A canonical representation of the path integral

Using an identity

$$\int_{-i\infty}^{+i\infty} \frac{dp}{2\pi i}\, e^{dt\left[Dp^2 - px\right]} = \frac{1}{\sqrt{4\pi D dt}}\, e^{-\frac{dt}{4D}\cdot x^2}$$

we write the path integral in Eq (2) as

$$G_T(x_T|x_0) = \lim_{\substack{dt\to 0\\ N\to\infty}} \int \prod_{k=1}^{N-1} dx_k \prod_{l=1}^{N} \frac{dp_l}{2\pi i}\, e^{-dt\sum_{n=0}^{N-1} p_n\left(\frac{x_{n+1}-x_n}{dt}\right)}$$
$$e^{dt\sum_{n=0}^{N-1}\left[Dp_n^2 + p_n F\left(\frac{x_{n+1}+x_n}{2}\right)\right]}$$
$$e^{-dt\cdot\frac{1}{2}\cdot\sum_{n=0}^{N-1} F'\left(\frac{x_{n+1}+x_n}{2}\right)}$$
$$= \int_{x_0}^{x_T} \mathcal{D}[x,p]\, e^{-S[x,p]}$$

with Action

$$S[x,p] = \int_0^T dt \left\{ p\dot{x} - \underbrace{\left[Dp^2 + pF - \tfrac{1}{2}F'\right]}_{\text{effective Hamiltonian.}} \right\}$$

Remark: This form of the Action is an example of Martin-Siggia-Rose-Janssen-De Dominicis Action. The field $p(t)$ is known as response field because of the following reason.

consider a small perturbation in the Force

$$F \to F + h\,\delta(t-t_0) \qquad \text{at time } 0<t_0<T$$

This will lead to a change in the probability at time T,

$$\Delta G_T(x_T|x_0) \simeq h\cdot\frac{\partial G_T}{\partial h}\Big|_{h=0} = \int \mathcal{D}[x,p]\, p(t_0)\, e^{-S_0[x,p]}$$

here S_0 is the Action for $h=0$ (unperturbed state)

Then, change in average value of x_T

$$\langle \Delta x_T \rangle = \langle x_T \rangle_h - \langle x_T \rangle_{h=0}$$

$$\simeq h \cdot \int dx_T \cdot \left.\frac{\partial G}{\partial h}\right|_{h=0} \cdot x_T \qquad \text{for small } h.$$

$$= h \int dx_T \int_{x_0}^{x_T} \mathcal{D}[x,p] \; x_T \, p(t_0) \cdot e^{-S_0}$$

$$= h \langle x_T \, p(t_0) \rangle$$

For arbitrary $h(t)$,

$$\langle \Delta x_T \rangle \simeq \int^T dt \; \underbrace{\langle x_T \, p(t) \rangle}_{\text{Response fn}^c \; R(T,t)} h(t)$$

<u>Further reading</u>: lecture note by Kay Wiese on "Advanced Statistical Field theory." available at www.phys.ens.fr/~wiese/masterENS.

Is there an analogue of Itô-Stratonovich in Quantum mechanics?

[Ref. Ashok Das, Field theory book, ch2]

Classical to quantum: When we describe a quantum system, we associate (x, p) to operators $(\hat{x}, \hat{p})$ and define a Hamiltonian operator from a classical counter part.

For example, classical harmonic oscillator

$$H_{class}(x,p) := \frac{p^2}{2m} + \frac{1}{2}\omega x^2$$

is used to describe quantum harmonic oscillator

$$\hat{H}_{quant}(\hat{x},\hat{p}) := \frac{\hat{p}^2}{2m} + \frac{1}{2}\omega \hat{x}^2$$

However, $[\hat{x},\hat{p}] = i\hbar$, ie they do not commute and this leads to ambiguities.

Most common convention for quantization is by Weyl ordering.

