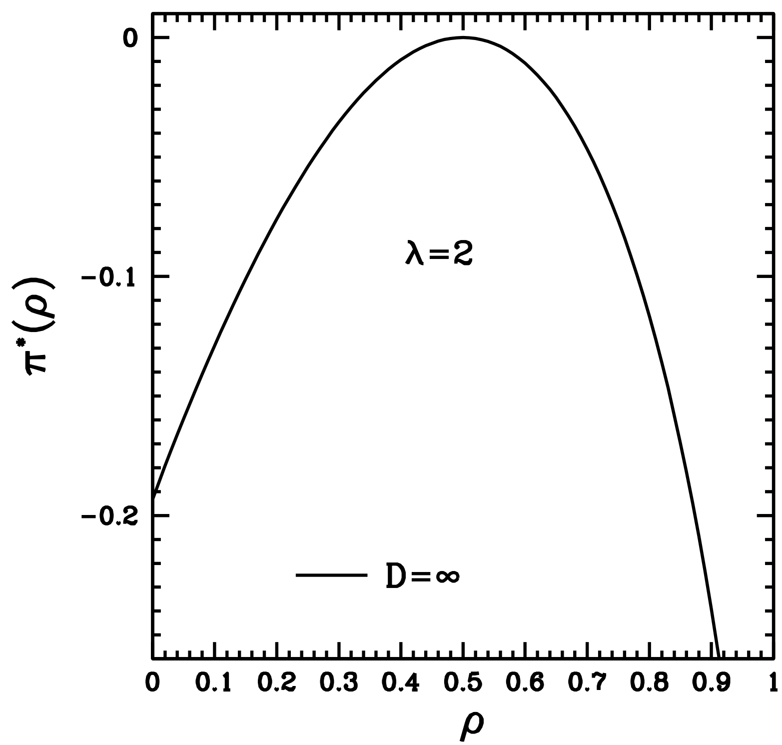
$$P(\rho, t) = e^{-N\pi(\rho,t)}$$



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We would like a reusable tool.

Translation into a field theory

Quantum formalism

DOI (1976), PELITI (1985), ...

We write the master equation with quantum operators (exact mapping):

A state of the graph is the list of occupation numbers (0=empty, 1=full):

$$\vec{s} = \{s_1, s_2, \ldots, s_N\}$$

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A state of the graph is the list of occupation numbers (0=empty, 1=full):

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On each site i we define two basis vectors: $|0\rangle_i$ (empty) and $|1\rangle_i$ (full) so that the state of the graph is one of the 2^N vectors like:

$$|\vec{s}\rangle = |1\rangle_1 \otimes |1\rangle_2 \otimes |0\rangle_3 \otimes \ldots \otimes |1\rangle_N$$

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On different sites operators commute:

$$[a_i, a_j] = [a_i, a_j^+] = [a_i^+, a_j^+] = 0$$

Quantum formalism

The master equation can be written:

$$\frac{\mathrm{d}}{\mathrm{d}t}|P(t)\rangle = \hat{W}|P(t)\rangle \quad , \quad |P(T)\rangle = \exp(T\hat{W})|P(0)\rangle$$

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For the contact process

$$\hat{W} = \hat{W}_{\mathrm{ann}} + \lambda\hat{W}_{\mathrm{cre}}$$

with (spontaneous health recovery)

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$$\begin{aligned}(1 - a^+)a\ |0\rangle &= 0 \\ (1 - a^+)a\ |1\rangle &= |0\rangle - |1\rangle\end{aligned}$$

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For the contact process

$$\hat{W} = \hat{W}_{\mathrm{ann}} + \lambda \hat{W}_{\mathrm{cre}}$$

with (spontaneous health recovery)

$$\hat{W}_{\mathrm{ann}} = \sum_i (1 - a_i^+) a_i$$

and (contamination)

$$\hat{W}_{\mathrm{cre}} = \frac{1}{z} \sum_i \sum_{j \in i} (a_j^+ (1 + a_j) - 1) a_i^+ a_i$$

$\longrightarrow$ path integral

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$\rightsquigarrow$ let's introduce a path integral.

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$\rightsquigarrow$ let's introduce a path integral.

For that, coherent states are useful.

KLAUDER, Ann. Phys. (1960)

$$|\phi,\psi\rangle = (1-\phi)^{-\frac{1}{2}} \left((1-\phi)\ |0\rangle + \phi\ \exp(\psi)\ |1\rangle \right)$$

$$\langle\phi,\psi| = (1-\phi)^{\frac{1}{2}} \left(\langle 0| + \exp(-\psi)\ \langle 1| \right)$$

with $\phi \in [0,1]$ and $\psi = -\frac{1}{2}\ln[\phi/(1-\phi)] + \hat{\imath}\ \theta$ with $\theta \in [0, 2\pi]$ and $\hat{\imath}^2 = -1$.

$\rightarrow$ path integral

Trotter's formula yields:

$$\langle\vec{\phi}_T,\vec{\psi}_T|\exp(T\,\hat{W})|\vec{\phi}_0,\vec{\psi}_0\rangle = \int_{\vec{\phi}(0)=\vec{\phi}_0,\vec{\psi}(0)=\vec{\psi}_0}^{\vec{\phi}(T)=\vec{\phi}_T,\vec{\psi}(T)=\vec{\psi}_T} \mathcal{D}\vec{\phi}(t)\,\mathcal{D}\vec{\psi}(t)\;\exp\left(-\mathcal{S}[\{\vec{\phi},\vec{\psi}\}]\right)$$

with

$$\mathcal{S}[\{\vec{\phi},\vec{\psi}\}] = \int_0^T \mathrm{d}t\,\left\{\sum_{i=1}^{N}\phi_i(t)\frac{\mathrm{d}\psi_i(t)}{\mathrm{d}t} - \tilde{W}(\vec{\phi}(t),\vec{\psi}(t))\right\}$$

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$\tilde{W}$ is deduced from $\hat{W}$...

