Optimal Fluctuation Method

Lecture 1. Geometrical optics of Brownian motion

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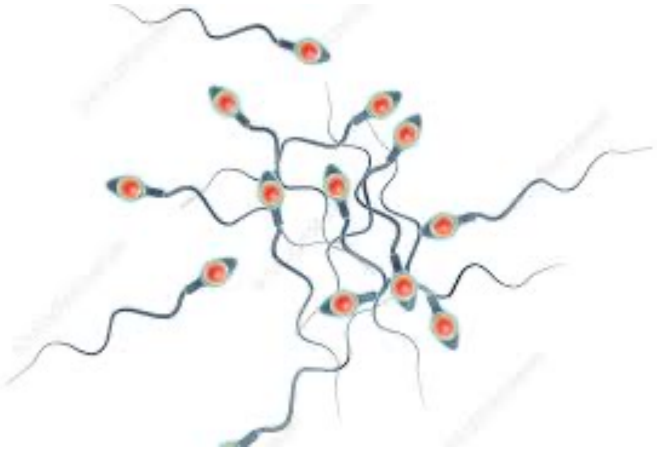
Looking for student(s) who would participate in preparing notes

"Large deviations and applications", Summer School in Les Houches, 1-26/07/2024

One motivation comes from *Redundancy* in biology

A very large number of agents (molecules, ions, cells, …) is often needed in situations where only one agent ultimately does the job.

A striking example: 3×10^8 sperm cells initially attempt to reach the oocyte after copulation in humans, and only one (rarely, two) can fertilize the oocyte.



Why such a huge redundancy? Can it be just to reduce the random search time?

BM and S. Redner, Phys. Rev. Lett. **114**, 198101 (2015)
Z. Schuss, K. Basnayake and D. Holcman, Phys. Life Rev. **28**, 52 (2019)

The first arrival is unusually fast, and it must have an atypical path: A large deviation

Outline

- Large deviations of Brownian motion $\Longrightarrow$ geometrical optics
- Example 1: survival of Brownian motion against a moving absorbing wall
- Example 2: winding angle distribution of Brownian motion
- Example 3: tail of the Airy distribution
- Summary

This lecture is based on two papers:

1. BM and N. R. Smith, J. Phys. A: Math. Theor. **52**, 415001 (2019).

2. T. Agranov, P. Zilber, N. R. Smith, T. Admon, Y. Roichman and BM, Phys. Rev. Res. **2**, 013174 (2020).

Different names for same or similar methods

- Geometrical optics of Brownian motion
- Dissipative WKB approximation
- Weak-noise theory
- Onsager-Machlup principle
- Macroscopic fluctuation theory (MFT)
- Instanton method
- Optimal fluctuation method (OFM)

Lecture 1 has some overlaps with lectures of E. Vanden-Eijnden and V. Lecomte and, to a lesser degree, of B. Derrida and P. Hurtado

Brownian motion x(t) as the Wiener process

$$\frac{dx}{dt} = \xi(t)$$

$\xi(t)$ Gaussian white noise

$$< \xi(t) > \; = 0, \qquad < \xi(t_1)\xi(t_2) > = 2\mathrm{D}\,\delta(\mathrm{t}_1 - \mathrm{t}_2)$$

D diffusion constant

The probability distribution P(x,t) obeys the diffusion equation

$$\frac{\partial P(x,t)}{\partial t} = D\,\frac{\partial^2 P(x,t)}{\partial x^2}$$

$$\frac{\partial P(x,t)}{\partial t} = D\ \frac{\partial^2 P(x,t)}{\partial x^2} \qquad -\infty < x < \infty$$

Simplest example: a Brownian particle starts at t=0 at x=0:

$$P(x, t = 0) = \delta(x)$$

The solution: $$P(x,t) = \frac{1}{\sqrt{4\,\pi\,Dt}}\, e^{-\frac{x^2}{4\,Dt}}$$

This P(x,t) is unconditional probability density

$\sqrt{Dt}$: characteristic length scale of unconditioned Brownian motion

Path-integral formulation for the Wiener process

What is the probability of a Brownian path x(t)?

Let us start with discrete-in-time Brownian motion in 1d: $x_{i+1} = x_i + \xi_i$

ξ_i are normally distributed, uncorrelated, with zero mean and variance σ^2

$$\mathrm{Prob}[\{x_i\}] \sim \exp\left[-\sum_i \frac{{\xi_i}^2}{2\sigma^2}\right] \sim \exp\left[-\frac{1}{2\sigma^2}\sum_i (x_i - x_{i-1})^2\right]$$

In the continuous-time limit $\sigma^2 = 2D\,\Delta t$ and $(x_i - x_{i-1})/\Delta t = dx/dt$, and we arrive at

$$\mathrm{Prob}[x(t)] \sim \exp\left[-\frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt\right]$$

Probability of a Brownian path x(t)

$$\mathrm{Prob}[x(t)] \sim \exp\left[-\frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt\right]$$

Large-deviation regimes, where this probability is exponentially small, are often dominated by a single Brownian path x(t) – the optimal path, for which the action functional

$$S[x(t)] = \frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt$$

is minimal subject to problem-specific constraints.

This is the essence of the optimal fluctuation method (OFM) in general, and geometrical optics of Brownian motion in particular

A. Grosberg and H. Frisch 2003, N. Ikeda and H. Matsumoto 2015, D. Holcman *et al.* 2018, N.R. Smith and BM 2019, BM and N.R. Smith 2019, …

A warm-up exercise: evaluate the probability density P(x=X,t=T) if P(x,t=0)=δ(x).

$$S = \min_{x(t)} \frac{1}{4D} \int_0^T \left(\frac{dx}{dt}\right)^2 dt$$

Boundary conditions in time: $x(t=0)=0, \;\; x(t=T)=X$.

Very simple problem of classical mechanics, or geometrical optics.

