A path integral approach to Kramer's escape problem.

Why this approach?

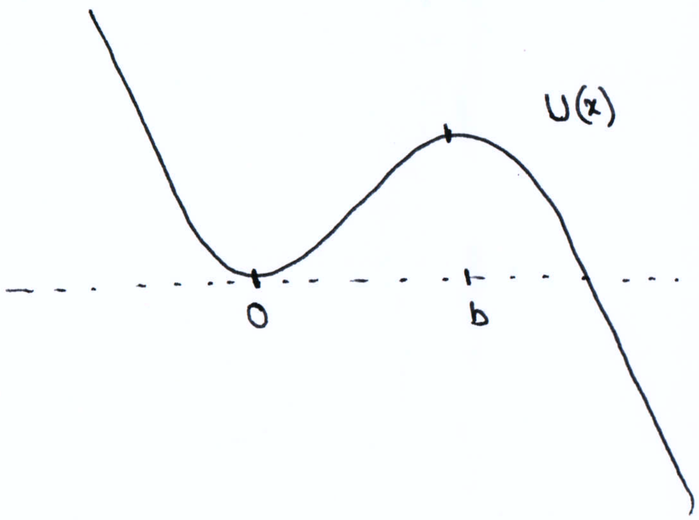
(i) gives an idea of least action paths in Langevin equation.

(2) Can be generalized straightforwardly, particularly for higher dimensional fields.

Ref: [1] "Diffusion in a bistable potential", Caroli, Caroli, Roulet. J. Stat. Phys., 26, 83 (1981).

[2] "Formulating the Kramer's problem in field theory" Berera, Mintz, and Ramos, PRD 100, 076005 (2019).

Solution: Consider the probability ~~of a path from~~ of transition from the point 0 to point b at time T.



$$G_T(b|0) = \int_0^b \mathcal{D}[x,p]\, e^{-S[x,p]}$$

with

$$S[x,p] = \int_0^T dt \left\{ p\dot{x} - \left[Dp^2 - pU' + \frac{1}{2}U'' \right] \right\}$$

We showed earlier that, by rearranging terms we can write

$$G_T(b|0) = e^{-\frac{U(b)-U(0)}{2D}} \cdot R$$

where

$$R = \int_0^b \mathcal{D}[x,p]\, e^{-\int_0^T dt \left\{ p\dot{x} - [Dp^2 - V(x)] \right\}}$$

$$V(x) = \frac{(U')^2}{4D} - \frac{U''}{2}$$

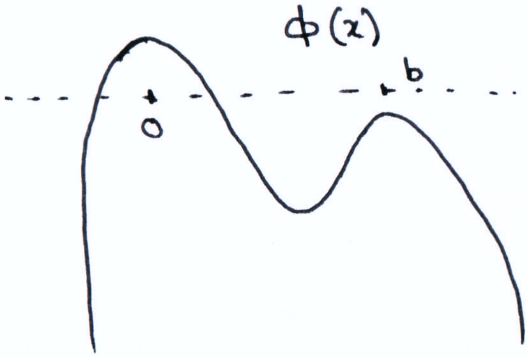
By redefining $p \to \frac{p}{D}$

$$R = \int_0^b \mathcal{D}[x,p]\, e^{-\frac{1}{D}\tilde{S}[x,p]}$$

$$\tilde{S} = \int_0^T dt \left\{ p\dot{x} - H(p,x) \right\}$$

$$H(p,x) = p^2 + \phi(x) \quad \text{with}$$

$$\phi(x) = -\frac{(U')^2}{4} + D\frac{U''}{2}$$



Note the similarity of a classical mechanics particle in potential $\phi(x)$.

Kramer's answer is for the case where D is small. In this limit, leading contribution comes from saddle point (least action).

Let's denote the least action paths as (x_{cl}, p_{cl}) drawing analog with "classical paths" in QM.

Least action path:

$$\dot{p}_{cl} = -\frac{\partial H}{\partial x_{cl}} = -\phi'(x_{cl})$$

$$\dot{x}_{cl} = \frac{\partial H}{\partial p_{cl}} = 2p_{cl}$$

boundary condition

$x_{cl}(0) = 0$

$x_{cl}(T) = b$

Solution:

$$p_{cl} = \pm\sqrt{A - \phi(x_{cl})}$$

$$\dot{x}_{cl} = 2p_{cl} = \pm 2\sqrt{A - \phi(x_{cl})}$$

easy to guess using $H = A$ (conserved). or constant of motion.