...with the table:

operator in $\widehat{W}$	expression in $\widetilde{W}$
1	1
a	$\phi\ \exp(\psi)$
a^+	$(1-\phi)\ \exp(-\psi)$
a^+a	ϕ
aa^+	$1-\phi$

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Intuition:

- ϕ = density of full sites (or probability of presence)
- ψ tests the response to a perturbation

MARTIN, SIGGIA, ROSE (1973)

Observables

We wrote

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- We finish with the projection state $\langle O|$ (projects on all possible configurations)

$$\langle O| \exp(T\,\hat{W}) |P(0)\rangle = 1$$

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but, for an actual computation:

- We put the initial distribution instead of $|\vec{\phi}_0, \vec{\psi}_0\rangle$
- We finish with the projection state $\langle O|$ (projects on all possible configurations)
- We can insert operators to do measurements : the density at time t is

$$\langle O| \exp((T-t)\,\hat{W}) \frac{1}{N} \sum_i a_i^+ a_i \exp(t\,\hat{W}) |P(0)\rangle = \langle \hat{\rho}(t) \rangle$$

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And often for bosonic systems (here we have spins-$\frac{1}{2}$ or hard core bosons)

Can we also get non universal properties? Quantitative predictions for non-critical quantities?

Intermezzo:

exercise of classical mechanics

Equations of motion

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We have to study

$$\int\int \mathcal{D}\phi(t)\mathcal{D}\psi(t)\exp\left(-\mathcal{S}[\{\phi,\psi\}]\right)$$

with

$$\mathcal{S}[\{\phi,\psi\}] = \int_0^T \mathrm{d}t\ \left(\phi(t)\frac{\mathrm{d}\psi(t)}{\mathrm{d}t} - \tilde{W}(\phi(t),\psi(t))\right)$$

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Optimizing $\mathcal{S} \Rightarrow$ equations of motion (Hamilton-Jacobi !):

$$\begin{aligned} \frac{\mathrm{d}\psi}{\mathrm{d}t}(t) &= \partial_\phi \tilde{W}(\phi(t),\psi(t)) \\ \frac{\mathrm{d}\phi}{\mathrm{d}t}(t) &= -\partial_\psi \tilde{W}(\phi(t),\psi(t)) \end{aligned}$$

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with

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with

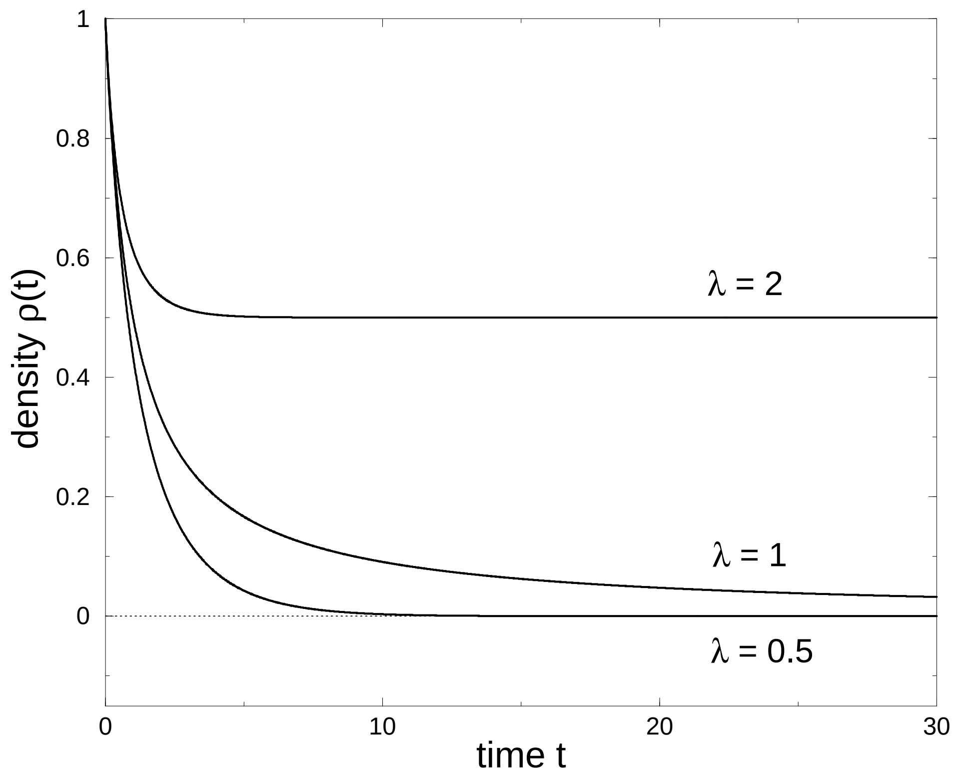
$$\tilde{W}(\phi,\psi) = \phi(e^{\psi}-1) + \lambda\phi(1-\phi)(e^{-\psi}-1)$$

$\tilde{W}$ is a conserved quantity.