The Euler-Lagrange equation is $\ddot{x}=0$, and the solution is $x(t)=\frac{Xt}{T}$

Then $S=\frac{X^2}{4DT}$ and $P \sim e^{-\frac{X^2}{4DT}}$

Compare with exact result $$P(X,T)=\frac{1}{\sqrt{4\,\pi\,DT}}e^{-\frac{X^2}{4\,DT}}$$ The OFM misses a pre-exponential factor, but the leading, exponential dependence is correct

Applicability condition: $$\frac{X^2}{4\,DT} \gg 1$$

S>>1 = short-time limit

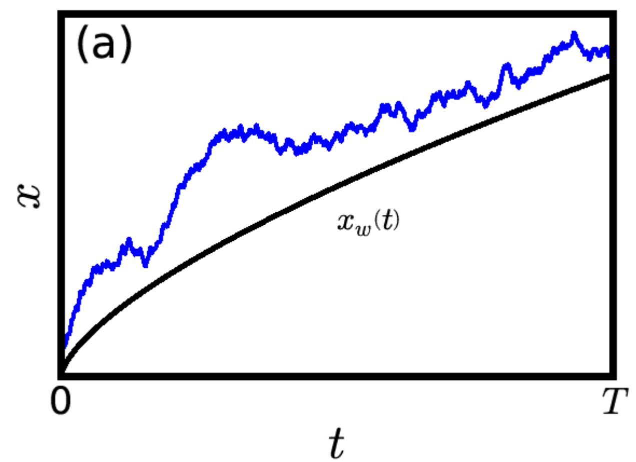
Example 1: survival of Brownian motion against invading wall

BM and N. R. Smith, J. Phys. A: Math. Theor. **52**, 415001 (2019).

A Brownian particle is released at t=0 at x=ε > 0. An absorbing wall, initially at x=0, is moving to the right according to a power law

$$x_w(t) = Ct^\gamma, \qquad \gamma > 0, C > 0$$

What is the probability P(T) that, at long time T, the particle has not yet been absorbed by the wall?



Early work by mathematicians: A.A. Novikov, Math. USSR Sb. **38**, 495 (1981) and references there. Physics papers: P.L. Krapivsky and S. Redner (1996,1999)

The result strongly depends on γ

$$x_w(t) = Ct^\gamma, \qquad \gamma > 0, C > 0$$

$\gamma < \frac{1}{2}$: P(T) goes down as $T^{-1/2}$, that is slowly: only as a power law. This regime is beyond geometrical optics

$\gamma > \frac{1}{2}$: P(T) is exponentially small, and can be described by geometrical optics:

Minimize $S = \frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt$

under conditions $x(0) = \varepsilon > 0,\ x(t) > x_w(t) = C\, t^\gamma$

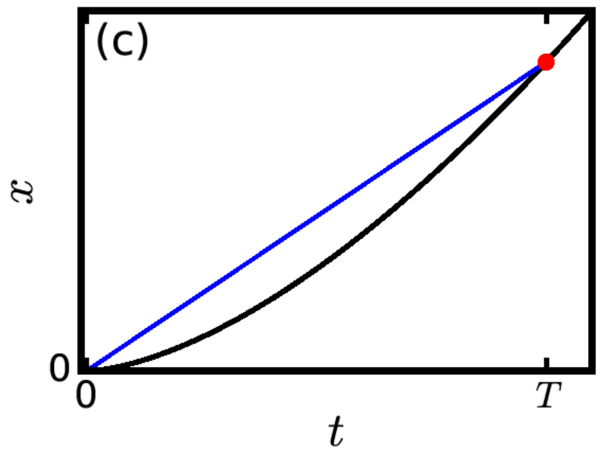
We need to satisfy an inequality: one-sided variations

Minimize $S = \frac{1}{4D} \int_0^T \left(\frac{dx}{dt}\right)^2 dt$

under conditions $x(0) = \varepsilon > 0, x(t) > x_w(t) = C\, t^\gamma$

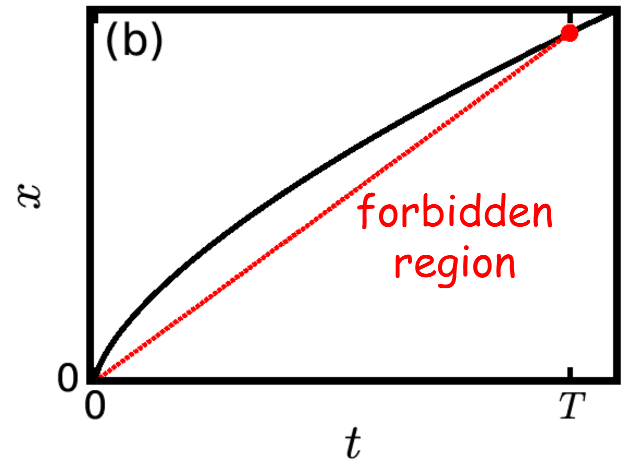
One-sided variations

$\gamma > 1$



Optimal path: $x(t) = C\, T^{\gamma-1} t$

$1/2 < \gamma < 1$



Optimal path coincides with the wall function: $x(t) = x_w(t) = C\, t^\gamma$

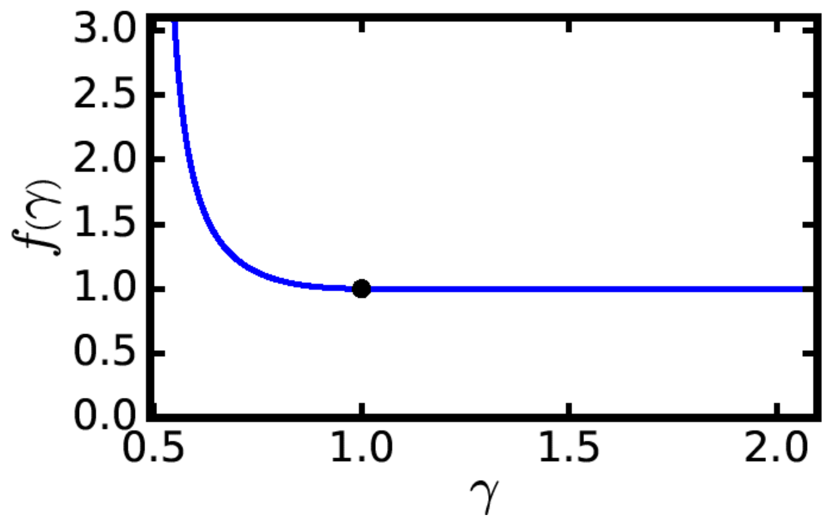
Evaluate the action $S = \frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt$

$$-\ln P(T) \cong S = \frac{C^2 f(\gamma) T^{2\gamma-1}}{4D}$$

coincides with Novikov (1981), but here it is a one-line calculation

$$f(\gamma) = \begin{cases} \frac{\gamma^2}{2\gamma-1}, & 1/2 < \gamma \le 1 \\ 1, & \gamma \ge 1 \end{cases}$$

f(γ) diverges at γ = 1/2



Applicability: large action ⇒ $\gamma > 1/2$, long-time limit $T \to \infty$

What happens in the marginal case $\gamma=1$?

