Part II – Markov dynamics and large deviation functions: first steps

MOTIVATIONS:

- Classical thermodynamics provides a frame to understand the <u>mean-value</u> of macroscopic observables (energy, density, susceptibility, ...)
- Physical systems are composed of numerous but finite # of particles → one wants to understand <u>fluctuations</u> of those observables.
- In particular: even at equilibrium, fluctuation of <u>time-integrated</u> observables are difficult to catch

e.g: currents, # events

GENERIC SETUP:

- Set of configurations $\{\mathcal{C}\}$ (finite or discrete)
  e.g: occupation numbers $\{n_i\}$ on sites i of a network/lattice.

- Transition <u>rates</u> $W(\mathcal{C}\to\mathcal{C}')$ between configurations $(\mathcal{C}\neq\mathcal{C}')$ (continuous-time dynamics)

- Evolution of the probability $P(\mathcal{C},t)$ of being in $\mathcal{C}$ at time t:

Master Equation

$$\boxed{\begin{aligned}\partial_t P(\mathcal{C},t) &= \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})P(\mathcal{C}',t) - r(\mathcal{C})P(\mathcal{C},t)\\ \text{with}\quad r(\mathcal{C}) &= \sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}') \quad \text{(escape rate from conf. } \mathcal{C})\end{aligned}}$$

one assumes $W(\mathcal{C}\to\mathcal{C})=0$

- Where does this come from? Come back to discrete time

$$P(\mathcal{C},t+dt) = \sum_{\mathcal{C}'} \underbrace{dt\,W(\mathcal{C}'\to\mathcal{C})}_{\substack{\text{probability to have}\\ \text{jumped from } \mathcal{C}' \text{ to } \mathcal{C}\\ \text{between } t \text{ and } t+dt}} P(\mathcal{C}',t) + \underbrace{\Big(1-dt\overbrace{\sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}')}^{r(\mathcal{C})}\Big)}_{\substack{\text{probability to have}\\ \text{remained in } \mathcal{C} \text{ btw}\\ t \text{ and } t+dt}} P(\mathcal{C},t)$$

This is also what we wrote $P(\mathcal{C},t+dt|\mathcal{C}',t)$

- To understand/remember/recover the second term, one remarks that it ensures probability conservation:

$$\sum_{\mathcal{C}} P(\mathcal{C},t+dt) = \sum_{\mathcal{C}} P(\mathcal{C},t)$$

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PROPERTIES :

- **Conservation of probability**: one has

$$\partial_t \sum_{\mathcal{C}} P(\mathcal{C},t) = 0$$

indeed $= \sum_{\mathcal{C}\mathcal{C}'} \{ W(\mathcal{C}'\to\mathcal{C})\, P(\mathcal{C}',t) - W(\mathcal{C}\to\mathcal{C}')\, P(\mathcal{C},t) \}$

as directly checked. Since $\sum_{\mathcal{C}} P(\mathcal{C},0) = 1$ this property remains valid at all times

- **Steady state**:

[This is the case if one can reach any state from any other through $\{W(\mathcal{C}\to\mathcal{C}')\}$, and if there are no recurrent states]

One assumes there exist a unique steady state $P_{st}(\mathcal{C})$ solution of $\partial_t P(\mathcal{C},t) = 0$

i.e. verifying the ~~detailed~~ global balance condition

$$\sum_{\mathcal{C}'} W(\mathcal{C}\to\mathcal{C}')\, P_{st}(\mathcal{C}) = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\, P_{st}(\mathcal{C}') \qquad \forall \mathcal{C}$$

- also named: "reversible dynamics"
"Equilibrium dynamics": detailed balance condition

$$W(\mathcal{C}\to\mathcal{C}')\, P_{eq}(\mathcal{C}) = W(\mathcal{C}'\to\mathcal{C})\, P_{eq}(\mathcal{C}') \qquad \forall \mathcal{C}, \mathcal{C}'$$

- the steady state is then called "equilibrium state" $P_{st} = P_{eq}$
- this condition is much more restrictive
- interpretation 1: there is no current of probability in the steady state

$$0 = \sum_{\mathcal{C}'} \Big(\underbrace{W(\mathcal{C}'\to\mathcal{C})\, P_{eq}(\mathcal{C}') - W(\mathcal{C}\to\mathcal{C}')\, P_{eq}(\mathcal{C})}_{\text{current of probability in } \mathcal{C} \ (=0)} \Big)$$