Equations of motion: $\psi = 0$

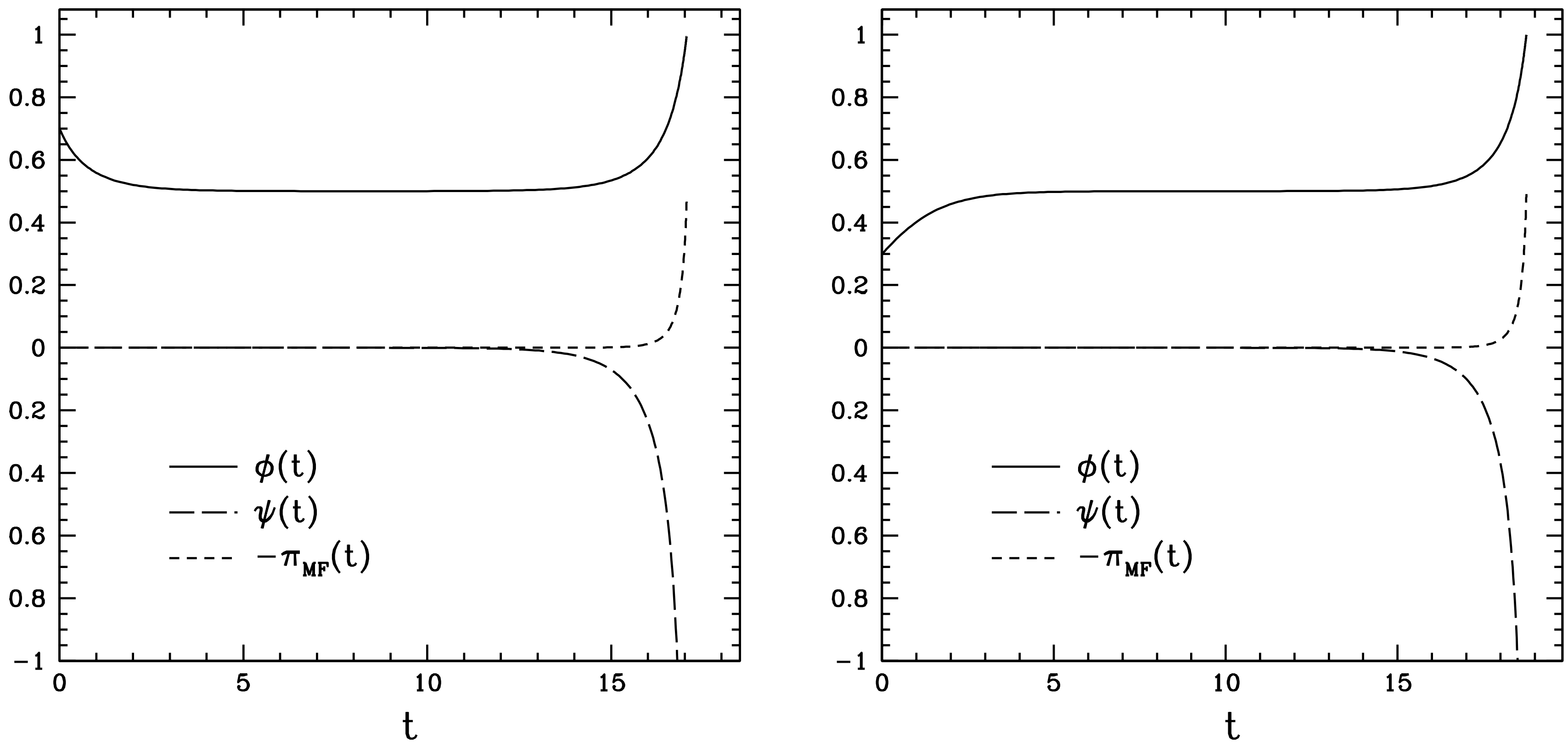
$\psi(t) = 0 \rightsquigarrow$ naive equation that one writes spontaneously, without taking care of fluctuations/correlations:

$$\frac{\mathrm{d}\phi(t)}{\mathrm{d}t} = -\lambda\phi(t)(\phi(t) - 1 + \frac{1}{\lambda})$$



Trajectories of the equations of motion

$$\psi(0) < 0$$



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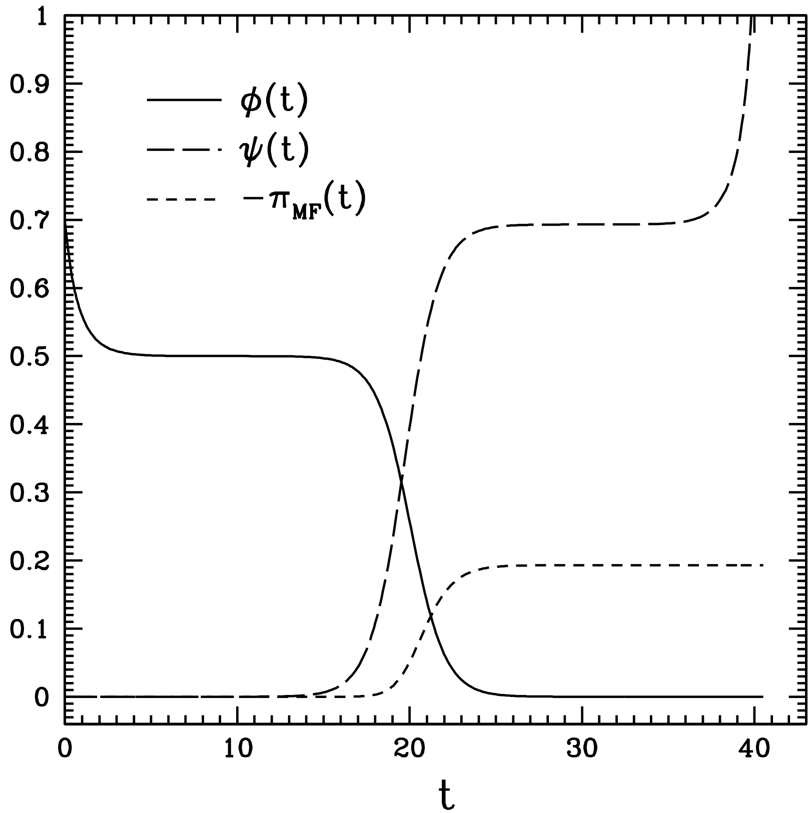

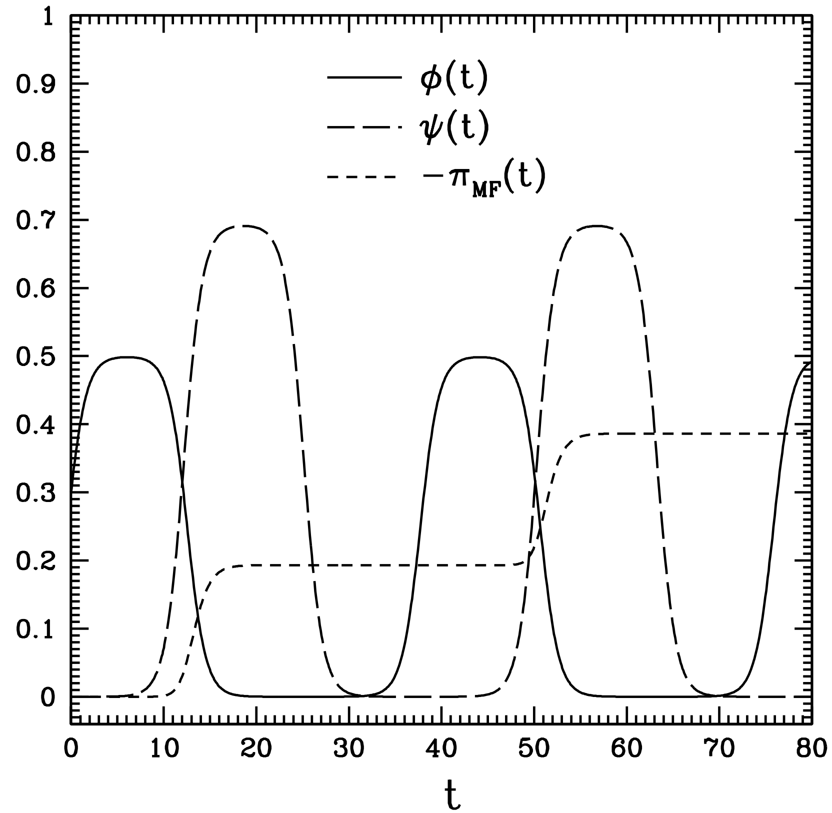

↑ Looks like an instanton ↑

Could it help calculate the large deviation function?