Classical		quantum
xp	$\longrightarrow$	$\frac{1}{2}(\hat{x}\hat{p} + \hat{p}\hat{x})$
$x^2 p$	$\longrightarrow$	$\frac{1}{3}(\hat{x}^2\hat{p} + \hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2)$
generally $e^{\alpha x + \beta p}$	$\longrightarrow$	$e^{\frac{\alpha}{2}\hat{x}} \cdot e^{\beta\hat{p}} \cdot e^{\frac{\alpha}{2}\hat{x}}$

using $[\hat{x},\hat{p}] = i\hbar$ and Baker-Campbell-Hausdorff formula.

A relevant consequence for us is that following this convention we can write elements of $\hat{H}_{wo}$ in terms of $H_{classical}$.

For this we note

- $\hat{x}, \hat{p}$ are Hermitian operators, their eigenbasis
- $\hat{x}|x\rangle = x|x\rangle$ and $\hat{p}|p\rangle = p|p\rangle$
- and
$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\frac{ip}{\hbar}x}$$
- and $\int dp\,|p\rangle\langle p| = \hat{\mathbb{1}}$ and $\int dx\,|x\rangle\langle x| = \hat{\mathbb{1}}$

Then,

$$\langle x'|\tfrac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x})|x\rangle = \int \frac{dp}{2\pi\hbar}\, e^{\frac{ip}{\hbar}(x'-x)}\, \frac{x'+x}{2}\cdot p$$

and more generally

$$\langle x'|\left[e^{\alpha x+\beta p}\right]_{W.O.}|x\rangle = \int \frac{dp}{2\pi\hbar}\, e^{\frac{ip}{\hbar}(x'-x)}\, e^{\alpha\frac{x'+x}{2}}\cdot e^{\beta p}$$

This finally means,

If we construct $\hat{H}_{w.o.}$ from $H_{cl}(x,p)$ by Weyl order convention, then

$$\boxed{\langle x'|\hat{H}_{w.o.}|x\rangle = \int \frac{dp}{2\pi\hbar}\, e^{\frac{ip}{\hbar}(x'-x)}\, H_{cl}\left(\frac{x+x'}{2}, p\right)}$$

See how this is analogous to Stratonovich-convention!

<u>Remark</u>: there is another convention, named Normal ordering,

where $x^n p^m \xrightarrow[N.O.]{} \hat{p}^m \cdot \hat{x}^n$ (always keep $\hat{p}$ at left)

following which

$$\langle x' | \hat{H}_{N.O.} | x \rangle = \int \frac{dp}{2\pi\hbar} \, e^{\frac{ip}{\hbar}(x'-x)} \, H_{cl}(x,p) \, .$$

See how this is analogous to Itô-convention.

Knowing that in statistics, stratonovich preserves standard calculus, let's construct quantum mechanical path integral using Weyl ordering.

Let's define quantum propagator

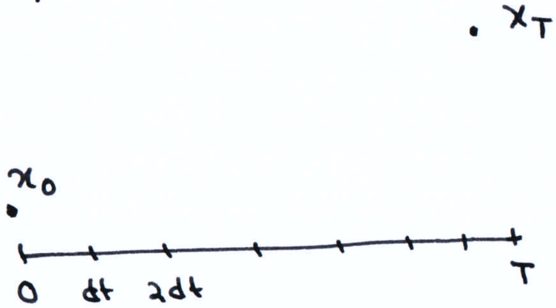
$$\hat{g}_T = \Theta(T) \cdot e^{-\frac{i}{\hbar} T \hat{H}_{W.O.}} \quad \cdots\cdots\cdots (3)$$

step function

time independent Hamiltonian

We are interested in the ~~probab~~ amplitude

$$g_T(x_T | x_0) = \langle x_T | \hat{g}_T | x_0 \rangle$$



splitting small time intervals dt, we write

$$g_T(x_T|x_0) = \int dx_1 \cdots dx_{N-1}$$

$$\langle x_N | \hat{g}_{dt} | x_{N-1} \rangle \langle x_{N-1} | \hat{g}_{dt} \cdots\cdots\cdots |x_1\rangle\langle x_1 | \hat{g}_{dt} | x_0 \rangle$$