$$x_w(t) = C\,t \qquad \gamma = 1\colon \quad -\ln P(T) \cong \frac{C^2 T}{4D}$$

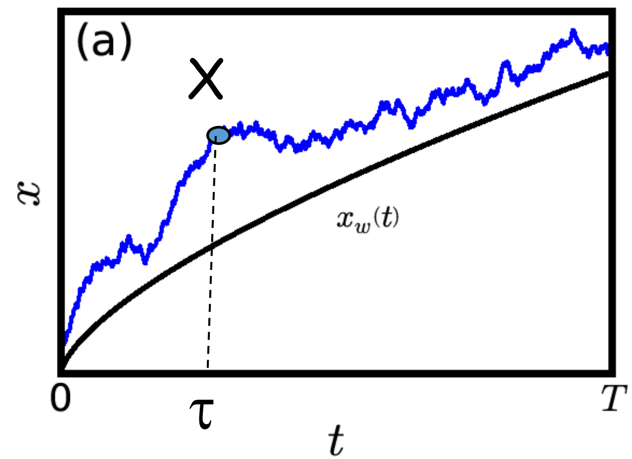
In fact, this case is exactly solvable. At long times the exact result becomes

$$P \cong \sqrt{\frac{4}{\pi}} \frac{L}{\sqrt{DT}} \frac{D}{C^2 T} e^{-\frac{C^2 T}{4D}}$$

Redner, *A Guide to First-Passage Processes (2001)*

The OFM misses pre-exponential factors,
but the exponential dependence is correct

What is the particle distribution $P(X,\tau,T)$ at intermediate time τ, given that the particle has not been absorbed until time T ?



Minimize $S = \frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt$

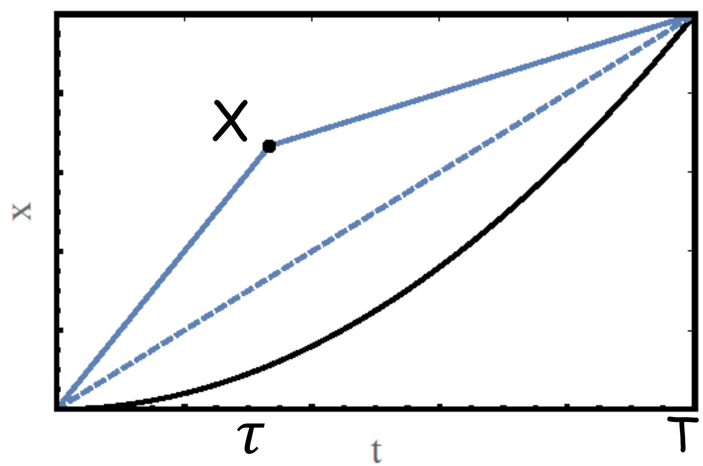
under conditions $x(0) = \varepsilon$, $x(\tau) = X$, and $x(t) > x_w(t) = C\,t^\gamma$

The conditional probability is equal to the ratio of the probabilities with and without the constraint $x(\tau) = X$.

In geometrical optics the corresponding action is equal to the difference of the actions of two different optimal paths that avoid absorption: with and without the constraint $x(\tau) = X$

Minimize $S = \frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt$

under conditions $x(0) = \varepsilon$, $x(\tau) = X$, and $x(t) > x_w(t) = C\, t^\gamma$



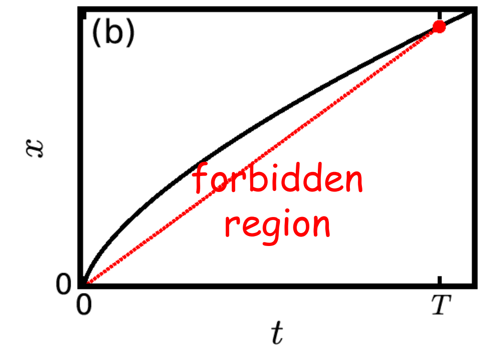
$\gamma > 1, \qquad T \to \infty$

$$-\ln P(X,\tau,T) \cong \frac{x_w(T)^2}{4DT} \frac{\left(\frac{X}{x_w(T)} - \frac{\tau}{T}\right)^2}{\frac{\tau}{T}\left(1 - \frac{\tau}{T}\right)}$$

A Gaussian distribution with the maximum at $X = (\tau/T)\, x_w(T)$, that is on the unconditioned path

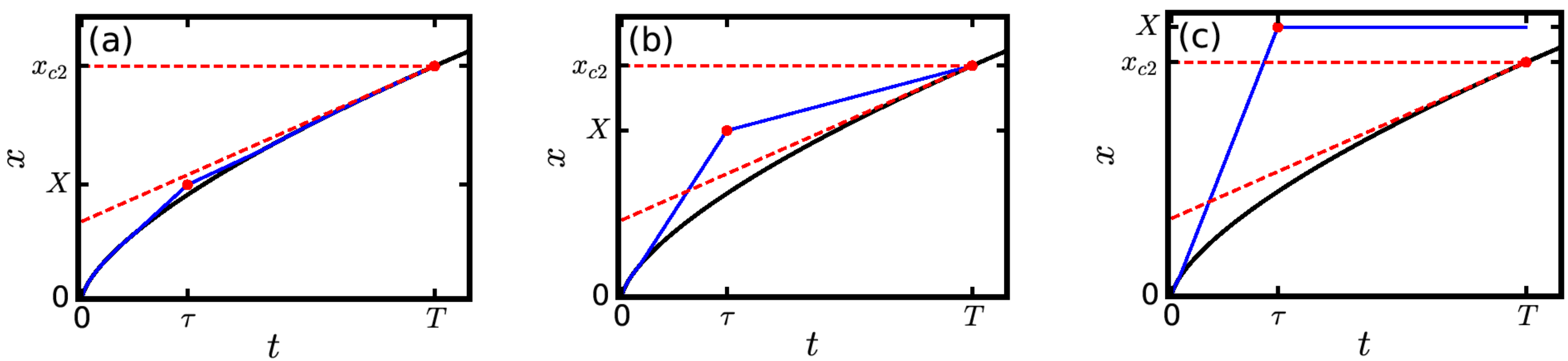
This asymptotic also applies to many other wall functions, for example those which are convex downward: $\ddot{x}_w(t) > 0$

The regime $\frac{1}{2} < \gamma < 1$ is more interesting



(a) and (b): tangent constructions for one-sided variations

e.g. L. Elsgolts, *Differential Equations and the Calculus of Variations*

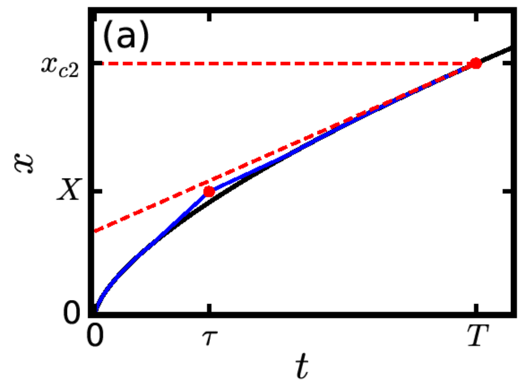


Three distinct regions of X: subcritical, first supercritical and second supercritical

$$-\ln P(X,\tau,T) \cong \frac{x_w(T)^2}{DT}\,\varphi\left(\frac{X}{x_w(T)},\frac{\tau}{T}\right)$$

φ is a non-analytic function of X at $X{=}X_{c1}$ and $X{=}X_{c2}$. Such non-analyticities are called dynamical phase transitions. Here they are of third and second order, respectively. The very far tail is a simple Gaussian.

