TD 7: Large Deviations of Radioactive Decay - Solutions

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We want to study the radioactive decay of some material. We denote $(x_n)_{i=1}^N$ the several particles, whose value is 1 is the particle remains excited and 0 if it has already disintegrated. Thus, $x_i \in \{0,1\}$ with initial condition $x_i(t=0)=1$ and a decay rate λ, *i.e.* its probability of disintegration at time t is $\lambda e^{-\lambda t}$. We assume the particles to be independent and denote

$$X_N(t) = \frac{1}{N}\sum_{i=1}^{N} x_i(t) \tag{1}$$

the density of radioactive particles.

1. What is the probability distribution of x_i.

Thermodynamic Limit. We consider the thermodynamic limit $N \to +\infty$.

2. Deduce the limit of X_N using the large number law.
3. What equation is fulfilled by this limit? Recall its physical meaning.

Dynamic Formalism for Large Deviations. We now want to study the large deviations of X_N, which depends on time t. We then want the dynamic version of X_N for $0 \le t \le T$. We start by considering M discrete time steps of length $\mathrm{d}t = \frac{T}{M}$. We then denote $X_N^j = X_N(j\mathrm{d}t)$. At the end, we are interested in the limit $M \to +\infty$. For teh moment we do not specify the law of x_i so that we remain general.

4. We denote $\mathbb{P}_x$ the probability given than the initial condition is $X_N = x$. Express
$$\mathbb{P}_{x_0}(X_N^1 = x_1, \dots X_N^M = x_M) \tag{2}$$
using only the random variable X_N^1.
5. Deduce that for any p,
$$\mathbb{P}_{x_0}(X_N^1 = x_1, \dots X_N^M = x_M) \le \exp\left(-N\mathrm{d}t \sum_{j=0}^{M-1}\left(p\frac{x_{j+1}-x_j}{\mathrm{d}t} - \mathcal{H}_M(x_j, p)\right)\right) \tag{3}$$
where we have defined
$$\mathcal{H}_M(x,p) = \frac{1}{N\mathrm{d}t}\ln\left(\mathbb{E}_x\left(e^{Np(X_N^1 - x)}\right)\right). \tag{4}$$
6. Going to the limit $M \to +\infty$, $\mathcal{H}_M(x,p) \to \mathcal{H}(x,p)$, the effective Hamiltonian. We consider a path $x(t)$ where we sample $x_j = x(j\mathrm{d}t)$. Deduce an upper bond of $\mathbb{P}_{x_0}(X_N(t) = x(t)$ for $0 \le t \le T)$.
7. Optimizing $p \in \mathbb{R}$, we perform a Legendre transform and find the Lagrangian
$$\mathcal{L}(x,\dot{x}) = \sup_{p\in\mathbb{R}}\left(p\dot{x} - \mathcal{H}(x,p)\right). \tag{5}$$
The inequality then becomes almost an equality (actually a log-equivalence). Define the action of large deviation and state the result of this section.

Application to the Radioactive Decay. We now come back to the initial problem.

8. Calculate the large deviation Hamiltonian.
9. Deduce that the Lagrangian is
$$\mathcal{L}(x,\dot{x}) = \lambda x + \dot{x}\left(1 - \ln\left(-\frac{\dot{x}}{\lambda x}\right)\right) \tag{6}$$
where we have assumed $\dot{x} < 0$ which is true physically.
10. Deduce the most probable trajectory? Comment.
11. Let us denote $\dot{x}(t=0) = -\lambda + v$ and let us remind that $x(t=0)=1$. Estimate $\mathcal{L}(x,\dot{x})$ for small v. Deduce the right initial condition and then the equation of the most probable trajectory.

Estimate of a Deviation. We consider a time T. We have proven that $\bar{x}(T) = \mathbb{E}(X_N(T)) = e^{-\lambda T}$. We are interested in a deviation to a and we want to estimate the probability that $X_N(T) = a$.

12. Going back to the time discretization, express the upper bound of the probability $\mathbb{P}(X_N(T) = a)$ using the discrete Hamiltonian.

13. When going to the limit $M \to +\infty$, there is an infinite number of integrals: this is a path integral. The probability then becomes:
$$\mathbb{P}(X_N(T) = a) = \int_{x(0)=1}^{x(T)=a} \mathcal{D}x\, e^{-N\mathcal{S}(x)}. \tag{7}$$
How to deduce the Gaussian approximation of this probability?