$$= \int dx_1 \cdots dx_{N-1} \int \frac{dp_1}{2\pi\hbar} \cdots\cdots \frac{dp_N}{2\pi\hbar} \left[e^{\frac{i}{\hbar} p_N (x_N - x_{N-1})} \cdot e^{-\frac{i\,dt}{\hbar} H_{cl}\left(\frac{x_N + x_{N-1}}{2}, p_N\right)} \right]$$

$$\cdots\cdots \left[e^{\frac{i}{\hbar} p_1 (x_1 - x_0)} \, e^{-\frac{i\,dt}{\hbar} H_{cl}\left(\frac{x_1 + x_0}{2}, p_1\right)} \right]$$

by using

$$\langle x_n | \hat{g}_{dt} | x_{n-1} \rangle = \langle x_n | e^{-\frac{i}{\hbar} dt \hat{H}_{w.o.}} | x_{n-1} \rangle$$

$$= \int \frac{dp_n}{2\pi\hbar} \cdot e^{\frac{ip}{\hbar}(x_n - x_{n-1})} \cdot e^{-\frac{i}{\hbar} dt H_{cl}\left(\frac{x_n + x_{n-1}}{2}, p_n\right)}$$

The formula we obtained for $g_T(x_T|x_0)$ in the limit $dt \to 0$ is considered as path integral representation.

$$\boxed{g_T(x_T|x_0) = \int_{x_0}^{x_T} \mathcal{D}[x,p]\, e^{\frac{i}{\hbar} S[x,p]}}$$

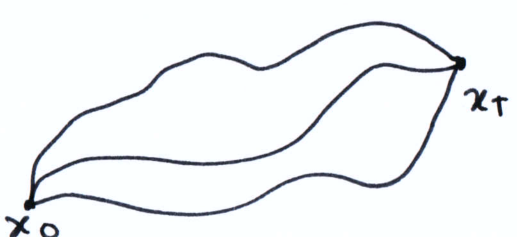
with $S[x,p] = \int_0^T dt \left\{ p(t) \cdot \dot{x}(t) - H_{cl}(x(t), p(t)) \right\}$

Their precise definition is in the discrete form.

$$g_T(x_T|x_0) = \lim_{dt \to 0} \lim_{N \to \infty} \int \prod_{k=1}^{N-1} dx_k \prod_{j=1}^{N} \frac{dp_j}{2\pi\hbar}\, e^{\frac{i\,dt}{\hbar} \sum_{n=0}^{N-1} p_{n+1}\left(\frac{x_{n+1} - x_n}{dt}\right)}$$

$$\cdot e^{-\frac{i}{\hbar} dt \sum_{n=0}^{N-1} H_{cl}\left(\frac{x_{n+1} + x_n}{2}, p_n\right)}$$

<u>Remark</u>: advantage of path integral is that everything on the right hand side is ~~classical~~ (no operator)!
Also it gives idea about contribution of paths



Each path is weighted by a phase factor $\frac{i}{\hbar} S$.

Relation of Langevin eq. to quantum mechanics

Case 1: Gradiant force / equilibrium condition.

$$F(x) = -U'(x)$$

Recall from earlier lectures that for this special case the F-P equation

$$\frac{\partial P_t(x)}{\partial t} = D \frac{\partial^2}{\partial x^2} P_t(x) + \frac{\partial}{\partial x} U'(x) P_t(x)$$