Let us look more closely at the subcritical regime



$$\frac{1}{2} < \gamma < 1,$$
$$T \to \infty$$

What happens when $x(\tau) = X$ is close to the wall $x_w(\tau) = C\tau^\gamma$?
Asymptotic of the geometrical-optics result:

$$-\ln P(X,\tau) \cong \frac{2\sqrt{2\,\gamma(1-\gamma)}C^2\tau^{2\gamma-1}}{3D}\left(\frac{X}{C\tau^\gamma} - 1\right)^{3/2} \qquad (1)$$

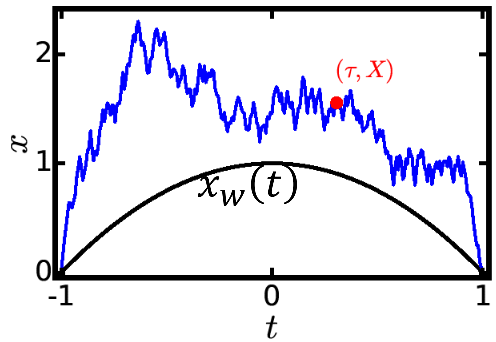
No dependence on T: the conditional distribution is local in time!

Equation (1) coincides (up to a pre-exponent) with the tail of the Ferrari-Spohn distribution.

Why?

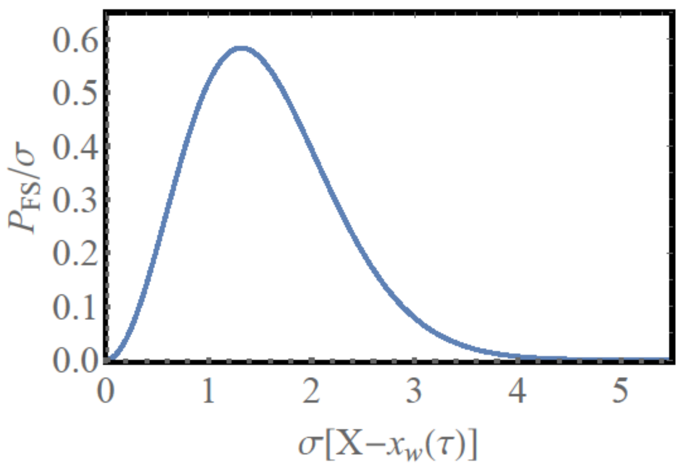
The Ferrari-Spohn distribution

P.L. Ferrari and H. Spohn, Ann. Probab. **33**, 1302 (2005)



A Brownian excursion $x(t)$, conditioned to stay away from a swinging wall $x_w(t)$

At $T \to \infty$, typical (that is, small) fluctuations of $\Delta X = X - x_w(\tau)$ are distributed according to FS distribution that depends only on the second derivative $\ddot{x}_w(\tau)$.



$$P_{\mathrm{FS}}(\Delta X, \tau) = \frac{\sigma \mathrm{Ai}[\sigma\, \Delta X + a_1]^2}{\mathrm{Ai}'\,(a_1)^2},$$

$$\sigma = \left[\frac{-\ddot{x}_w(\tau)}{2D^2}\right]^{1/3}$$

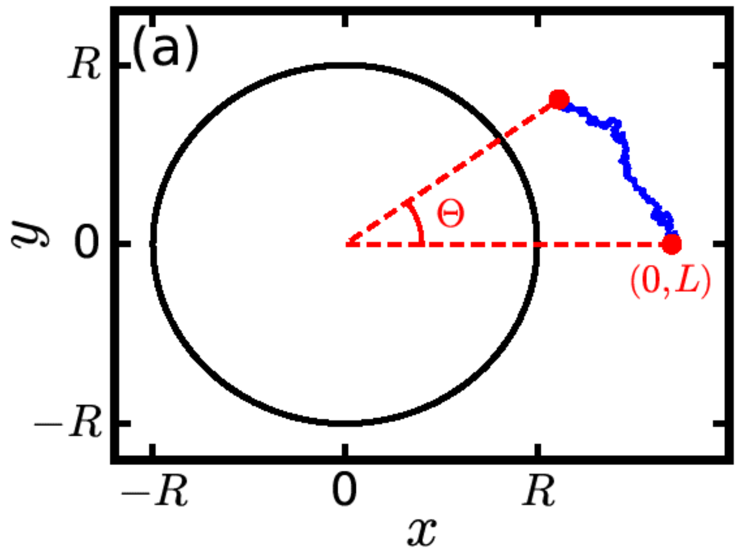
Ai(...) is the Airy function,
a_1 =-2.33810... is its first root

The Ferrari-Spohn (FS) distribution $P_{\mathrm{FS}}(\Delta X, \tau)$ and our large-deviation tail $P(X, \tau)$ have a joint validity region. It is described by the large-ΔX asymptotic of the FS dist., but a small-ΔX asymptote of geometrical optics. Overall, this gives complete statistics.

Example 2: the winding angle distribution of BM

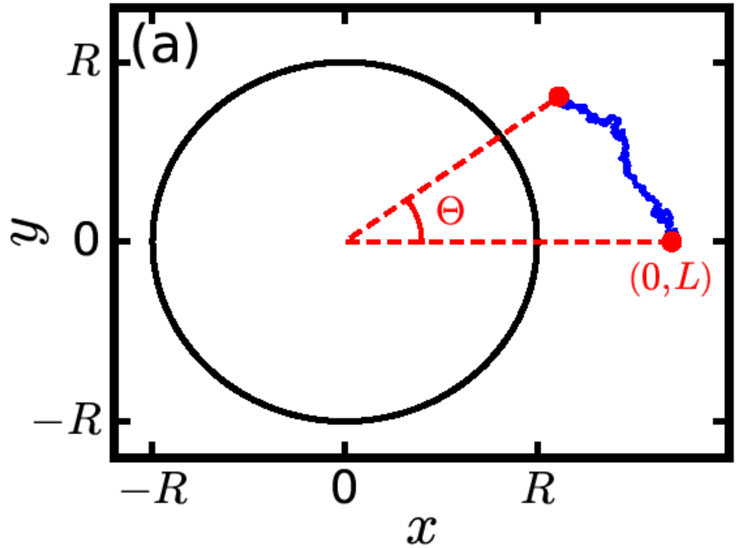
BM and N. R. Smith (2019)

A Brownian particle is released at t=0 at a distance L from the center of a reflecting disk with radius R<L



What is the distribution $P(\theta, T)$ of the winding angle θ at time T?