Correction

1. The random variable $x_i(t)$ is 0 or 1. Since its initial condition is 1,
$$\mathbb{P}(x_i(t) = 0) = \int_0^t \lambda e^{-\lambda s} \mathrm{d}s = 1 - e^{-\lambda t} \tag{8}$$
and then
$$\mathbb{P}(x_i(t) = 1) = \int_0^t \lambda e^{-\lambda s} \mathrm{d}s = e^{-\lambda t}. \tag{9}$$

2. The large number law states that $X_n(t)$ converges toward
$$\mathbb{E}(x(t)) = 1 \times e^{-\lambda t} + 0 \times (1 - e^{-\lambda t}) = e^{-\lambda t}. \tag{10}$$

3. We find back that the limit is solution of the equation
$$\dot{x} = -\lambda x \tag{11}$$
which is natural physically: the numbers of decays during $\mathrm{d}t$ is $\lambda x \mathrm{d}t$.

4. The exponential decay is a no memory law so we can write
$$\begin{aligned} \mathbb{P}_{x_0}(X_N^1 = x_1, \dots X_N^M = x_M) &= \mathbb{P}_{x_0}(X_N^1 = x_1)\mathbb{P}_{x_0}(X_N^2 = x_2 | X_N^1 = x_1) \dots & (12)\\ &= \mathbb{P}_{x_0}(X_N^1 = x_1)\mathbb{P}_{x_1}(X_N^1 = x_2) \dots \mathbb{P}_{x_{M-1}}(X_N^1 = x_M). & (13)\end{aligned}$$

5. We denote p the probability distribution of X_N^1 and calculate
$$\begin{aligned} \mathbb{P}_{x_0}(X_N^1 = x_1) &= \int_{X_N^1 = x_1} \mathrm{d}p(x) = \int_{X_N^1 = x_1} \mathrm{d}p(x) e^{Np(X_N^1 - x_1)} & (14)\\ &\leq \int \mathrm{d}p(x) e^{Np(X_N^1 - x_1)} = \mathbb{E}_{x_0}\left(e^{Np(X_N^1 - x_1)}\right). & (15)\end{aligned}$$
We deduce
$$\begin{aligned} \mathbb{P}_{x_0}(X_N^1 = x_1, \dots X_N^M = x_M) &= \mathbb{P}_{x_0}(X_N^1 = x_1)\mathbb{P}_{x_1}(X_N^1 = x_2) \dots \mathbb{P}_{x_{M-1}}(X_N^1 = x_M) & (16)\\ &\leq \mathbb{E}_{x_0}\left(e^{Np(X_N^1 - x_1)}\right) \dots \mathbb{E}_{x_{M-1}}\left(e^{Np(X_N^1 - x_M)}\right) & (17)\\ &= \exp\left(\sum_{j=0}^{M-1} \ln\left(\mathbb{E}_{x_j}\left(e^{Np(X_N^1 - x_j)} e^{Np(x_j - x_{j+1})}\right)\right)\right) & (18)\\ &= \exp\left(-N\mathrm{d}t \sum_{j=0}^{M-1}\left(p\frac{x_{j+1} - x_j}{\mathrm{d}t} - \mathcal{H}_M(x_j, p)\right)\right) & (19)\end{aligned}$$

6. Going to the limit, the sum becomes an integral and we find
$$\mathbb{P}_{x_0}(X_N(t) = x(t) \text{ for } 0 \leq t \leq T) \leq \exp\left(-N \int_0^T (p\dot{x}(t) - \mathcal{H}(x(t), p))\, \mathrm{d}t\right). \tag{20}$$

7. We define $\mathcal{S}(x) = \int_0^T L(x(t), \dot{x}(t))\mathrm{d}t$ and we have proven that
$$\mathbb{P}_{x_0}(X_N(t) = x(t) \text{ for } 0 \leq t \leq T) \sim \exp\left(-N\mathcal{S}(x)\right). \tag{21}$$

8. We start from the discrete Hamiltonian
$$\mathcal{H}_M(x, p) = \frac{1}{N\mathrm{d}t} \ln\left(\mathbb{E}_x\left(e^{Np(X_N^1 - x)}\right)\right). \tag{22}$$
At first order in $\mathrm{d}t$, $X_N^1 = x - \frac{1}{N}$ with probability $\lambda N x \mathrm{d}t$ and x with $1 - \lambda N x \mathrm{d}t$, then
$$\mathbb{E}_x\left(e^{Np(X_N^1 - x)}\right) = 1 - \lambda N x \mathrm{d}t + \lambda N x \mathrm{d}t e^{-p} + o(\mathrm{d}t). \tag{23}$$
Thus,
$$\mathcal{H}_M(x, p) = \frac{1}{N\mathrm{d}t} \ln\left(1 + (e^{-p} - 1)\lambda N x \mathrm{d}t + o(\mathrm{d}t)\right) \to (e^{-p} - 1)\lambda x. \tag{24}$$