- interpretation 2: the dynamics starting from P_{eq} is **reversible**

using detailed balance condition

$$\underbrace{P_{eq}(\mathcal{C}_0)\, W(\mathcal{C}_0\to\mathcal{C}_1) \ldots W(\mathcal{C}_{K-1}\to\mathcal{C}_K)}_{} = \underbrace{P_{eq}(\mathcal{C}_K)\, W(\mathcal{C}_K\to\mathcal{C}_{K-1}) \ldots W(\mathcal{C}_1\to\mathcal{C}_0)}_{}$$

probability density of the history $\mathcal{C}_0 \to \ldots \to \mathcal{C}_K$ of the system

probability density of the time-reversed history $\mathcal{C}_K \to \ldots \to \mathcal{C}_0$ of the system

Those probabilities are the same: reversibility $\Leftrightarrow$ equilibrium.

very similar to the case of Langevin dynamics (part I)

OPERATOR NOTATION :

- One considers a vector space of basis $|\mathcal{C}\rangle$, $\mathcal{C}$ in the set of all configs.
- The space is orthonormal, the scalar product denoted $\langle\cdot|\cdot\rangle$:

$$\langle \mathcal{C}' | \mathcal{C} \rangle = \delta_{\mathcal{C}\mathcal{C}'} \qquad \text{(Kronecker delta)}$$

- Traduction of the Markov evolution : (master equation)

Defining the vector $|P(t)\rangle = \sum_{\mathcal{C}} P(\mathcal{C},t)\,|\mathcal{C}\rangle$ of components $P(\mathcal{C},t)$:

$$\partial_t |P(t)\rangle = \mathbb{W}\,|P(t)\rangle \quad \text{with} \quad \boxed{\mathbb{W}_{\mathcal{C}\mathcal{C}'} = W(\mathcal{C}'\to\mathcal{C}) - r(\mathcal{C})\delta_{\mathcal{C}\mathcal{C}'}}$$

$\mathbb{W}_{\mathcal{C}\mathcal{C}'}$ is the element $\mathcal{C}\mathcal{C}'$ of the matrix (or 'operator') $\mathbb{W}$.
named 'evolution operator'

- Traduction of the conservation of probability :

This vector is termed "the total vector", or "Attila's vector" (car toutes ses composantes sont des uns)

$$\partial_t \sum_{\mathcal{C}} P(\mathcal{C},t) = 0 \iff \sum_{\mathcal{C}} \mathbb{W}_{\mathcal{C}\mathcal{C}'} \;\; \forall \mathcal{C}' \iff \boxed{\langle -|\,\mathbb{W} = 0 \quad \text{with } \langle -| = \sum_{\mathcal{C}} \langle \mathcal{C}|}$$

in other words, the vector $\langle -|$ is a left eigenvector of $\mathbb{W}$ of eigenvalue 0.

- Traduction of the steady state property :
  - the global balance condition rewrites $\boxed{\mathbb{W}|P_{st}\rangle = 0}$

    in other words the vector $|P_{st}\rangle$ is a right eigenvalue of $\mathbb{W}$ of e.v. 0.
  - It must exists if probability is conserved, since $\mathbb{W}$ and $\mathbb{W}^T$ have the same spectrum (and a left eigenvector of $\mathbb{W}$ corresponds to a right e.v. of $\mathbb{W}^T$)

→ We thus see how, using Algebra, conservation of probability ensures the existence of a steady state.

- **Remark**: All other eigenvalues of $\mathbb{W}$ are of ~~modulus~~ real part <0.

This is the Perron-Frobenius theorem. It ensures that $e^{t\mathbb{W}}|P(0)\rangle = |P(t)\rangle \xrightarrow{t\to\infty} |P_{st}\rangle$.