Original motivation: polymer winding around an obstacle



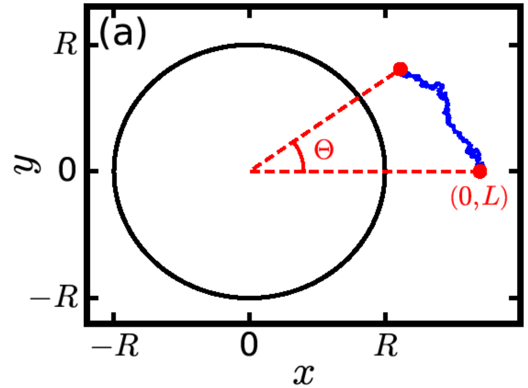
Previous work (Rudnick and Hu 1987, Saleur 1994, Grosberg and Frisch 2003) focused on the long-time limit:

$$DT \gg L^2$$

where the distribution becomes independent of L:

$$P(\theta,T)=\frac{\pi\chi}{4\cosh^2(\pi\chi\theta/2)}, \qquad \chi=\frac{2}{\ln\frac{4DT}{R^2}}$$

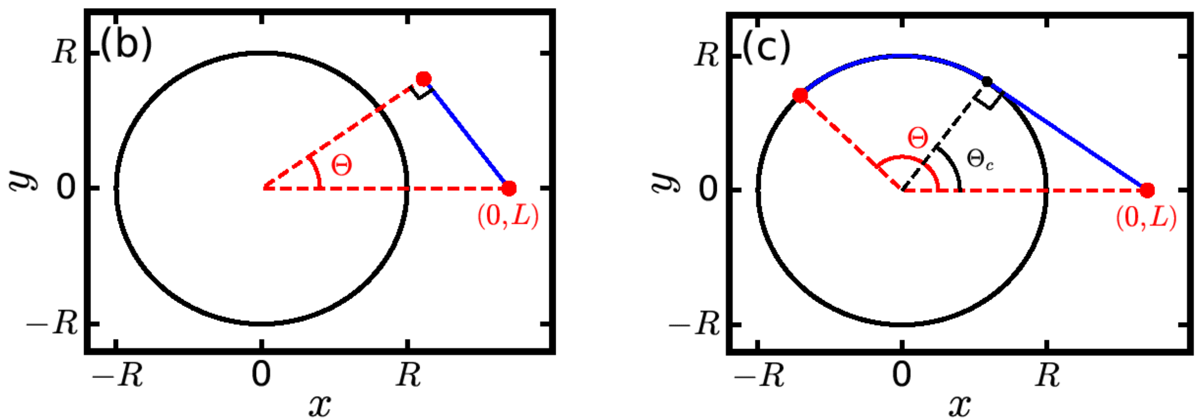
The long-time scaling $\theta \sim \ln T$



We are interested in the short-time limit: $\sqrt{DT} \ll L, L-R$

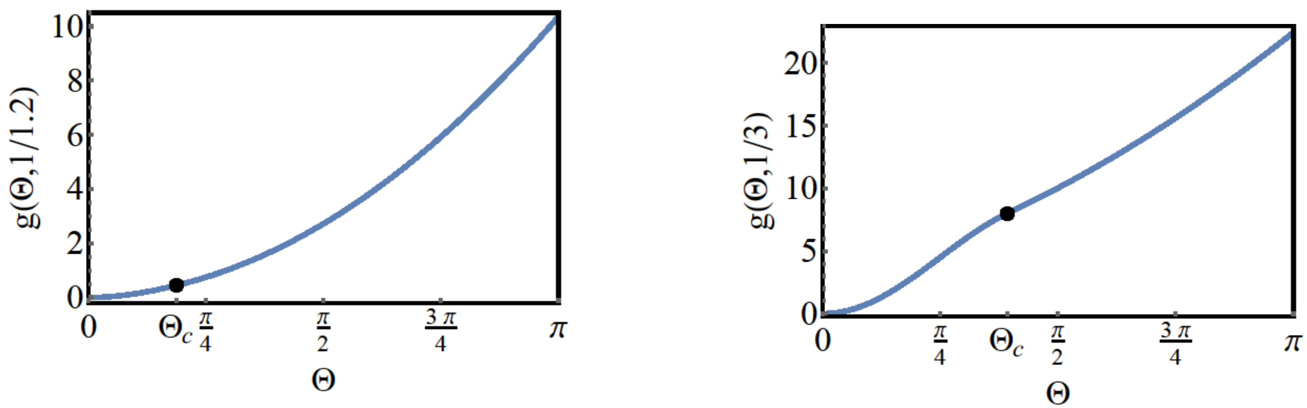
where a sizable θ is a large deviation, and use geometrical optics

We should find the shortest path leading to a specified θ at time T and avoiding the disk



$$-\ln P = \frac{R^2}{4DT} g\left(\theta, \frac{R}{L}\right) \qquad \frac{R^2}{4DT} \gg 1$$

$$g(\theta, z) = \begin{cases} z^{-2}\sin^2\theta\,, & |\theta| \le \arccos z \\ \left(|\theta| + \sqrt{z^{-2}-1} - \arccos z\right)^2, & |\theta| \ge \arccos z \end{cases}$$



The second derivative $\partial^2 g/\partial\theta^2$ has a jump at $\theta = \theta_c = \arccos\left(\frac{R}{L}\right)$: a second-order transition

For $\frac{L}{R} > \sqrt{2}$ $\quad g(\theta, L/R)$ is non-convex. Non-convex rate functions appear relatively rarely.