Only the (+) solution ~~has~~ $x=0$ as repulsive point and $x=b$ as attractive for $0<x<b$.

This is the solution relevant for us.

The constant A is determind by

$$\dot{x}_{cl} = 2\sqrt{A-\phi(x_{cl})}$$

$$\Rightarrow \quad \frac{dx_{cl}}{2\sqrt{A-\phi(x_{cl})}} = dt$$

$$\Rightarrow \quad \boxed{\int_0^b \frac{dx_{cl}}{2\sqrt{A-\phi(x_{cl})}} = T}$$

This is an example of integral equations.

The minimal Action

$$\tilde{S}[x_{cl}, p_{cl}] = \tilde{S}_0 = \int_0^T dt \left\{ p_{cl}\cdot\dot{x}_{cl} - \underbrace{\left[p_{cl}^2 + \phi_{cl}\right]}_{A} \right\}$$

$$= \int_0^T dt \left\{ 2\left(A - \phi(x_{cl})\right) - A \right\}$$

$$= \int_0^b \frac{dx_{cl}}{2\sqrt{A-\phi}} \cdot (A - 2\phi)$$

$$\Rightarrow \quad \boxed{\tilde{S}_0 = \frac{1}{2}\int_0^b dx_{cl} \, \frac{A-2\phi(x_{cl})}{\sqrt{A-\phi(x_{cl})}}}$$

Then,

$$R = e^{-\frac{1}{D}\tilde{S}_0} \times \underbrace{\int_{u=0}^{u=0} \mathcal{D}[u,v] \cdot e^{-\frac{1}{D}\left\{ S(x_{cl}+u,\, p_{cl}+v) - S_0(x_{cl}, p_{cl}) \right\}}}_{\text{fluctuation}}$$

where we defined $x = x_{cl} + u(t)$ and $p = p_{cl} + v(t)$

In general it is hard to calculation the fluctuation part. For small D, ~~the ca~~ where least action paths is dominating, we can estimate by expanding upto quadratic order.

$$S(x_{cl}+u, p_{cl}+v) = S(x_{cl}, p_{cl}) + \int_0^T dt \left\{ v\dot{u} - v^2 - \frac{\phi''(x_{cl})}{2} u^2 \right\}$$

$$+ \cdots$$

Gives the

$$\text{fluctuation part} = \int_{u=0}^{u=0} \mathcal{D}[u,v]\, e^{-\frac{1}{D}\int dt \left\{ v\dot{u} - v^2 - \frac{\phi''(x_{cl})}{2} u^2 \right\}}$$

$$= \int_0^0 \mathcal{D}[u,v]\, e^{+\frac{1}{D}\int_0^T dt \left(v - \frac{\dot{u}}{2}\right)^2} \cdot e^{-\frac{1}{4D}\int_0^T dt \left(\dot{u}^2 - 2\phi'' \cdot u^2\right)}$$

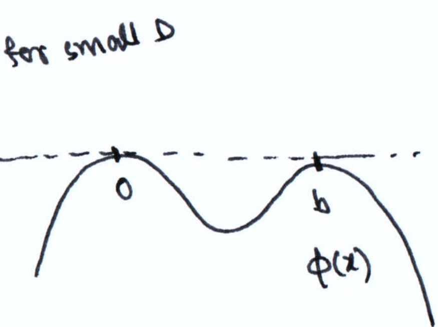
$$= \int_0^0 \mathcal{D}[u]\, e^{-\frac{1}{4D}\int_0^T dt \left(\dot{u}^2 + m^2 u^2\right)}$$