• Translation of the detailed balance condition:

$$W(\mathcal{C}'\to\mathcal{C})\, P_{eq}(\mathcal{C}') = W(\mathcal{C}\to\mathcal{C}')\, P_{eq}(\mathcal{C}) \qquad \forall\, \mathcal{C}\,\mathcal{C}'$$

$$\Leftrightarrow \quad \mathbb{W}_{\mathcal{C}\mathcal{C}'}\, P_{eq}(\mathcal{C}') = \mathbb{W}_{\mathcal{C}'\mathcal{C}}\, P_{eq}(\mathcal{C})$$

$$\Leftrightarrow \quad P_{eq}^{-1/2}(\mathcal{C})\, \mathbb{W}_{\mathcal{C}\mathcal{C}'}\, P_{eq}(\mathcal{C}')^{1/2} = P_{eq}(\mathcal{C}')^{-1/2}\, \mathbb{W}_{\mathcal{C}'\mathcal{C}}\, P_{eq}(\mathcal{C})^{1/2}$$

Hence $\mathbb{W}^{sym}$ can be interpreted as a quantum Hamiltonian (see also Langevin case)

$$\Leftrightarrow \quad \boxed{\text{the 'symetrised operator' } \mathbb{W}^{sym} = \hat{P}_{eq}^{-1/2}\, \mathbb{W}\, \hat{P}_{eq}^{1/2} \text{ is symmetric}}$$

where $\hat{P}_{eq}$ is the diagonal operator of elements $P_{eq}(\mathcal{C})$.

In this case, $\mathbb{W}^{sym}$ (and hence $\mathbb{W}$) can be diagonalized in an orthonormal basis.

• Formal solution through matrix exponentiation:

* form 1: $\begin{cases} \partial_t |P(t)\rangle = \mathbb{W}\, |P(t)\rangle \\ |P(0)\rangle = |P_0\rangle = \sum_{\mathcal{C}} P_0(\mathcal{C})|\mathcal{C}\rangle \end{cases}$ has a solution $|P(\mathcal{C},t)\rangle = e^{t\mathbb{W}}\,|P_0\rangle = \sum_{n\geq 0} \frac{t^n}{n!}\, \mathbb{W}^n\, |P_0\rangle$

  but this form is not very useful.

* form 2: description in terms of a jump process. To eliminate the diagonal term in $\partial_t |P(t)\rangle_{\mathcal{C}} = \sum_{\mathcal{C}'} W(\mathcal{C}'\to\mathcal{C})\, |P(t)\rangle_{\mathcal{C}'} - r(\mathcal{C})|P(t)\rangle_{\mathcal{C}}$

  one sets $Q(\mathcal{C},t) = e^{-t\, r(\mathcal{C})}\, P(\mathcal{C},t)$ which verifies:

  Remark: if rates depend on time, set $Q(\mathcal{C},t) = e^{-\int_0^t r(\mathcal{C}(\tau))\,d\tau}\, P(\mathcal{C},t)$

$$(*) \quad \underline{\partial_t |Q(t)\rangle = W(t)\, |Q(t)\rangle} \quad \text{with } W(t)_{\mathcal{C}\mathcal{C}'} = W(\mathcal{C}'\to\mathcal{C})\, e^{t(r(\mathcal{C}')-r(\mathcal{C}))}$$

  this is a linear evolution with time-dependent operator $W(t)$

  The solution is $|Q(t)\rangle = \mathcal{T}exp\left(\int_0^t W\right) |Q(0)\rangle$ $(**)$

  where the time-ordered exponential $\mathcal{T}exp$ writes

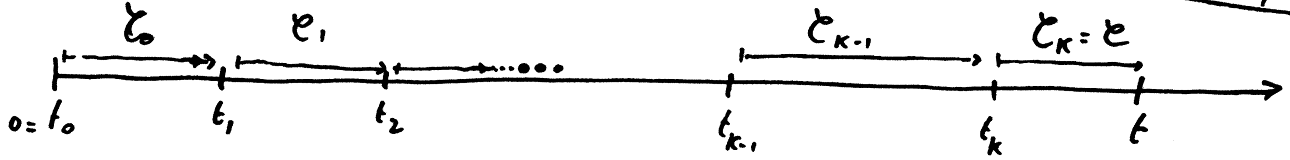
  $K \in \mathbb{N}$

$$\mathcal{T}exp\left(\int_0^t W\right) = \sum_{K\geq 0} \mathcal{T}\left(\int_0^t W\right)^K = \sum_{K\geq 0} \int_0^t dt_K \int_0^{t_K} dt_{K-1} \cdots \int_0^{t_2} dt_1\, W(t_K)\ldots W(t_1)$$

$$= \sum_{K\geq 0} \int_0^t dt_1 \int_{t_1}^t dt_2 \cdots \int_{t_{K-1}}^t dt_K\, W(t_K)\ldots W(t_1)$$

check that $(**)$ solves $(*)$ using this expression

Final form of the result: coming back to $P(\mathcal{C},t)$ from $Q(\mathcal{C},t)$:



sum over the number of jumps — sum over the histories of configurations — integrals over the time jump t_k's between $\mathcal{C}_{k-1}$ and $\mathcal{C}_k$

$$P(\mathcal{C},t) = \sum_{K\geq 0} \sum_{\mathcal{C}_0\cdots\mathcal{C}_K} \int_{t_0}^{t} dt_1 \int_{t_1}^{t} dt_2 \cdots \int_{t_{K-1}}^{t} dt_K$$