$(* \; D \equiv k_B T)$

under a transformation

$$P_t(x) = e^{-\frac{U(x)}{2D}} \psi_t(x)$$

reduces to

$$-\frac{\partial}{\partial t} \psi_t(x) = -D\, \psi_t''(x) + V(x)\, \psi_t(x)$$

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

Similarity with Schrödinger equation can be made even more strong by a change of variables

$$\boxed{t \to \frac{i}{\hbar} t \;, \quad D \to \frac{\hbar^2}{2m}} \quad \text{and} \quad \psi_t(x) \equiv \psi_t(x)$$

which gives

$$\boxed{i\hbar \frac{\partial}{\partial t} \psi_t(x) = -\frac{\hbar^2}{2m} \cdot \psi_t''(x) + V(x)\, \psi_t(x)}$$

In operator form, the quantum mechanical Hamiltonian

$$\hat{H}(\hat{x},\hat{p}) := \frac{\hat{p}^2}{2m} + V(\hat{x}) \quad \text{with } \hat{p} = -i\hbar \frac{\partial}{\partial x}$$

$$\text{and } V(x) = \frac{m}{2\hbar^2} (U')^2 - \frac{U''}{2}$$

This gives the propagator for FP-equation in terms of propagator in quantum mechanics.

$$\underbrace{G_T(x_T|x_0)}_{\big\downarrow\; e^{T\hat{\mathcal{L}}}} = e^{-\frac{U(x_T)}{2D}} \underbrace{\Big[g_T(x_T|x_0)\Big]_{T\to -i\hbar T}}_{\big\downarrow\; e^{-\frac{i}{\hbar}T\hat{H}}} \cdot e^{+\frac{U(x_0)}{2D}}$$

How do we see this in their path integral?

Start with path integral for Langevin (in canonical form).

$$G_T(x_T|x_0) = \int \mathcal{D}[x,p]\, e^{-S[x,p]}$$

with
$$S = \int_0^T dt \left\{ p\dot{x} - \left[Dp^2 + pF - \tfrac{1}{2}F'\right]\right\}$$

← following Stratonovich discretization ($\alpha = \frac{1}{2}$) therefore usual calculus.

$$= \underbrace{-\int_0^T dt\cdot \frac{F}{2D}\cdot\dot{x}}_{\xrightarrow{F=-U'}\ \frac{U(x_T)}{2D}-\frac{U(x_0)}{2D}} + \int_0^T dt\left\{\left(p+\frac{F}{2D}\right)\cdot\dot{x} - \left[D\left(p+\frac{F}{2D}\right)^2 - \underbrace{\left(\frac{F^2}{2D}+\frac{F'}{2}\right)}_{V(x)}\right]\right\}$$

gives us

$$G_T(x_T|x_0) = e^{-\frac{U(x_T)}{2D}}\cdot R\cdot e^{+\frac{U(x_0)}{2D}}$$

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

where we redefined $p + \frac{F}{2D} \to p$

Now, using the change of variables

$$t \to \frac{i}{\hbar} t \,, \quad D \to \frac{\hbar^2}{2m} \quad \text{and} \quad p \to -\frac{i}{\hbar} p$$

we get

$$R = \int \mathcal{D}[x,p] \, e^{\frac{i}{\hbar} \int_0^{-i\hbar T} dt \left\{ p\dot{x} - \left(\frac{p^2}{2m} + V(x) \right) \right\}}$$

$$= \Big[g_T(x_T | x_0) \Big]_{T \to -i\hbar T}$$

Quantum propagator with $H_{cl}(x,p) = \frac{p^2}{2m} + V(x)$

Remark: Note that we started with Stratonovich discretization $(\alpha = \frac{1}{2})$, which for the quantum propagator gives Weyl ordering discretization $\quad H_{cl}\left(\frac{x_{n+1} + x_n}{2}, p_n \right)$.

This demonstrates the equivalence between Stratonovich and Weyl ordering. It is straightforward to see the equivalence extends for other choices of discretization, e.g. $\alpha = 0 \Rightarrow$ normal order.