Speculation

At very large θ $$-\ln P = \frac{R^2\theta^2}{4DT},$$ should hold for any fixed time T

But its scaling $\theta \sim \sqrt{T}$ is very different from the late-time scaling of typical fluctuations $\theta \sim \ln T$

→ There should be a nontrivial (and unexplored) intermediate region at $\theta \sim \frac{T}{\ln T}$

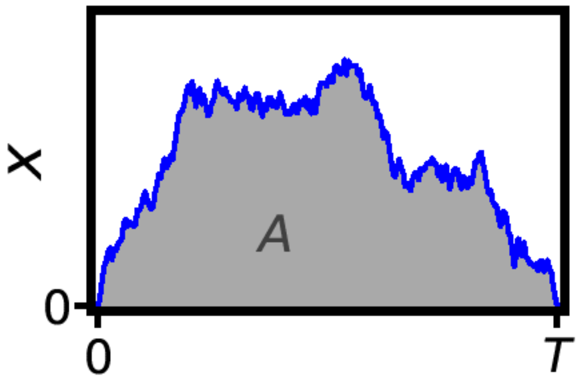
where the long-time and short-time behaviors predict a comparable probability.

One way to study it: the distribution $P(\theta, T)$ can be found exactly from the solution of the diffusion equation in 2d subject to the reflecting boundary condition on the disk and a delta-function initial condition. The exact result involves triple integrals of combinations of Bessel functions and trigonometric and/or exponential functions (J. Rudnick and Y. Hu 1987, A. Grosberg and H. Frisch 2003). Asymptotics?

Example 3: the Airy distribution and additional statistics

T. Agranov, P. Zilber, N.R. Smith, T. Admon, Y. Roichman and BM, Phys. Rev. Res. **2**, 013174 (2020)

The Airy distribution is the distribution of the area $A_T = \int_0^T x(t)dt$ under a Brownian excursion



D. A. Darling, Ann. Probab. **11**, 803 (1983).
G. Louchard, J. Appl. Probab. **21**, 479 (1984).

Many applications in computer science and graph theory. More recently, in physics:

Height of fluctuating interfaces S. N. Majumdar and A. Comtet, Phys. Rev. Lett. **92**, 225501 (2004); J. Stat. Phys. **119**, 314 (2005).
Sizes of avalanches in sandpile models M. A. Stapleton and K. Christensen J. Phys. A: Math. Gen. **39**, 9107 (2006).
Positions of laser-cooled atoms E. Barkai, E. Aghion, and D. A. Kessler, Phys. Rev. X **4**, 021036 (2014).
Sizes of ring polymers S. Medalion, E. Aghion, H. Meirovitch, E. Barkai and D. A. Kessler, Sci. Rep. **6**, 27661 (2016).

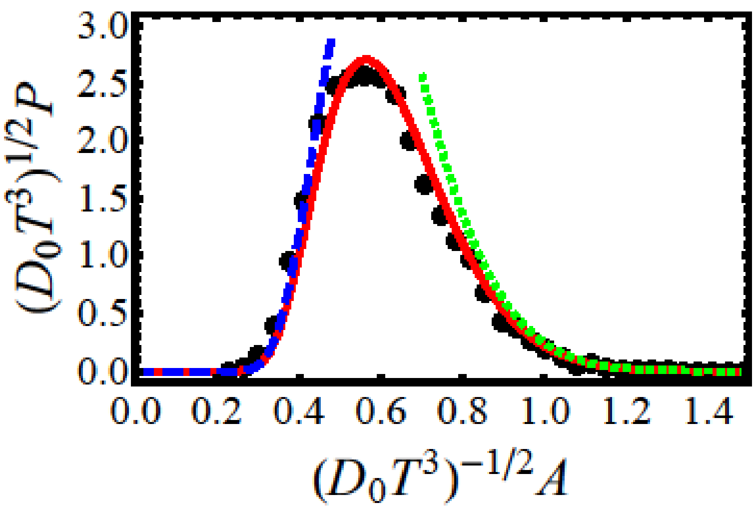
The Airy distribution

$$P(A,T) = \frac{1}{\sqrt{D\,T^3}} f\left(\frac{A}{\sqrt{D\,T^3}}\right)$$ from dimensional analysis

$$f(\xi) = \frac{2\sqrt{6}}{\xi^{10/3}} \sum_{k=1}^{\infty} e^{-\beta_k/\xi^2} {\beta_k}^{2/3} U\left(-\frac{5}{6}, \frac{4}{3}, \frac{\beta_k}{\xi^2}\right),$$

$\beta_k = \frac{2\,\alpha_k^3}{27}$. α_k are ordered abs. values of zeros of the Airy function $\mathrm{Ai}(\xi)$.

L. Takács, Adv. Appl. Prob. **23**, 557 (1991); J. Appl. Prob. **32**, 375 (1995).



$$-\ln P(A,T) \cong \begin{cases} \frac{2\,{\alpha_1}^3}{27}\frac{DT^3}{A^2}, & A \ll \sqrt{D\,T^3} \\ \frac{6\,A^2}{DT^3}, & A \gg \sqrt{D\,T^3} \end{cases}$$

The $A \gg \sqrt{D\,T^3}$ tail can be obtained from geometrical optics

- experimental data Agranov *et al.* (2020)

colloidal suspensions of silica spheres (1.50 ± 0.08 μm diameter) in water. Quasi-2D monolayers. Imaging + particle tracking

Minimize $$S = \frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt$$

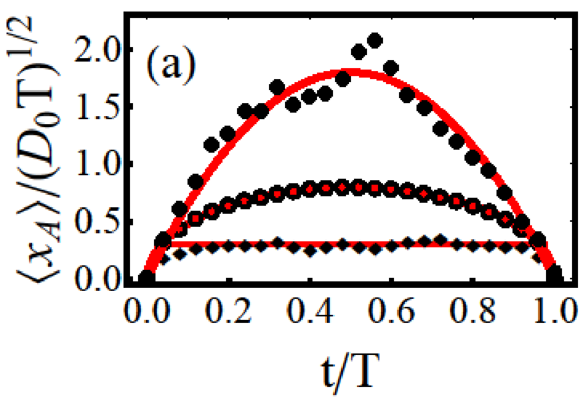
under conditions $x(0) = x(T) = 0, \;\; x(0 < t < T) > 0, \;\; \int_0^T x(t)dt = A$

One-sided variations

integral constraint

The constrained action $$S = \int_0^T \left[\frac{1}{4D}\left(\frac{dx}{dt}\right)^2 - \lambda x\right] dt$$ λ: Lagrange multiplier

Optimal path is a parabola: $x(t) = \left(\frac{6At}{T^2}\right)\left(1 - \frac{t}{T}\right)$