Ⓐ → $$r(\mathcal{C}_0)\, e^{-(t_1-t_0)\, r(\mathcal{C}_0)} \times \cdots \times r(\mathcal{C}_{K-1})\, e^{-(t_K-t_{K-1})\, r(\mathcal{C}_{K-1})}\, e^{-(t-t_K)\, r(\mathcal{C}_K)}$$

Ⓑ → $$\times \frac{W(\mathcal{C}_0\to\mathcal{C}_1)}{r(\mathcal{C}_0)} \times \cdots \times \frac{W(\mathcal{C}_{K-1}\to\mathcal{C})}{r(\mathcal{C}_{K-1})}$$

sampling of the initial condit° → $\times\ P_0(\mathcal{C}_0)$

- in Ⓐ: all the $r(\mathcal{C}_{k-1})\, e^{-(t_k-t_{k-1})\, r(\mathcal{C}_{k-1})}$ $(1\leq k\leq K)$ represent the probability that the time t_k of jump between $\mathcal{C}_{k-1}$ and $\mathcal{C}_k$ is t_k.
  - $e^{-(t-t_K)\, r(\mathcal{C}_K)}$ represents the probability not to jump between t_K and t

hence Ⓐ is the probability distribution of the times of jump $\{t_k\}$.

- in Ⓑ: $\dfrac{W(\mathcal{C}_{k-1}\to\mathcal{C}_k)}{r(\mathcal{C}_{k-1})}$ represents the (normalised) probability to jump to $\mathcal{C}_k$ starting from $\mathcal{C}_{k-1}$.

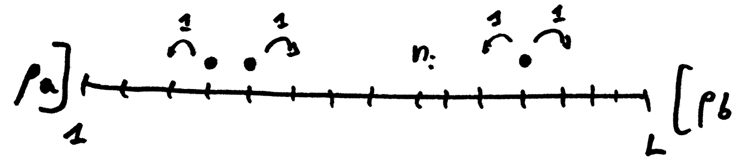
hence Ⓑ represents the probability of the history of configurations $\mathcal{C}_0 \ldots \mathcal{C}_K$

<u>Remark</u>: one can rewrite Ⓐ $= \prod_{k=0}^{K-1} r(\mathcal{C}_k) \cdot e^{-\int_0^t dt'\, r(\mathcal{C}_{t'})}$

check that this is the correct solution when rates depend on time and hence $r(\mathcal{C}) = r(\mathcal{C},t)$

LARGE DEVIATION FUNCTIONS

- **Examples and motivation:**



$n_i \in \{0,1\}$ occupation number

. total current on a time interval $[0,t]$: $Q = \#\{\text{jumps to the right}\} - \#\{\text{jumps to the left}\}$

in time: $Q \mapsto Q+1$ each time a particle jumps to the right

$Q \mapsto Q-1$ — — — left.

. total time and space integrated density:

$$\rho = \frac{1}{L} \int_0^t d\tau \sum_{i=1}^{L} n_i(t)$$

evolution in time: continuous (no jumps)

on each interval $[t_{k-1}, t_k[$ where the system does not change configurat°:

$$\rho \mapsto \rho + \frac{1}{L} \int_{t_{k-1}}^{t_k} d\tau \sum_{i=1}^{L} \overbrace{n_i(t_{k-1})}^{\text{constant}} = \rho + (t_k - t_{k-1}) \frac{1}{L} \sum_{i=1}^{L} n_i(t_{k-1})$$

. 'dynamical activity' K: on a time interval $[0,t]$, $K = \#\{\text{change of configurat°}\}$

in time: $K \mapsto K+1$ each time a configuration changes

. 'integrated escape rate' R: configuration at time τ, constant $\mathcal{C}_\tau = \mathcal{C}_{k-1}$ for $\tau \in [t_{k-1}, t_k[$

$$R = \int_0^t d\tau \, r(\mathcal{C}_\tau)$$

$$R = \sum_{k=1}^{K} (t_k - t_{k-1})\, r(\mathcal{C}_{k-1}) + (t - t_K)\, r(\mathcal{C}_K)$$

→ What is the distribution of those history-dependent observables?
What can we learn from those distribution in terms of
dynamical phase transitions?