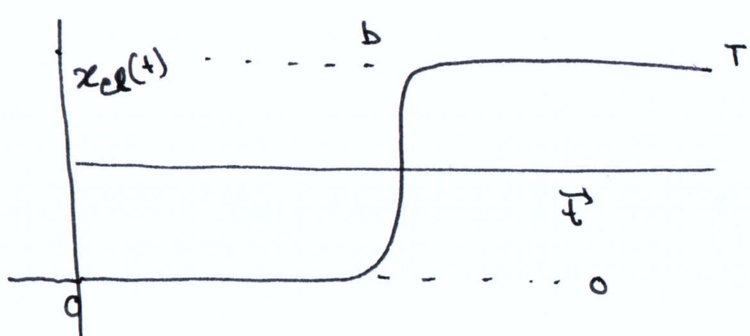
where $m^2 = -2\phi''(x_{cl}) = \left(U''(x_{cl})\right)^2 + U'(x_{cl}) \cdot U'''(x_{cl})$

$$- 2D\, \phi''''(x_{cl})$$

~~In general, where m(t) dep~~

For our case, $m(x_{cl}(t))$ depends on time and it is hard to do the path integration over u. Simplification comes if we observe the trajectory for small D-limit





The transition path is almost instantaneous compared to the time spent around $x=0$ and $x=b$. These least action paths are called instantons in field theory.

This means, for the small D limit, we can do the Gaussian path integral in u by considering $m(x(t))$ at $x=0$ and at $x=b$, where

$$m^2(x_{cl}=0) \simeq U''(0)^2$$

$$m^2(x_{cl}=b) \simeq U''(b)^2$$

For constant m, the Gaussian path integral is ~~st~~ known

$$\boxed{\int_0^0 \mathcal{D}[u]\, e^{-\frac{1}{4D}\int_0^\tau dt\,(\dot{u}^2 + m^2 u^2)} = \sqrt{\frac{m}{2\pi D}} \cdot \frac{e^{-\frac{m\tau}{2}}}{\sqrt{1-e^{-2m\tau}}}}$$

Ref: Feynmann and Hibbs book on path integral

or

Ashok Das field theory book

or

Lecture note by Kay Wiese, ENS-Paris on statistical field theory.

Typically, in field theory, the above integral is derived using Gelfand-Yaglom method.

One easy way for us is to derive the formula by solving the Langevin equation in a harmonic potential $\frac{1}{2}mx^2$.

~~corresponding~~ [See assignment question]

~~Finally~~ Using this formula we get, for small D and large T,

$$\text{fluctuation part} \simeq \sqrt{\frac{m(0)}{2\pi D}} \times \sqrt{\frac{m(b)}{2\pi D}} \times e^{-\frac{m(0)}{2}t_1 - \frac{m(b)}{2}t_2}$$

(t_1, t_2 are the time spent near 0 and b)

Finally, we get the transition path probability

$$G_T(b|0) \simeq e^{-\frac{U(b)-U(0)}{2D}} \times e^{-\frac{1}{D}\tilde{S}_0 - \frac{m(0)}{2}t_1 - \frac{m(b)}{2}t_2} \times \frac{\sqrt{m(0)\cdot m(b)}}{2\pi D}$$

with $m(0) \simeq U''(0)$ and $m(b) \simeq |U''(b)|$

To get the Kramer's formula, in small D limit we use that

$$\frac{1}{D}\tilde{S}_0 = \frac{1}{2D}\int_0^b dx_{cl}\, \frac{A - 2\phi(x_{cl})}{\sqrt{A - \phi(x_{cl})}}$$

for small D, A is order D.

$$\simeq \frac{1}{2D}\int_0^b dx_{cl}\left(2\sqrt{-\phi(x)}\right)$$

$$\simeq \frac{1}{2D}\int_0^b dx_{cl}\sqrt{(U'(x_{cl}))^2 - D\,\frac{U''(x_{cl})}{2}}$$

$$\simeq \frac{1}{2D}\int_0^b dx_{cl}\, U'(x_{cl}) + \text{Subleading in } D$$

$$= \frac{U(b)-U(0)}{2D} + \text{subleading}$$

term cancels with the $\frac{m(0)}{2}t_1 + \frac{m(b)}{2}t_2$ but takes effort to show, and we shall avoid.