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$$= \int_{\psi(0)}^{\psi(T)} \phi(\psi) \mathrm{d}\psi - T \; E$$

with $T(E) \; E \to 0$ when $E \to 0$ (t and ψ are related)

Action of the instanton

And $\psi(0) \approx 0$:

$$\mathcal{S} = \int_{\psi(0)}^{\psi(T)} \phi(\psi)\mathrm{d}\psi = \int_{0}^{\psi(T)} (1 - \frac{e^{\psi}}{\lambda})\mathrm{d}\psi$$

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$\Rightarrow$ large deviation function in the $t \to \infty$ limit:

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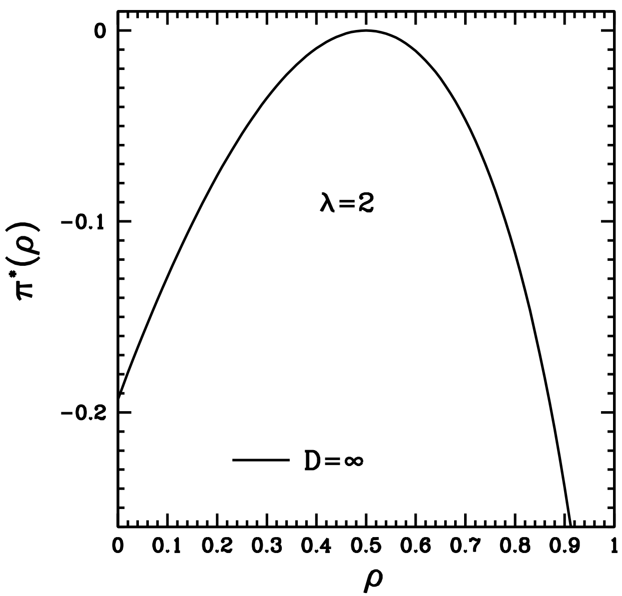

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Works numerically!

The mean field case —

full treatment

The mean field case

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and $\langle \rho_T |$ is the projection on states with density ρ_T.

The mean field case

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$$= \int_{\vec{\phi}(0)=\vec{\phi}_0, \vec{\psi}(0)=\vec{\psi}_0}^{\vec{\phi}(T)=\vec{\phi}_T, \vec{\psi}(T)=\vec{\psi}_T} \mathcal{D}\vec{\phi}(t)\,\mathcal{D}\vec{\psi}(t)\ \exp\left(-\mathcal{S}[\{\vec{\phi},\vec{\psi}\}]\right)$$

with

$$\mathcal{S}[\{\vec{\phi},\vec{\psi}\}] = \int_0^T \mathrm{d}t\ \left\{\sum_{i=1}^{N} \phi_i(t)\frac{\mathrm{d}\psi_i(t)}{\mathrm{d}t} - \tilde{W}(\vec{\phi}(t),\vec{\psi}(t))\right\}$$

and $\langle \rho_T |$ is the projection on states with density ρ_T.

How to compute this?

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How to compute this?

Let us compute the weight of a particular solution that we impose with Lagrange multipliers.

GAUNT & BAKER (1970), GEORGES & YEDIDIA (1990), GEORGES & YEDIDIA (1991)

Introducing multipliers

$\overline{\phi}_i(t)$ and $\overline{\psi}_i(t)$ are arbitrary functions.

Let $\overline{\chi}_i(t) = (1 - \overline{\phi}_i(t))(\exp(-\overline{\psi}_i(t)) - 1)$ and $\hat{\chi}_i = a_i^+(1 + a_i) - 1$.

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We constrain ϕ_i and ψ_i to follow $\overline{\phi}_i$ and $\overline{\psi}_i$. More precisely, we impose
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$\langle a_i^+ a_i(t)\rangle = \overline{\phi}_i(t)$ and $\langle\hat{\chi}_i\rangle(t) = \overline{\chi}_i(t)$
thanks to Lagrange multipliers $h_i(t)$ and $g_i(t)$:

$$\hat{W} = \hat{W}_{\text{ann}} + \lambda\hat{W}_{\text{cre}}$$

is changed for

$$\hat{W}(t) = \mu\hat{W}_{\text{ann}} + \lambda\hat{W}_{\text{cre}} + \sum_i \Big(h_i(t)(\hat{\phi}_i - \overline{\phi}_i(t)) - g_i(t)(\overline{\chi}_i(t) - \hat{\chi}_i)\Big)$$

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- And we optimize $\Pi[\{\overline{\phi}_i(t), \overline{\psi}_i(t)\}]$: after optimization $h_i = g_i = 0$ thus $\Pi = \Pi_0$.

The mean field case

$$\hat{W}(t) = \mu \hat{W}_{\text{ann}} + \lambda \hat{W}_{\text{cre}} + \sum_i \Big(h_i(t)(\hat{\phi}_i - \overline{\phi}_i(t)) - g_i(t)(\overline{\chi}_i(t) - \hat{\chi}_i) \Big)$$

We may separate the time dependent, non-operator part:

$$\hat{W}(t) = \hat{W}' + W''(t)$$

with

$$\hat{W}' = \mu \hat{W}_{\text{ann}} + \lambda \hat{W}_{\text{cre}} + \sum_i \Big(h_i(t)\hat{\phi}_i + g_i(t)\hat{\chi}_i \Big)$$

$$W''(t) = \sum_i \left(-h_i(t)\overline{\phi}_i(t) - g_i(t)\overline{\chi}_i(t) \right)$$

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For $\lambda > 0$, sites are coupled through $\hat{W}_{\rm cre}$ so we can't compute things easily. Let's take $\lambda = 0$; sites decouple:

$$\hat{W}' = \hat{W}'_1 \otimes \hat{W}'_2 \otimes \ldots \otimes \hat{W}'_N$$

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If we also take $\mu = 0$, $\hat{W}'_i$ has a triangular matrix. We can compute $\exp(T\hat{W}'_i)$, then $h_i(t)$ and $g_i(t)$: we find

$$\int_0^T W''_i(t)\mathrm{d}t = -\int_0^T \overline{\phi}_i(t)\frac{\mathrm{d}\overline{\psi}_i(t)}{\mathrm{d}t} + \text{boundary terms}$$

This is the kinetic part of the path integral action!

