ICFP M2 – Selected Topics in Statistical Field Theory
TD n° 6 – Kramers' escape problem, two ways

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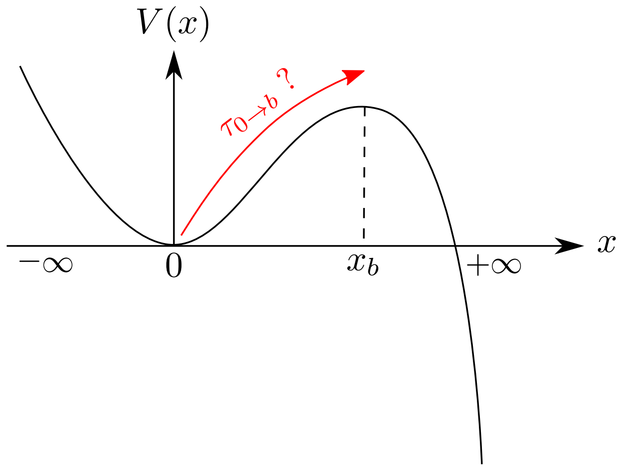

Figure 1: Kramers' escape problem: What is the typical time it takes for thermal fluctuations to help a particle pass the potential barrier?

Let us consider a particle of coordinate $x(t)$ undergoing overdamped dynamics at temperature T in a static one-dimensional potential $V(x)$ such as the one represented in Fig. 1. The corresponding Langevin equation reads

$$\eta \partial_t x(t) = -V'(x) + \xi(t)\,, \tag{1}$$

where $\eta > 0$ is a friction coefficient and $\xi(t)$ is a Gaussian white noise: $\langle \xi(t) \rangle = 0$ and $\langle \xi(t)\xi(t') \rangle = 2\eta T \delta(t-t')$ where T is measured in units k_{B}. Below, we set $\eta = 1$ by re-scaling time accordingly.

The particle is initially located in a local minimum of the potential at $x = 0$. The closest local maximum is at $x = x_b$. We aim at computing the typical time $\tau_{0\to b}$ for the particle to escape the local minimum $x = 0$ and pass the barrier at $x = x_b$.

A – Fokker-Planck's approach

We slightly modify the problem to a situation where the particle is automatically re-injected at $x = -\infty$ each time it reaches $x = x_b$. This consists in setting an absorbing boundary condition at $x = x_b$ and periodic boundary conditions. This non-equilibrium situation corresponds to a finite current of particles, which is expected to reach a non-equilibrium steady-state value, $J_{\mathrm{NESS}} > 0$, and which can be used to deduce the typical escape time *via* the relation $\tau_{0\to b} \sim J_{\mathrm{NESS}}^{-1}$.

(1) Write down the Fokker-Planck equation governing the evolution of the probability distribution $P(x,t)$. Express the absorbing boundary condition.

(2) Identify the current $J(x,t)$ defined such that the Fokker-Planck equation reads as a probability conservation equation

$$\partial_t P(x,t) + \partial_x J(x,t) = 0\,, \tag{2}$$

(3) In the non-equilibrium steady-state, $P(x,t)$ and $J(x,t)$ converge to the constant $P_{\rm NESS}(x)$ and $J_{\rm NESS}$, respectively. Solve for $P_{\rm NESS}(x)$ in terms of $J_{\rm NESS}$ and another constant α_0 to be determined by the absorbing boundary condition.

(4) Use the normalization of $P_{\rm NESS}(x)$ to express $J_{\rm NESS}$, and Kramers' escape time $\tau_{0\to b}$, in terms of two nested integrals.

(5) Restricting the analysis to temperatures T much smaller than the typical variations of $V(x)$, perform the following saddle-point approximations,

$$V(x) \simeq V(0) + \frac{1}{2}\,V''(0)\,x^2 \text{ around } x=0\,, \tag{3}$$

$$V(x) \simeq V(x_b) + \frac{1}{2}\,V''(x_b)\,(x-x_b)^2 \text{ around } x=x_b\,, \tag{4}$$

to simplify the expression of $\tau_{0\to b}$ into nested Gaussian integrals.

(6) Decouple the nested Gaussian integrals and arrange their boundaries of integration in order to obtain an explicit formula for $\tau_{0\to b}$, Kramers' escape time.

(7) Comment and discuss the domain of validity of the final result.

B – Martin-Siggia-Rose's approach

(1) Write down the MSR action functional $S[x,\hat{x}]$ corresponding to the dynamics in Eq. (1).

(2) Write down $P_{0\to b}(\tau)$, the probability for the particle to go from $x=0$ to $x=x_b$ in a given time τ, in terms of a MSR path integral.

(3) Write down the Euler-Lagrange equations (saddle point equations) on the fields x and $\mathrm{i}\hat{x}$.

(4) Identify a trivial pair of solutions, $x_{\rm cl}(t)$ and $\mathrm{i}\hat{x}_{\rm cl}(t)$, of the saddle point equations. Compute $S[x_{\rm cl},\hat{x}_{\rm cl}]$, and the corresponding probability $P_{0\to b}(\tau)$.

(5) There is another pair of solutions of the saddle point equations, $x_{\rm q}(t)$ and $\mathrm{i}\hat{x}_{\rm q}(t)$. If you manage to guess it (and check it is indeed a solution), go directly to question (8). Otherwise, we make an analogy with Quantum Mechanics by replacing $x\to q$ and $\mathrm{i}\hat{x}\to p$ where q and p will be interpreted as position and momentum. Show that the MSR action functional can be re-written in a quite standard Lagrangian formulation

$$S[x,\hat{x}] \to S[q,p] = \int_0^\tau \mathrm{d}t\ \left[p\dot{q} - H(q,p)\right] \tag{5}$$

where $H(p,q)$ is a Hamiltonian to be expressed. Note that we started from dissipative and stochastic dynamics and mapped them onto a Hamiltonian problem with purely unitary dynamics.

(6) Show that the trivial pair of solution corresponds to the zero-energy ground state $H(p,q)=0$. Show that there is another solution to $H(q,p)=0$.

(7) Draw the phase portrait of $H(q,p)$ –the lines of equal energy in the $p-q$ plane– at zero energy. Represent the two pairs of solutions and analyze their stability in the $p-q$ plane. Compute the action $S[q,p]$ of both solutions.

(8) Deduce the second non-trivial solution of the original saddle point equations, $x_{\mathrm{q}}(t)$ and $\mathrm{i}\hat{x}_{\mathrm{q}}(t)$. Compute $S[x_{\mathrm{q}}, \hat{x}_{\mathrm{q}}]$, and the corresponding probability $P_{0\to b}(\tau)$.

(9) Extract the expression for Kramers' escape time, $\tau_{0\to b}$.

C – Challenge

Write down the first law of thermodynamics for the non-equilibrium steady state considered in Section A. Identify the work and the heat in this Kramers' problem.