1. Propagator and the saddle-point approximation.

Consider a process in zero spatial dimensions, which is fully characterised by an integer number n and by the probability $P_n(t)$ that this integer takes the value n at time t. Assuming that $n = 0$ at time $t = 0$ write down, within the Doi-Peliti formalism,

(a) the formal expression of $P_n(t)$ as the expectation value of a suitable operator on the vacuum $|0\rangle$, denoting by H the normally-ordered Hamiltonian of the system. *[Remember that $\langle n'|n\rangle = n!\delta_{n',n}$]*

(b) the corresponding expression as a coherent-state path integral and cast it in the form $P_n(t) = \int \mathscr{D}\phi\mathscr{D}\phi^* \mathrm{e}^{-S_{n,t}[\phi^*,\phi]}$, with suitable $S_{n,t}$.

(c) the saddle-point equations for the action $S_{n,t}[\phi^*,\phi]$, which determine the saddle-point fields $\bar{\phi}^*$ and $\bar{\phi}$. *[Due to the presence of boundary terms, care is required when considering the variations of $S_{n,t}$ with respect to the boundary fields ϕ_0, ϕ_t, ϕ_0^*, and ϕ_t^*.]*

As an application, consider the Poisson process defined by transitions $n \to n+1$ occurring with a rate $W(n \to n+1) = \lambda$.

(d) Write down the master equation for $P_n(t)$ and solve it by introducing the generating function $g(x,t) = \sum_{n=0}^{\infty} x^n P_n(t)$.

(e) Determine the (Doi-Peliti) Hamiltonian H corresponding to this Poisson process.

(f) For this Hamiltonian, solve the saddle-point equations determined at point (c) and calculate the corresponding value of the action $\bar{S}_{n,t} \equiv S_{n,t}[\bar{\phi}^*,\bar{\phi}]$. Compare the saddle-point estimate $\simeq \mathrm{e}^{-\bar{S}_{n,t}}$ of the path-integral for $P_n(t)$ at point (b) with the exact expression determined at point (d) and comment on this result.

Consider, now, the "phase-space" path integral for the Poisson process, with the same rules and initial conditions as those introduced above.

(g) Write down the Hamiltonian of the process, such that $\dot{P}_n(t) = -H(\hat{p},n)P_n(t)$, where $\hat{p} = -i\partial_n$ is the "momentum operator".

(h) Derive the phase-space path integral representation of $P_n(t)$.

(i) Estimate $P_n(t)$ from the saddle-point approximation of the path integral determined at point (h). Compare this result to that of points (f) and (d) and comment.

2. Activation over a potential barrier

Consider the master equation for a system described by an integer n and generic transition rates $W(n \to n+r)$ and cast it in the form discussed in the lecture, i.e.,

$$\partial_t P(n,t) = -H(\hat{p},n)P(n,t), \tag{1}$$

where $\hat{p} = -i\partial_n$ is the "momentum operator".

(a) Expand $H(\hat{p},n) = \hat{p}A(n) + \hat{p}^2B(n) + \mathscr{O}(\hat{p}^3)$: determine the expression of $A(n)$ and $B(n)$ in terms of the transitions rates and argue that they correspond to the "drift" and "diffusion" coefficients of the variable n (e.g., n could be the position of a random walker along a line).

Assume that, within the approximation discussed at point (a), one takes the continuum limit (think of the random walker), such that $n \to q$, where the variable q takes continuous values and $\hat{p} = -i\partial_q$, with $P(n,t) \to P(q,t)$.

(b) Assuming that $B = \gamma k_B T$ (with γ a kinetic coefficient and T the temperature, see below) does not depend on q and that higher-orders in the expansion at point (a) can be neglected, determine the (equilibrium) stationary distribution $P_{\text{eq}}(q)$. Fix $A(q)$ such that $P_{\text{eq}}(q)$ corresponds to the thermal equilibrium distribution $\propto \exp\{-V(q)/(k_BT)\}$ at temperature T of an overdamped particle with coordinate q in a potential $V(q)$.

Assume that the potential $V(q)$ is such that $V \to \pm\infty$ for $q \to \mp\infty$, with only two stationary points: a local minimum for $q = 0$, with $V(q = 0) = 0$, and a local maximum for $q = q_M > 0$.

(c) Write down the phase-space path-integral expression for $P_{1|1}(q,t|q_0,t_0)$. Determine the equation of motion along the optimal paths which are extremal trajectories of the associated action and sketch these paths in the "phase space" (p,q).

(d) Assuming that $q \simeq 0$ at $t = 0$, determine the probability to reach q_M along the stationary paths. Show that this implies that the probability to overcome the potential barrier is $\propto \exp\{-V(q_M)/(k_BT)\}$. How long does it take to reach q_M?