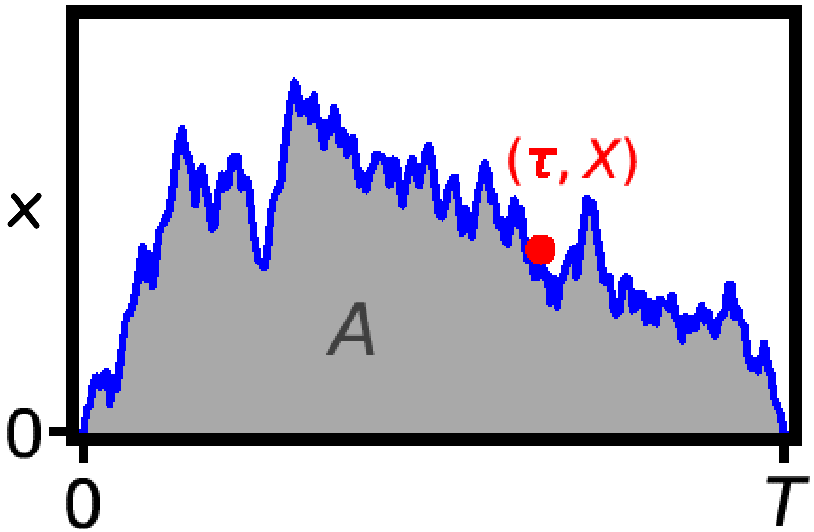


● experimental data relevant to this tail

One-sidedness of variations plays no role as yet!

The action $S = \dfrac{6\,A^2}{DT^3}$ exactly reproduces the $A \gg \sqrt{D\,T^3}$ tail of the Airy distribution

What is the position distribution $P(X, \tau, T, A)$
of the Brownian excursion at intermediate time τ conditioned on area A?



From dimensional analysis

$$P(X, \tau, T, A) = \frac{T}{A} F\left(\frac{TX}{A}, \frac{t}{T}, \frac{A}{\sqrt{D\,T^3}}\right)$$

$$\frac{A}{\sqrt{D\,T^3}} \gg 1$$

Minimize $$S = \frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt$$

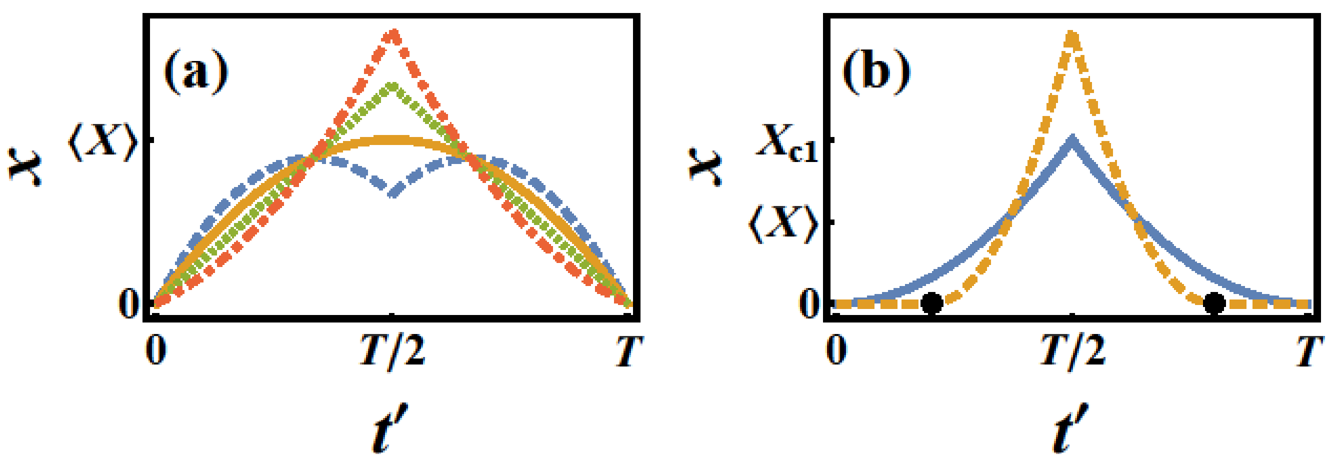
under conditions $x(0) = x(T) = 0, \;\; x(0 < t < T) > 0, \;\; \int_0^T x(t)dt = A, \; x(\tau) = X$

In geometrical optics, this conditional probability is equal to the ratio of the probabilities (and the action is equal to the difference of the actions) of two different optimal paths that enclose area A: with and without the constraint $x(\tau) = X$

Minimize $$S = \frac{1}{4D}\int_0^T \left(\frac{dx}{dt}\right)^2 dt$$

under conditions $x(0) = x(T) = 0$, $x(0 < t < T) > 0$, $\int_0^T x(t)dt = A$, $x(T/2) = X$

The optimal path is composed of two parabolic segments

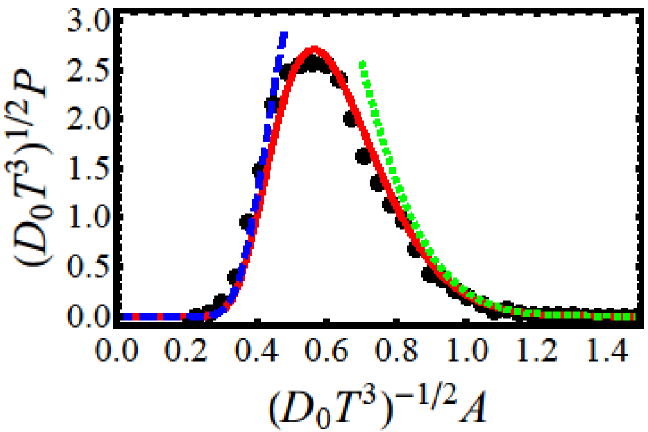


At $X > X_c = \frac{3A}{T}$ the one-sidedness $x(0 < t < T) > 0$ kicks in via tangent construction. This leads to a dynamical phase transition of third order

A sharp transition appears only in the limit $\frac{A}{\sqrt{D\,T^3}} \to \infty$; it is smoothed out at finite $\frac{A}{\sqrt{D\,T^3}}$

Does geometrical optics describe all types of large deviations of Brownian motion? The answer is no.

Example: the small-A tail of the Airy distribution



$$-\ln P(A,T) \cong \begin{cases} \dfrac{2\,\alpha_1{}^3}{27}\,\dfrac{DT^3}{A^2}, & A \ll \sqrt{D\,T^3} \\ \dfrac{6\,A^2}{DT^3}, & A \gg \sqrt{D\,T^3} \end{cases}$$

The $A \ll \sqrt{D\,T^3}$ tail follows from a different large-deviation formalism

Let $\bar{x} = \frac{A_T}{T} = \frac{1}{T}\int_0^T x(t)dt$ $\quad C\,\frac{DT^3}{A^2} = Tg(a),\ a = \frac{A}{T}, g(a) = C\ \frac{D}{a^2},\ \ \bar{x} \ll \sqrt{DT}$

Donsker-Varadhan large deviation principle

The constant $C = \frac{2\,\alpha_1{}^3}{27}$ can be found by using the tilted generator technique,
See the lectures of H. Touchette, or H. Touchette, Physica A **504**, 5 (2018)

In this regime there are many non-typical paths which lead to small $\bar{x}$

Some other applications of geometrical optics of Brownian motion

1. BM, Mortal Brownian motion: Three short stories, Int. J. Mod. Phys. B **33**, 1950172 (2019).

2. S. N. Majumdar and BM, Statistics of first-passage Brownian functionals, J. Stat. Mech. (2020) 023202.

3. S. N. Majumdar and BM, Toward the full short-time statistics of an active Brownian particle on the plane, Phys. Rev. E **102**, 022113 (2020).