Remark: Schrödinger equation associated to g_T is with Hamiltonian

$$\hat{H} := \frac{\hat{p}^2}{2m} + \left[\frac{1}{2} \frac{m}{\hbar^2} (U')^2 - \frac{U''}{2} \right]$$

as we have found directly by similarity transformation.

and

$$\left(i\hbar \partial_t - \hat{H} \right) g_t(x|x_0) = i\hbar \, \delta(t) \, \delta(x - x_0)$$

case 2: The previous mapping relies on the fact that $F(x) = -U'(x)$, i.e. a gradiant force. The equivalent quantum problem is with a self-adjoint Hamiltonian. For non-gradiant force this not the case, but still we can follow the ~~correspondance~~ correspondance mathematically to derive the Fokker-Planck equation from the path integral representation.

For arbitrary $F(x)$, the Langevin propagator

$$G_T(x_T|x_0) = \int \mathcal{D}[x,p]\, e^{-S}$$

with stratonovich ~~choice~~ discretization

$$S = \int dt \left\{ p\dot{x} - \left[Dp^2 + pF - \tfrac{1}{2}F' \right] \right\}$$

$$\rightarrow -\frac{i}{\hbar} \int_0^{-i\hbar T} dt \left\{ p\dot{x} - \left[\frac{p^2}{2m} + \frac{i}{\hbar} pF(x) + \frac{1}{2}F'(x) \right] \right\}$$

where we used ~~the~~ the earlier transformation

$$t \rightarrow \frac{i}{\hbar} t, \quad D \rightarrow \frac{\hbar^2}{2m}, \quad p \rightarrow -\frac{i}{\hbar} p$$

Evidently

$$G_T(x_T|x_0) = \Big[g_T(x_T|x_0) \Big]_{T \rightarrow -i\hbar T}$$

with $H_{el} = \dfrac{p^2}{2m} + \dfrac{i}{\hbar} pF + \dfrac{1}{2}F'$

[See the definion of g_T and H_{el}].

As we started with stratonovich convention, clearly the transformed path integral (associated to g_T) is the one that corresponds to weyl ordered action. This means, g_T is the path integral for a quantum Hamiltonian

$$\hat{H}_{w.o.} := \frac{\hat{p}^2}{2m} + \frac{i}{\hbar}\,\frac{\left(\hat{p}\,F(\hat{x}) + F(\hat{x})\,\hat{p}\right)}{2} + \frac{1}{2}F'(\hat{x})$$

This means, $g_t(x|x_0)$ follows

$$i\hbar\,\partial_t \hat{g}_t = \hat{H}_{w.o.}\,\hat{g}_t + i\hbar\,\delta(t)$$

$p = -i\hbar\partial_x$

$$\Rightarrow i\hbar\,\partial_t g_t(x|x_0) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2 g}{\partial x^2} + \frac{1}{2}\frac{\partial}{\partial x}Fg + \frac{1}{2}g\cdot F' + \frac{1}{2}F'g\right] + i\hbar\,\delta(t)\,\delta(x-x_0)$$

$$= -\frac{\hbar^2}{2m}g'' + (Fg)' + i\hbar\,\delta(t)\,\delta(x-x_0)$$

To see what equation $G_T(x|x_0)$ satisfies, we $G_T = \left[g_T\right]_{T\to -i\hbar T}$ ~~and~~
~~take the "inverse" change of variables~~ with $\frac{\hbar^2}{2m} = D$,

~~$t \to -i\hbar t$~~

which gives

$$\boxed{\partial_t G_T(x|x_0) = D\,G_T'' - (F\,G)' + \delta(t)\,\delta(x-x_0)}$$

as we have expected from the FP equation of the Langevin equation $\dot{x} = F(x) + \eta(t)$ with $\langle \eta(t)\eta(t')\rangle = 2D\,\delta(t-t')$.