- Generic cases: A_1 A_2 observables depending on the history of the system on $[0,t]$

A_1 defined as: $\begin{cases} A_1\big|_{t=0}=0 \ , & A_1 \mapsto A_1 + a_1(\mathcal{C}\to\mathcal{C}') \\ & \text{at each jump } \mathcal{C}\to\mathcal{C}' \end{cases}$

(A_1 only changes at jump times)

A_2 defined as $\quad A_2 = \int_0^t d\tau \; a_2(\mathcal{C}_\tau) = \sum_{k=1}^{K} (t_k - t_{k-1})\, a_2(\mathcal{C}_{k-1}) + (t-t_K)\, a_2(\mathcal{C}_K)$

(A_2 evolves continuously in time)

- Large deviation function:

× in direct space: for A an observable of type A_1 or A_2:

. the probability density of being in $\mathcal{C}$ at time t, having observed a value A of the observable, is denoted $P(\mathcal{C},A,t)$.

. the probability distribution of A at time t is

$$P(A,t) = \sum_{\mathcal{C}} P(\mathcal{C},A,t) \quad \text{and scales as}$$

$$\boxed{P(A,t) \sim \exp\left(+t\,\pi(A/t)\right)} \quad \text{as } t\to\infty$$

Other scalings are possible, but for finite systems, this is the most generic.

π is a dynamical equivalent of the entropy

$\pi(a)$ describes more than the mean and the variance of a → "large deviation function"

. π is difficult to determine in general ("microcanonical problem")

one prefers to go to the "canonical dynamical ensemble"

× in Laplace space: one has the $t\to\infty$ scaling

$$\boxed{\left\langle e^{-sA}\right\rangle \sim \exp\left(t\,\psi(s)\right)} \quad \text{as } t\to\infty$$

average taken on histories on time interval $(0,t)$

$\psi(s)$ is the cumulant generating function: (ψ is a "dynamical free energy")

$$\boxed{\partial_s^k \psi\big|_{s=0} = (-1)^k \frac{1}{t}\langle A^k\rangle_c}$$

$\langle A^k\rangle_c$ is the k^{th} cumulant of A.

- Interpretation of s; link between $\psi(s)$ and $\pi(a)$:

× Starting from $\langle e^{-sA}\rangle = \int dA\, P(A,t)\, e^{-sA}$ $A = at$

$$e^{+t\psi(s)} \sim \int da\, e^{\underbrace{t[\pi(a)-sa]}}$$

in the $t\to\infty$ limit, one may use the saddle point theorem

One has $\boxed{\psi(s) = \max_a(\pi(a)-sa)}$ ψ and π are legendre transformed.

If π is convex, one may perform the inverse legendre transform:

$$\boxed{\pi(a) = \min_s(\psi(s)+sa)}$$

× If $a^*(s)$ is the a where the $\max_a$ is reached
or if $s^*(a)$ — s —— $\min_s$ —— one says that $a^*(s)$ and s / $s^*(a)$ and a are 'conjugated'

× ⚠ s plays a role similar to the inverse temperature β:
it fixes the average value of A (in the same way as β fixes the average value of the energy E in thermodynamics)

× Indeed, in the large time limit: the mean value of an observable $\mathcal{O}$ in the 's-state' writes

$$\langle \mathcal{O}(\mathcal{C})\rangle_s \equiv \frac{\langle \mathcal{O}(\mathcal{C}(t))e^{-sA}\rangle}{\langle e^{-sA}\rangle} = \frac{1}{\langle e^{-sA}\rangle}\sum_{\mathcal{C},A} \overbrace{P(\mathcal{C},A,t)}^{\sim e^{t\pi(A/t)}\tilde{P}(\mathcal{C},A/t)}\, \mathcal{O}(\mathcal{C})\, e^{-sA} \qquad A = at$$