4. T. Bar and BM, Geometrical optics of large deviations of Brownian motion in inhomogeneous media, J. Stat. Mech. (2023) 093301.

Summary of this part

- Geometrical optics is a simple and efficient tool for studying Brownian motion, “pushed” to a large-deviation regime by imposed constraints. Optimal paths are visual, instructive and observable in experiment and simulations.

- Predicts dynamical phase transitions of purely geometrical origin.

Geometrical optics can also be obtained from the Fokker-Planck equation via dissipative WKB approximation

Freidlin and Wentzel, … in mathematics
Graham, Dykman et al, … in physics

$$\frac{\partial P(x,t)}{\partial t} = D\ \frac{\partial^2 P(x,t)}{\partial x^2} \qquad -\infty < x < \infty$$

$$P(x, t=0) = \delta(x)$$

$$\text{WKB ansatz } P(x,t) = \exp[-\frac{s(x,t)}{D}]$$

Compare with quantum mechanics!

$$\frac{1}{D}\frac{\partial s}{\partial t} + \frac{1}{D}\left(\frac{\partial s}{\partial x}\right)^2 + \frac{\partial^2 s}{\partial x^2} = 0$$

This equation is exact

In WKB approximation (formally $D \to 0$, "weak−noise" theory) we can neglect the second derivative term:

$$\frac{\partial s}{\partial t} + \left(\frac{\partial s}{\partial x}\right)^2 = 0$$

a Hamilton − Jacobi equation
for a free 1d particle motion with Hamiltonian $H(x,p) = p^2$

Hamilton′s equations are $\dfrac{dx}{dt} = \dfrac{\partial H}{\partial p} = 2p, \quad \dfrac{dp}{dt} = -\dfrac{\partial H}{\partial x} = 0 \qquad p = p_0 = \text{const.}$

Hamilton's equations are $\dfrac{dx}{dt} = \dfrac{\partial H}{\partial p} = 2p, \quad \dfrac{dp}{dt} = -\dfrac{\partial H}{\partial x} = 0 \qquad p = p_0 = \text{const.}$

$$x(t) = 2p_0 t = Xt/T$$

$$s(X,T) = \int_0^T [p(dx/dt) - H]\,\mathrm{dt} = \int_0^T (2{p_0}^2 - {p_0}^2)\,\mathrm{dt} = X^2/(4T)$$

$$P(X,T) \sim \exp\left[-\frac{s(X,T)}{D}\right] = \exp\left[-\frac{X^2}{4DT}\right]$$

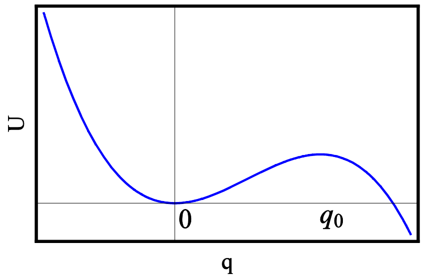
again reproducing the propagator of the diffusion equation

A more interesting example: Kramers problem

$$\partial_t q = f(q) + \sqrt{\varepsilon}\,\xi(t)$$

$$\langle \xi(t)\xi(t+\tau)\rangle = \delta(\tau)$$

$$f(q) = -dU(q)/dq$$



Over-damped particle in a potential

ε<<1

The evolution of the probability distribution *P(q,t)* is described by the Fokker-Planck eqn.

$$\partial_t P = -\partial_q [f(q)P] + \frac{\varepsilon}{2}\partial_{qq} P$$

WKB ansatz for long-lived metastable PDF

$$P(q,t) \sim \exp[-\frac{S(q,t)}{\varepsilon}]$$

In the leading order in 1/ε we obtain

$$\partial_t S + f(q)\partial_q S + \frac{1}{2}(\partial_q S)^2 = 0,$$

a Hamilton-Jacobi equation

$$H(q,p) = (1/2)p^2 + f(q)p = \text{const}$$

$$dq/dt = \partial H/\partial p = f(q) + p,$$

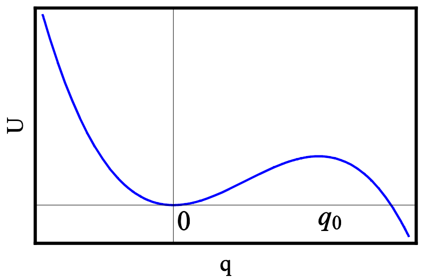
$$dp/dt = -\partial H/\partial q = -f'(q)p$$

$$H(q,p)=\frac{p^2}{2}+f(q)p=\text{const}$$

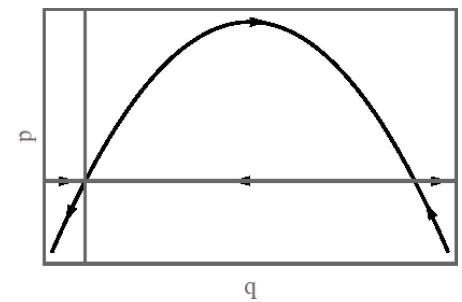
$$dq/dt=\partial H/\partial p=f(q)+p,$$

$$dp/dt=-\partial H/\partial q=-f'(q)p$$

p=0 is an invariant manifold, *dq/dt=f(q)* relaxation trajectories.
Escape requires an *activation* trajectory, *p≠0*



Boundary conditions in time:
q(t=-∞)=0, q(t=T)=q0



$$H=0\Rightarrow p=-2f(q)\Rightarrow dq/dt=-f(q),$$

1) heteroclinic trajectory
2) time-reversed relaxation trajectory

$$S(q_0,t)=\int_0^{q_0}p(q)dq=-2\int_0^{q_0}f(q)dq \;=2U(q_0)$$

$$P(q_0,t)\sim\exp[-\frac{2U(q_0)}{\varepsilon}]$$

Kramers' formula

Pre-exponential factor can be calculated in the sub-leading order in ε