The mean field case

Now we do a perturbative expansion:

$$\Pi = \sum_{a=0}^{\infty} \sum_{b=0}^{\infty} \lambda^a \mu^b \Pi_{a,b}$$

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e.g. $$\langle a_i(t')a_i(t)\rangle = \overline{\phi}_i(t)(1 - \overline{\phi}_i(t')) \quad \text{if} \quad t < t',$$

$$\langle a_i(T)V_i(t)a_j^+(0)a_j(0)\rangle = \ldots$$

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In the mean field case (complete graph), if we look for a translation invariant solution ($\overline{\phi}$ and $\overline{\psi}$ independent on i)
only a few terms contribute and give

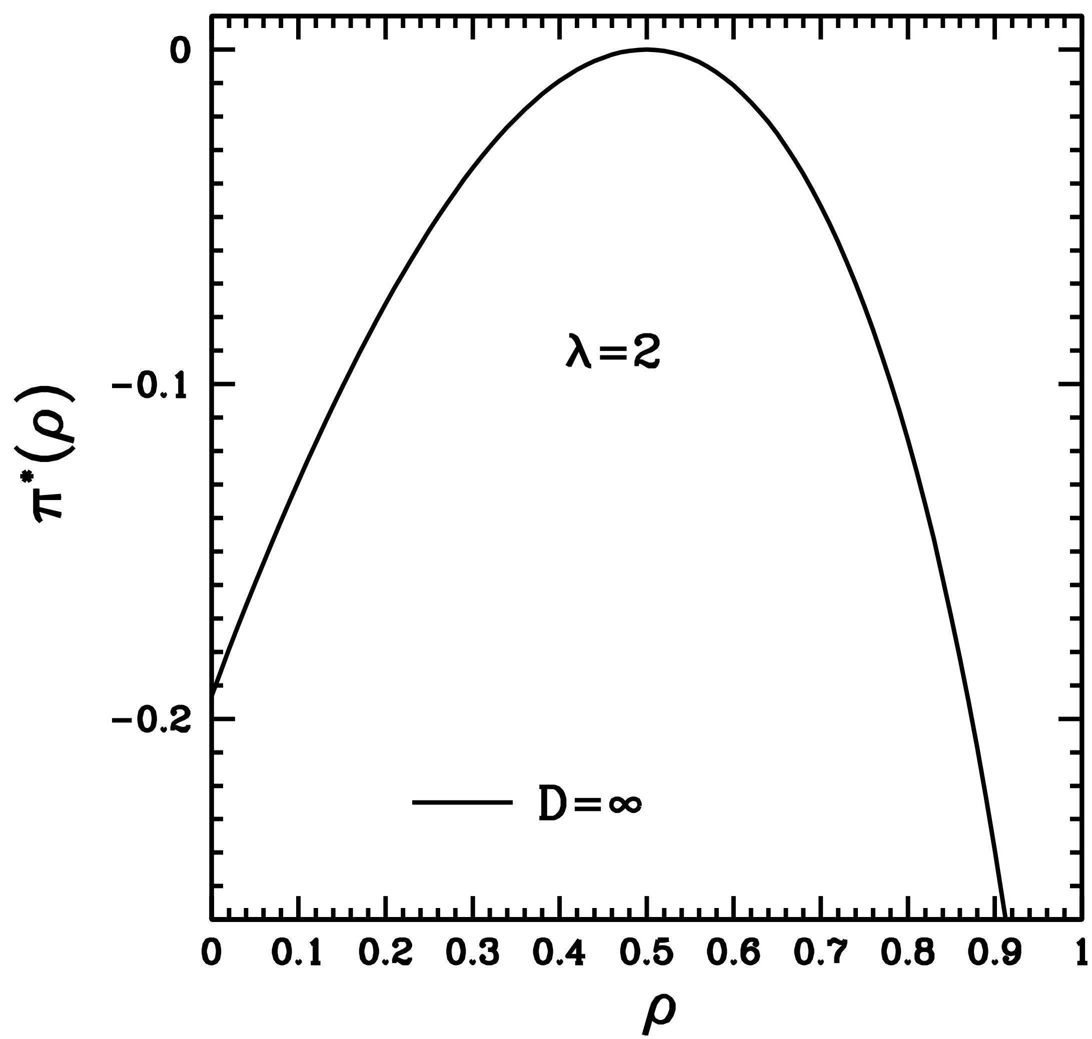
$$\Pi_{\mathrm{MF}}[\overline{\phi}(t),\overline{\psi}(t)] = N\int_0^T \mathrm{d}t \left(-\overline{\phi}(t)\frac{\mathrm{d}\overline{\psi}(t)}{\mathrm{d}t} + \tilde{W}_{\mathrm{MF}}(\overline{\phi}(t),\overline{\psi}(t))\right)$$

(boundary terms omitted) with

$$\tilde{W}_{\mathrm{MF}}(\phi,\psi) = \phi\,\big(\exp(\psi)-1\big) + \lambda\,\phi\,(1-\phi)\,\big(\exp(-\psi)-1\big)$$

The mean field case

This is what we studied in the classical mechanics exercise...



The mean field case

Bonus: discretizing the path integral (in a symmetric way between t and $t + \mathrm{d}t$), we get

$$\partial_t \pi_{MF}(\rho, t) = \tilde{W}_{\mathrm{MF}}\big(\rho, \partial_\rho \pi_{\mathrm{MF}}(\rho, t)\big)$$

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It helps understand the role of ψ:

$$\psi \quad \leftrightarrow \quad \partial_\rho \pi(\rho)$$

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But with the field theory we can get the corrections to mean field !

Beyond mean field

So far...