Together, we get

$$G_T(b|0) \simeq e^{-\frac{U(b)-U(0)}{D}} \times \frac{\sqrt{U''(0)\,|U''(b)|}}{2\pi D}$$

~~[illegible]~~

This is the probability to reach the peak of the barrier. Once there, the particle diffuses and has half-half probability to fall on the right side of the hill and escape. This rate is given by the diffusion constant D, so that the rate of escape

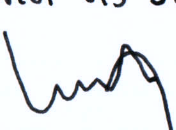
$$r = D \times G_T(b|0)$$

which is the expression obtained by Kramer. [You can argue this dimensionally as well]

<u>Remark:</u> We only looked at the trajectory from the minima of the well at $x=0$. This justified because the path from anywhere else inside the well, goes downhill very fast to $x=0$ and such paths do not "cost much" for small D, meaning probability $\mathcal{O}(1)$. This you can check similarly solving the minimal Action paths. This time the $(-)$ solution is the relevant solution.

<u>Remark:</u> ~~[illegible]~~

Note that the transition rate depends only on the height of the potential barrier and not its shape (except the prefactor).

This means  and  both have same escape rate.

This changes for nonequilibrium dynamics.

Ref: Woillez, Zhao, Kafri, Lecomte and Tailleur, PRL 122, 258001 (2019).

Remark: For a bistable potential the transition rate is modified.

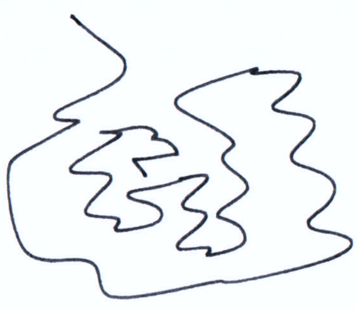
Further reading: "Lectures on the theory of dissipative tunneling" by Dykman & and Pryadko

Quantum tunneling.

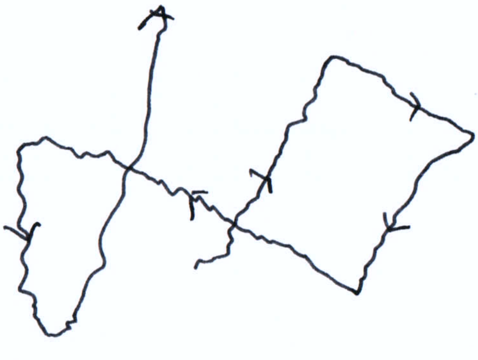
Remark: For non-equilibrium dynamics or for non-Markovian process, the escape rate may depend on the shape of the barrier, and not only on the barrier height.

① A common and a much discussed example of non-equilibrium dynamics: Active matter.

A ~~story~~ short description:



Brownian ptl.
(ideally zero persistence).



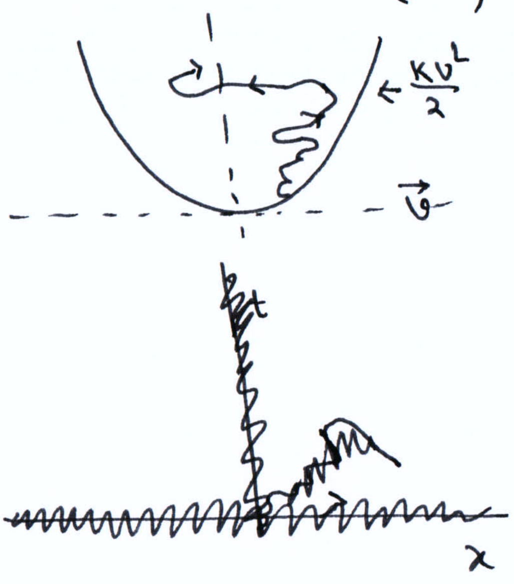
Active ptls: persistent motion

Examples: Bacteria movement, living organisms, birds.
Janus particle.

The persistence motion comes from internal source of energy in each particle. This breaks ~~[illegible]~~ fluctuation-dissipation relation (relation between noise and ~~[illegible]~~ viscous dissipation). This is very different from ~~particles~~ Brownian particles under uniform external field (which is also non-equilibrium and has persistent motion).