$$\sim \frac{\int da \sum_{\mathcal{C}} \tilde{P}(\mathcal{C},a)\mathcal{O}(\mathcal{C})\, e^{t(\pi(a)-sa)}}{\int da\; e^{t(\pi(a)-sa)}}$$

the saddle is reached at the same value $a = a^*(s)$

$$\langle \mathcal{O}(\mathcal{C})\rangle_s \sim \sum_{\mathcal{C}} \tilde{P}(\mathcal{C},a^*(s))\mathcal{O}(\mathcal{C}) \quad \text{i.e.} \quad \boxed{\langle \mathcal{O}(\mathcal{C})\rangle_s \overset{t\to\infty}{=} \langle \mathcal{O}(\mathcal{C})\rangle\big|_{A=a^*(s)t}}$$

mean value in the s-state, of $\mathcal{O}(\mathcal{C})$ at final time

Mean value of $\mathcal{O}(\mathcal{C})$ at final time for histories with $A = a^*(s)t$

In the same way, if $\pi(a)$ is convex: by inverse Legendre transform

$$\boxed{\langle O(\mathcal{C})\rangle\Big|_{A=at} \overset{t\to\infty}{=} \langle O(\mathcal{C})\rangle_{s=s^*(a)}}$$

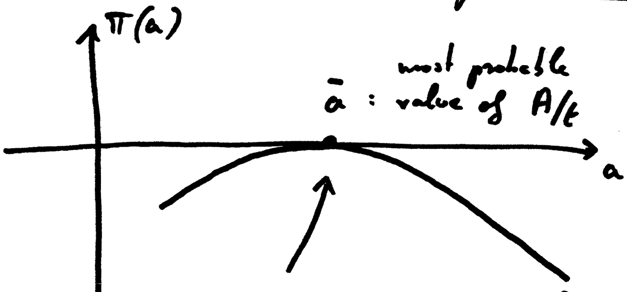
Mean value of $O(\mathcal{C})$ at final time for histories with a value $A=at$ of the observable A

Mean value in the s-state of $O(\mathcal{C})$ at final time:

$$\langle O(\mathcal{C})\rangle_s = \frac{\langle O(\mathcal{C}(t))\, e^{-sA}\rangle}{\langle e^{-sA}\rangle}$$

In other words, to characterize the value of the observable O in histories with a value $A\sim at$ of the observable A, one has to compute $\langle O(\mathcal{C})\rangle_s$ at $s=s^*(a)$.

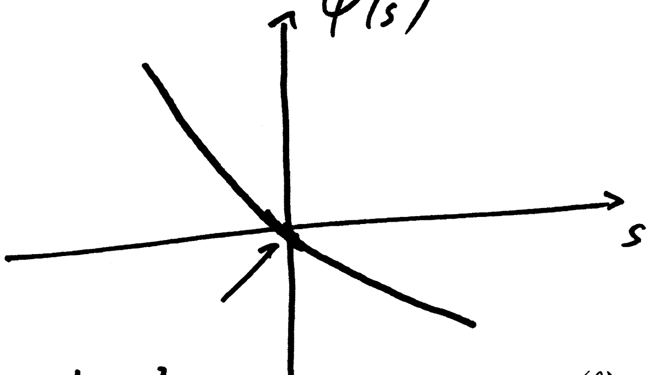
- Generic shape of the functions $\pi(a)$ and $\psi(s)$:



$$\bar{a} = a_1 = \frac{\langle A\rangle}{t} \quad \text{mean value}$$

$$a_2 = \frac{\langle A^2\rangle_c}{t} \quad \text{second cumulant}$$

$$\pi(a) \simeq 0 + 0 + -\frac{1}{2}\frac{(a-\bar{a})^2}{a_2} + \dots \Big\} \to P(A=at,t) \sim e^{-\frac{1}{2}\frac{(a-\bar{a})^2}{a_2}t} \quad [\text{Gaussian distribution}]$$



For a reference on large deviations, Laplace & Legendre transforms, see Hugo Touchette
The large deviation approach to statistical mechanics
Physics Reports 478 1 (2009)

$$\psi(s) \simeq -s a_1 + \frac{1}{2} a_2 s^2 + \dots$$

cf: $\dfrac{\langle A\rangle}{t} = -\dfrac{\partial\psi}{\partial s}\Big|_{s=0}$

$\dfrac{\langle A^2\rangle_c}{t} = \dfrac{\partial^2\psi}{\partial s^2}\Big|_{s=0}$