Stochastic process

$\downarrow$

Master equation

$\downarrow$

Quantum formalism

$\downarrow$

Field theory: $\Pi[\{\overline{\phi}_i(t), \overline{\psi}_i(t)\}]$

$\downarrow$

Large deviation function

$$\pi = \sum_{a=0}^{\infty} \sum_{b=0}^{\infty} \lambda^a \mu^b \pi_{a,b} \quad \text{with} \quad \mu \leftarrow 1$$

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Mean field:

$$\pi = \pi_{0,0} + \pi_{1,0} + \pi_{0,1} + \mathcal{O}(\frac{1}{z})$$

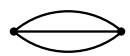
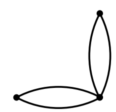
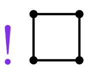
Graphical interpretation

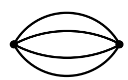
$\hat{V}$ writes as a sum over the links of the graph:

$$\hat{V} = \frac{1}{2D} \sum_i \sum_{j \in i} \int_0^T \mathrm{d}t \left((\hat{\phi}_i - \overline{\phi}_i(t))(\hat{\chi}_j - \overline{\chi}_j(t)) \right)$$

$\Rightarrow$ The terms of the λ-expansion can be drawn:

$$\pi = \pi_{\mathrm{MF}} + \frac{\lambda^2}{2!(2D)^2} D$$  $+$

$$\frac{\lambda^3}{3!(2D)^3} D$$  $$+ \frac{\lambda^4}{4!(2D)^4} D(2D-1)6$$  $$+ \frac{\lambda^4}{4!(2D)^4} \frac{D(D-1)}{2} 4!$$  $+$

$$\frac{\lambda^4}{4!(2D)^4} D$$  $+ \dots$

So that we know what terms are needed for each order in $\frac{1}{D}$.

The memory kernels

The resummation on μ yields memory kernels for non mean field terms:

$$\int_0^T \mathrm{d}t \int_0^T \mathrm{d}t' \, \langle (\tilde{\phi}_i(t) \; \tilde{\phi}_i(t') \rangle$$

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$$\int_0^T \mathrm{d}t \int_0^T \mathrm{d}t' \; \langle \tilde{\phi}_i(t) \tilde{\phi}_i(t') \rangle \; \exp\left(-\mu \int_{\min(t,t')}^{\max(t,t')} \mathrm{d}t'' \; \frac{\exp\left(\overline{\psi}_i(t'')\right)}{1 - \overline{\phi}_i(t'')} \right)$$

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Are the consequence of the projection of 2^N states onto the states $|\rho\rangle$ (even if the contact process is Markovian).

Results: λ_c hypercubic

We computed the equations of motion up to order $\frac{1}{D^2}$ included for hypercubic lattices.

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Easy result: setting $\psi(t) = 0$ yields the typical behaviour $\rho^*(\lambda)$ ($z = 2D$):

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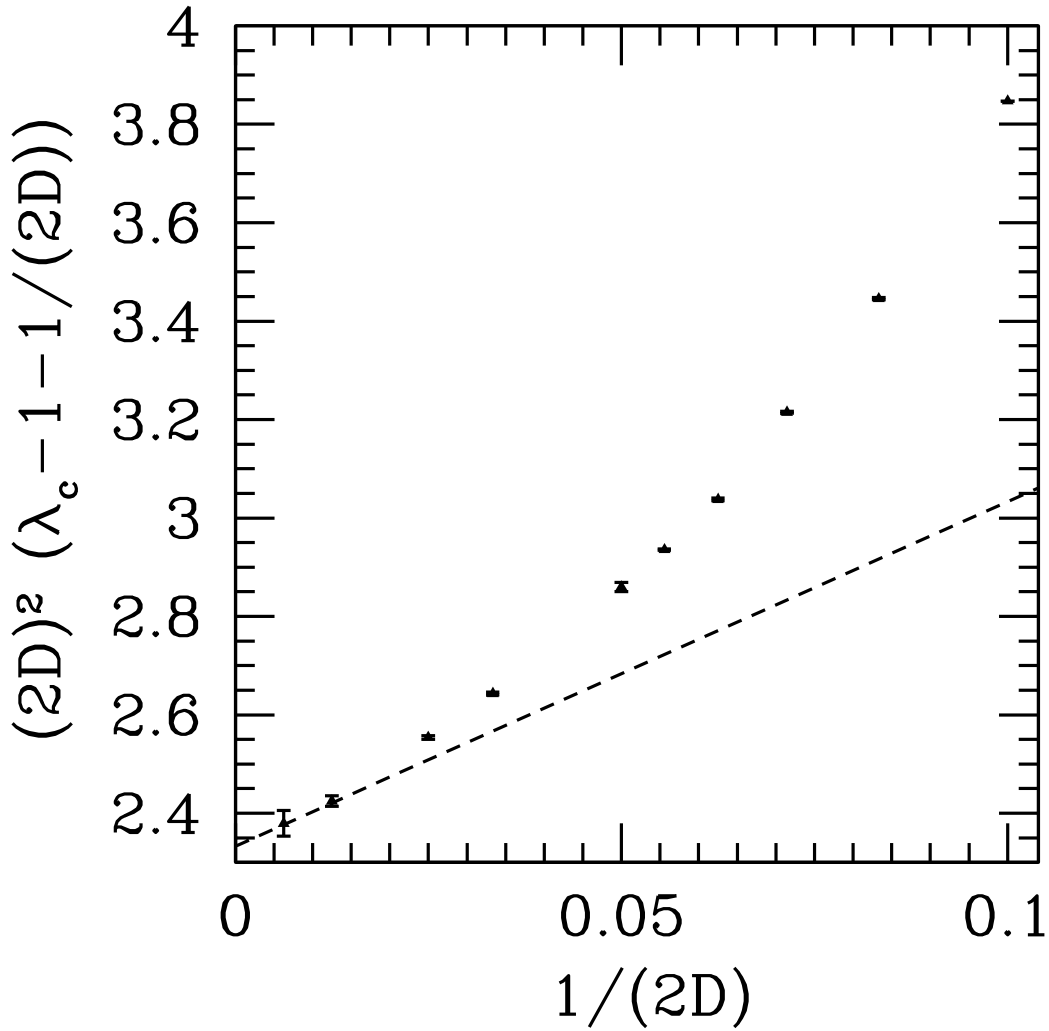
Satisfies the mathematicians' bounds.

LIGGETT, book of 1999

Results: λ_c hypercubic

Comparison with Monte-Carlo simulations:



Results: λ_c Cayley tree

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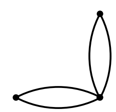
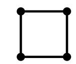
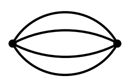
$\pi = \pi_{\mathrm{MF}} + \frac{\lambda^2}{2!z^2} z$  $+$

$\frac{\lambda^3}{3!z^3} z$  $+ \frac{\lambda^4}{4!z^4} \frac{z(z-1)}{2} 6$  $+ \frac{\lambda^4}{4!(2D)^4} \frac{D(D-1)}{2} 4!$  $+$

$\frac{\lambda^4}{4!z^4} \frac{z}{2}$  $+ \dots$

We just need to remove the loop terms.