9. We denote $f(p) = p\dot{x} - \mathcal{H}(x,p) = p\dot{x} - (e^{-p}-1)\lambda x$. We want its maximum in p, therefore we derive:
$$0 = f'(p) = \dot{x} + e^{-p}\lambda x \Longrightarrow p = -\ln\left(-\frac{\dot{x}}{\lambda x}\right) \tag{25}$$
assuming $\dot{x} < 0$, which is physical. Thus,
$$\mathcal{L}(x,\dot{x}) = -\dot{x}\ln\left(-\frac{\dot{x}}{\lambda x}\right) + \left(\frac{\dot{x}}{\lambda x}+1\right)\lambda x = \lambda x + \dot{x}\left(1 - \ln\left(-\frac{\dot{x}}{\lambda x}\right)\right) \tag{26}$$

10. To get the most probable trajectory, we minimize the action. We may use the Euler-Lagrange equations but here it is easier to use the energy conservation. The impulsion p can be written as
$$p = \frac{\partial \mathcal{L}}{\partial \dot{x}} = -\ln\left(-\frac{\dot{x}}{\lambda x}\right) \tag{27}$$
and then the Hamiltonian
$$\mathcal{H} = -\dot{x} - \lambda x. \tag{28}$$
Finally, the conservation of energy gives
$$\ddot{x} = -\lambda \dot{x}. \tag{29}$$
This is coherent with the firs part but disappointing since it is of second order. This comes from the initial condition for $\dot{x}$ which is to be specified. If chosen properly, we would have $\mathcal{H} = 0$ and then $\dot{x} = -\lambda x$.

11. We have $\mathcal{H} = -\dot{x} - \lambda x = v + \lambda - \lambda$ *i.e.* $-\dot{x} = v + \lambda x$. We may rewrite the Lagrangian for an extremal trajectory
$$\begin{aligned}
\mathcal{L} &= \lambda x + \dot{x}\left(1 - \ln\left(-\frac{\dot{x}}{\lambda x}\right)\right) && (30)\\
&= \lambda x - (v+\lambda x)\left(1 - \ln\left(1+\frac{v}{\lambda x}\right)\right) && (31)\\
&= \lambda x \ln\left(1+\frac{v}{\lambda x}\right) - v\left(1 - \ln\left(1+\frac{v}{\lambda x}\right)\right) && (32)\\
&= \lambda x\left(\frac{v}{\lambda x} - \frac{1}{2}\left(\frac{v}{\lambda x}\right)^2\right) - v\left(1 - \frac{v}{\lambda x}\right) + o\left(\left(\frac{v}{\lambda x}\right)^2\right) && (33)\\
&= \frac{\lambda x}{2}\left(\frac{v}{\lambda x}\right)^2 + o\left(\left(\frac{v}{\lambda x}\right)^2\right) && (34)
\end{aligned}$$
We conclude that the Lagrangian is minimal for $v = 0$ as expected. We then have $\dot{x} = -\lambda x$.

12. We have
$$\mathbb{P}(X_N(T) = a) \leq \int \prod_{j=1}^{M-1} \mathrm{d}x_j \exp\left(-N\mathrm{d}t \sum_{j=0}^{M-1}\left(p\frac{x_{j+1}-x_j}{\mathrm{d}t} - \mathcal{H}_M(x_j,p)\right)\right) \tag{35}$$
where we have setted $x_0 = 1$ and $x_M = a$.

13. The action is minimal close to the equilibrium path. We have $\mathcal{S}(\bar{x}) = 0$ and $\frac{\delta \mathcal{S}}{\delta x}(\bar{x}) = 0$ where δ is for the functional derivative. We then need to go to second order, the Gaussian order:
$$\mathcal{S}(x) \approx \frac{1}{2}(x-\bar{x})(t)\frac{\delta^2 \mathcal{S}}{\delta x(t)\delta x(s)}(\bar{x})(x-\bar{x})(s). \tag{36}$$
Thus the probability becomes
$$\mathbb{P}(X_N(T) = a) = \int_{y(0)=0}^{y(T)=a-\bar{x}(T)} \mathcal{D}x\, e^{-\frac{N}{2}y(t)\frac{\delta^2\mathcal{S}}{\delta x(t)\delta x(s)}y(s)}. \tag{37}$$
We recognize a Gaussian, thus it can be solved exactly using the inverse operator of $\frac{\delta^2 \mathcal{S}}{\delta x(t)\delta x(s)}$, but this is a story for next year.