A very simple model: Active Ornstein-Uhlenbeck process. (1d)

$$\boxed{\begin{aligned} \dot{x} &= v + \mu F(x) + \eta(t) \\ \dot{v} &= -Kv + \xi(t) \end{aligned}}$$



① $\langle \eta(t)\eta(t')\rangle = 2\mu K_B T\,\delta(t-t')$

② $\langle \xi(t)\xi(t')\rangle = 2\Gamma\,\delta(t-t')$

③ Easy to show that

$$v(t) = \int_0^t ds\, e^{-K(t-s)}\, \xi(s)$$

$$\Rightarrow \langle v(t)v(t')\rangle = \int_0^t ds \int_0^{t'} ds'\, e^{-K(t+t'-s-s')} \langle \xi(s)\xi(s')\rangle$$

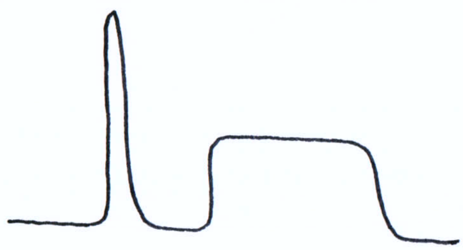
$$\approx e^{-K|t'-t|} \cdot \frac{\Gamma}{K} \quad \text{for large } t', t$$

This mean velocity is correlated ~~ove~~ upto a time scale $\tau \sim \frac{1}{K}$ therefore persistent (active).

These kind of Active systems are important because they exhibit collective non-equilibrium phases which are not possible in equilibrium.

For example, liquid-gas type transition for repulsive inter particle potential.

Kramer's escape rate for active particle depend on shape of the potential barrier, and not only on barrier height.

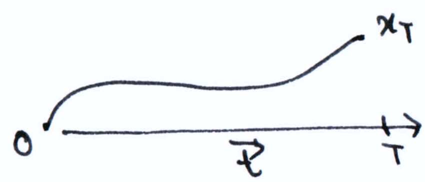


increasing persistent time τ (more activity) makes the particle escape from the left-higher barrier.

See the corresponding instanton (least action path) solution in Woillez et. al, PRL, 122, 258001 (2019).

② <u>An example of a common non-Markovian dynamics</u>: fractional Brownian motion.

Definition using path integral.



$$P_H[x(t)] \sim e^{-\frac{1}{2}\int_0^T dt_1\, dt_2\; x(t_1)\cdot c^{-1}(t_1,t_2)\cdot x(t_2)}$$

with $c(t_1,t_2) = D\left[t_1^{2H} + t_2^{2H} - |t_1-t_2|^{2H}\right]$

with $H \in [0,1]$ is called Hurst exponent.

c^{-1} and c are related by $\displaystyle\int_0^T dt\, c^{-1}(t_1,t)\, c(t,t_2) = \delta(t_1-t_2).$

Remark: ① The above probability is Gaussian with covariance

$$\langle x(t_1)\, x(t_2)\rangle = c(t_1,t_2)$$

[You may think of it as a continuous limit of multivariate Gaussian distribution]

② This is a generalization of Brownian motion, which corresponds to $H=\frac{1}{2}$.

$$\langle x(t_1)\, x(t_2)\rangle = c(t_1,t_2) = 2D\min(t_1,t_2).$$

$$\Rightarrow \boxed{\langle x(t)^2\rangle = 2Dt}$$

Moreover using $\langle \dot{x}(t_1)\, \dot{x}(t_2)\rangle = 2D\,\delta(t_1-t_2)$

and using integration by parts in the Action we get

$$P_{H=\frac{1}{2}}[x(t)] \sim e^{-\frac{1}{4D}\int_0^T dt\, (\dot{x}(t))^2}$$

The Feynmann-Kac Action.

③ Fractional Brownian motion is a fundamental process for anomalous diffusion.

$$\langle x(t)^2\rangle = 2D\cdot t^{2H} \qquad \begin{cases} \text{Superdiffusion for } H>\frac{1}{2} \\ \text{Subdiffusion for } H<\frac{1}{2}. \end{cases}$$

Unlike Lévy process, fractional Brownian motion is long-range correlated in time. The $H \to 0$ limit is an example of log-correlated Gaussian field.

④ The process is self-similar, stationary (time-translation invariant).

Many many natural processes are described by fractional Brownian motion.

<u>Examples:</u> solar flare activity, price in ~~the~~ a free market, water level in rivers Nile, movement inside a cell, monomer in a polymer chain etc.

<u>Open problem:</u> What is the Kramer's escape rate?