Results: λ_c Cayley tree

$$\rho^* = 1 - \frac{1}{\lambda} - \frac{1}{\lambda^2 z} - \frac{6\lambda^2 + 11\lambda - 3}{6\lambda^4 z^2} + O(1/z^3)$$

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$$\lambda_{\mathrm{c}} = 1 + \frac{1}{z} + \frac{4}{3z^2} + O(1/z^3)$$

Results: λ_c Cayley tree

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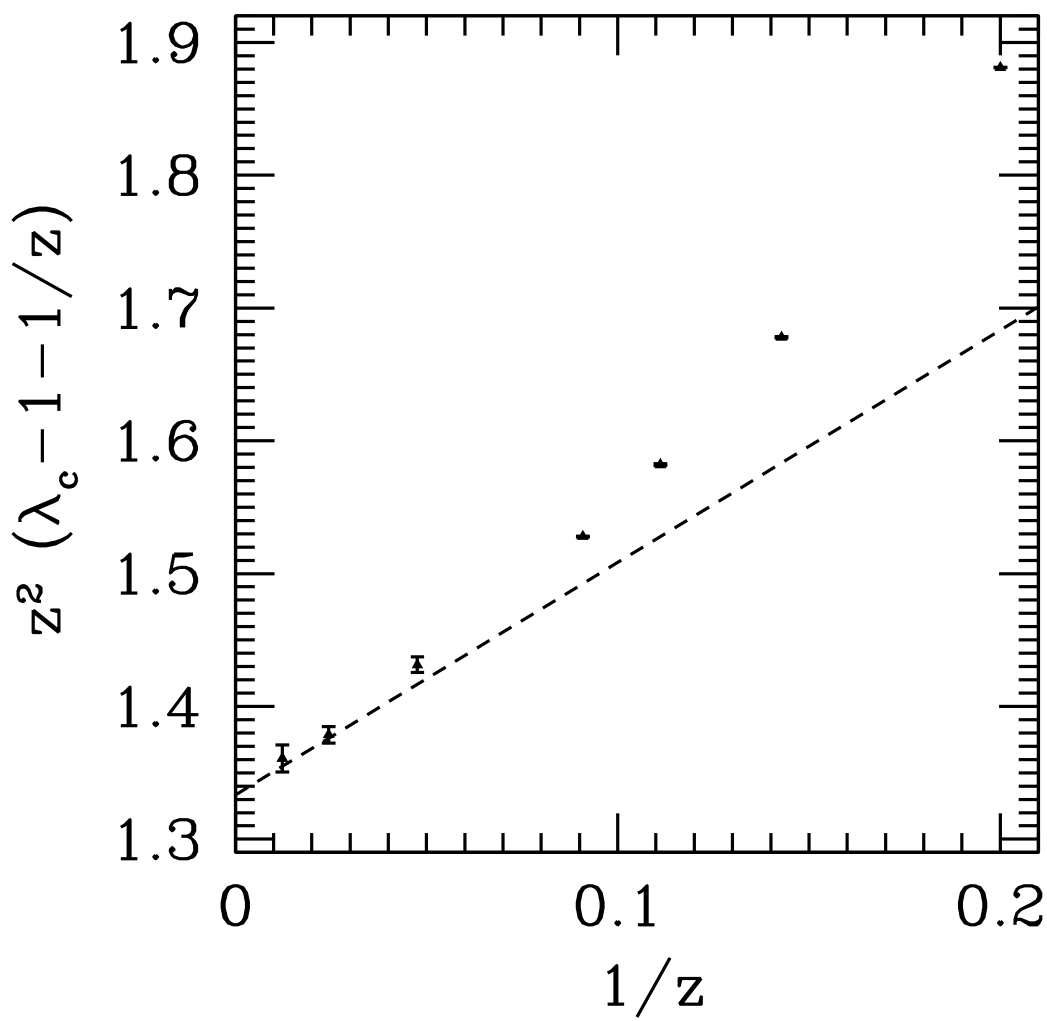
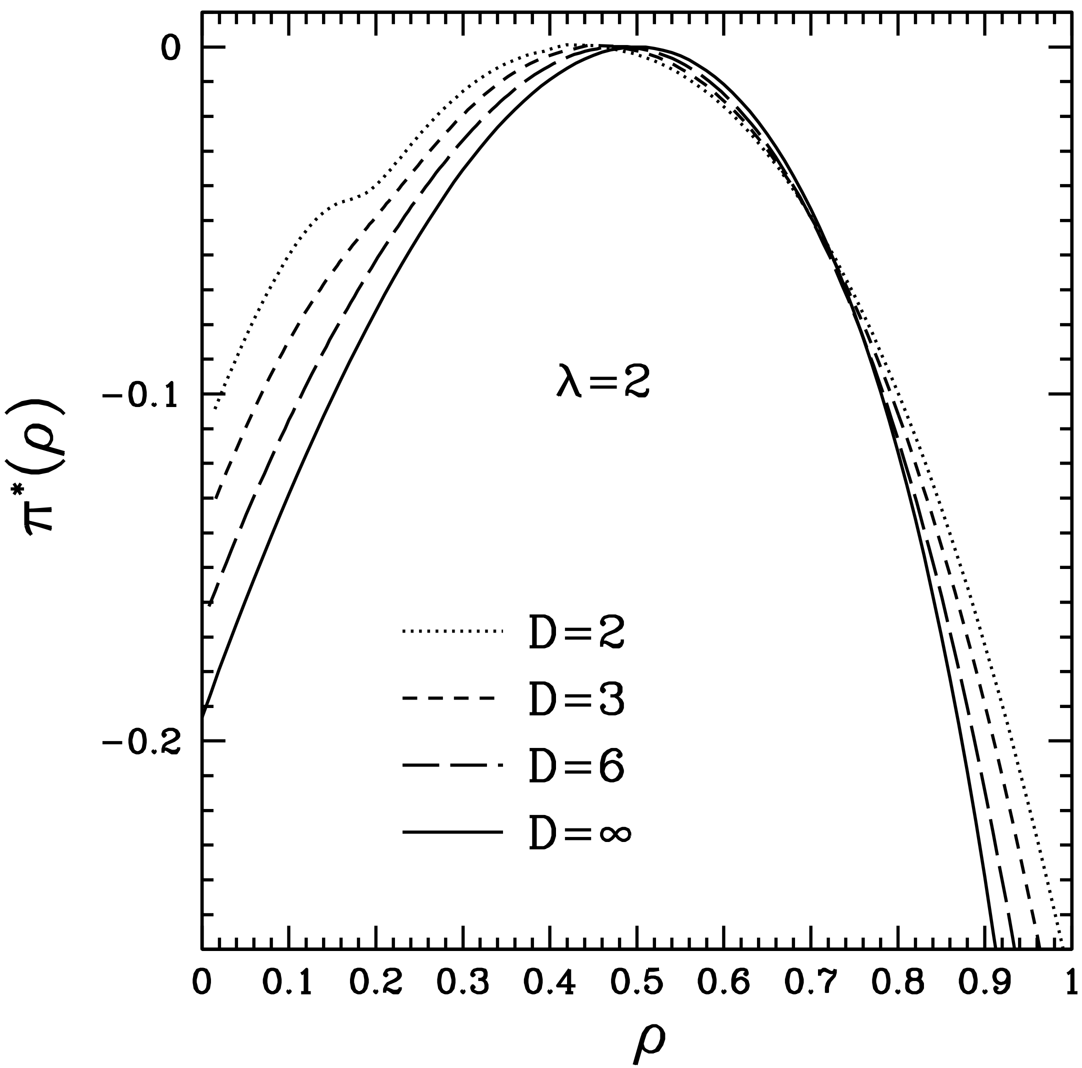


Results: large deviation function π

$\Rightarrow$ resolution for $\psi \neq 0$ (far more involving).
Here we stopped after order $\frac{1}{D}$.



Results: lifetime τ

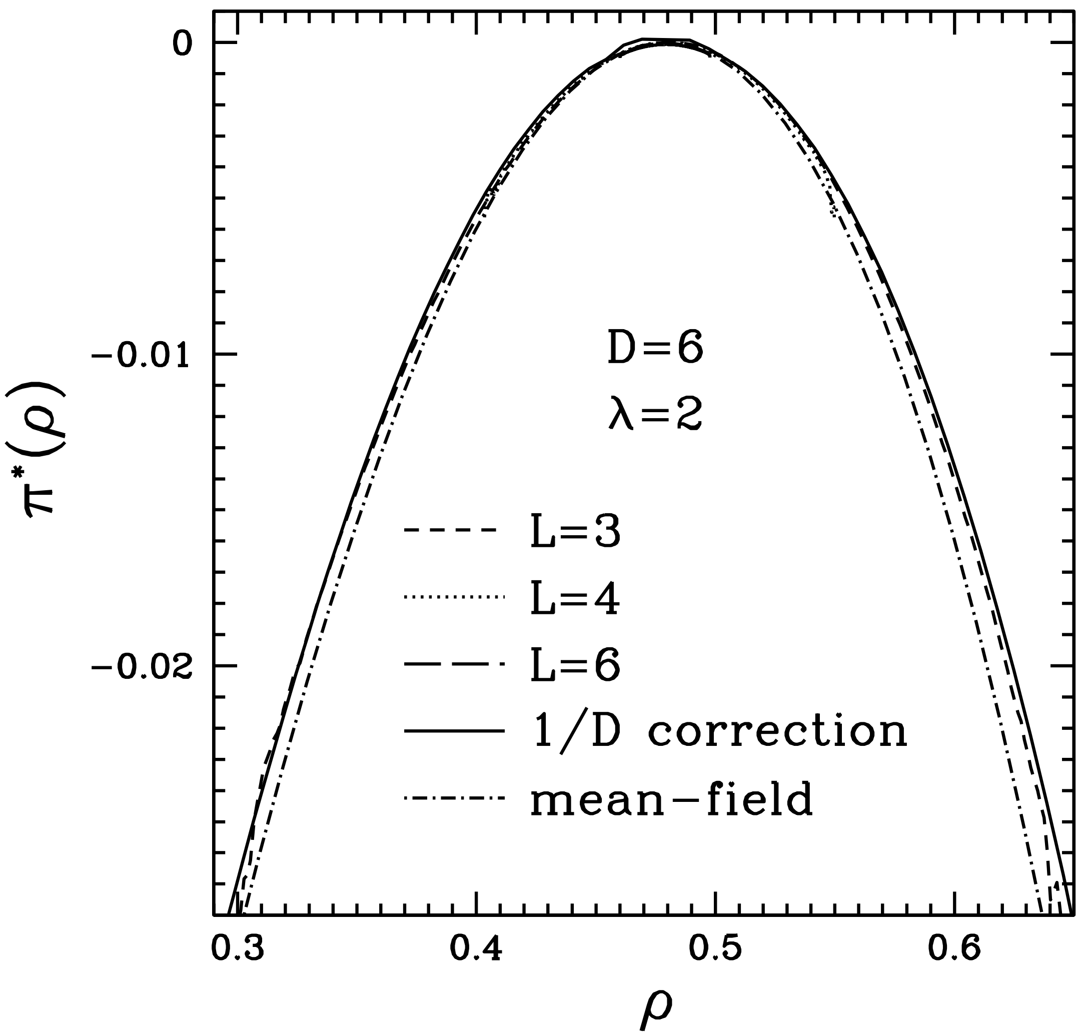
$\pi^*(\rho = 0) \rightarrow$ lifetime

In general needs hypergeometric functions, but special values of λ:

λ	$\pi(\rho = 0)$	Decimal approximation
3	$-\ln 3 + 2/3 + (-53/18 + \pi^2/3)/z$	$-0.432 + 0.345/z$
2	$-\ln 2 + 1/2 + (-107/36 + \pi^2/3)/z$	$-0.193 + 0.318/z$
5/3	$-\ln(5/3) + 2/5 + (-5413/1800 + \pi^2/3)/z$	$-0.111 + 0.283/z$
3/2	$-\ln(3/2) + 1/3 + (-1823/600 + \pi^2/3)/z$	$-0.072 + 0.252/z$
7/5	$-\ln(7/5) + 2/7 + (-270281/88200 + \pi^2/3)/z$	$-0.051 + 0.225/z$
$\ldots$	$\ldots$	$\ldots$

Results: large deviation function π

Comparison with Monte-Carlo simulations (after translation of the top point):
the curvature is OK



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Prospects:

- study of algorithms, glassy systems, ...
- requires to treat disorder