__Remark:__ note that $\hat{H}_{w.o.}$ is not self-adjoint (because of the i-term)
Never the less the algebra follows without a problem.
We took this root to emphasize the equivalence with Weyl ordering. One can straight away do the analysis of Path integral $\longrightarrow$ FP equation without the change of variables (and therefore not relating to QM).

• Why is path integral useful for Langevin equation?

Two examples

① Describing processes under "global constraints" and analysing path functionals.

② Gives optimal path (Instanton solutions).

For the first example we shall use the following.

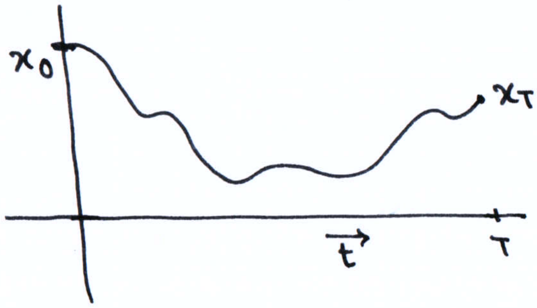
$$\boxed{\begin{array}{l}\text{The propagator} \\ \displaystyle G_T(x_T|x_0) = \int_{x_0}^{x_T} \mathcal{D}[x]\, e^{-\int_0^T dt \left\{ \frac{\dot{x}^2}{4D} + V(x) \right\}} \\ \text{satisfies} \\ \partial_t G_t(x|x_0) = D\, \partial_x^2 G_t(x|x_0) - V(x)\, G_t(x|x_0) + \delta(t)\,\delta(x-x_0)\end{array}} \quad (5)$$

[verify this]

__Remark:__ as there are no $\dot{x}V(x)$ terms, choise of discretization do not play a role.

__A very simple example:__ Survival probability of a Brownian motion.

What is the probability for a Brownian particle started at $x_0 > 0$ to not cross the origin upto time T.



This is given by

$$S_T(x_0) = \int_0^\infty dx_T \int_{x_0}^{x_T} \mathcal{D}[x]\, e^{-\int_0^T dt \frac{\dot{x}^2}{4D}} \prod_{t=0}^{T} \Theta(x(t))$$

$$= \int_0^\infty dx_T \lim_{\substack{dt \to 0 \\ N \to \infty}} \left(\frac{1}{4\pi D\, dt}\right)^{\frac{N}{2}} \int_{-\infty}^{\infty} dx_1 \cdots dx_{N-1} \prod_{n=1}^{N} \Theta(x_n)\, e^{-\frac{1}{4D}\sum_{n=0}^{N-1} \frac{(x_{n+1}-x_n)^2}{dt}}$$

We can write the path integral as

$$S_T(x_0) = \int_0^\infty dx_T \int_{x_0}^{x_T} \mathcal{D}[x_T]\; e^{-\int_0^T dt \left\{ \frac{\dot{x}^2}{4D} + V(x) \right\}} = \int_0^\infty dx_T\, G_T(x_T|x_0)$$

with $$V(x) = -\log \Theta(x) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x \leq 0. \end{cases}$$

~~From (5) and considering symmetry of (x_T, x_0), we see~~

$$\cancel{\partial_t S_t(x_0) = D\, \partial^2_{x_0} S_t(x_0) + V(x_0)\, S_t(x_0)}$$

Then, from (5) $G_t(x|x_0)$ is solution of a diffusion equation in presence of vanishing boundary at $x=0$, i.e.

$$G_t(x|x_0) = 0 \quad \text{for } x = 0$$

Corresponding solution

$$G_t(x|x_0) = \frac{1}{\sqrt{4\pi D t}} \left\{ e^{-\frac{(x-x_0)^2}{4Dt}} - e^{-\frac{(x+x_0)^2}{4Dt}} \right\}$$

[check that is satisfies $\partial_t G_t = \delta(t)\,\delta(x-x_0)$ with $G_t(0) = 0$]

[We could have obtained the solution using reflection principle]
or
Image method.

It gives

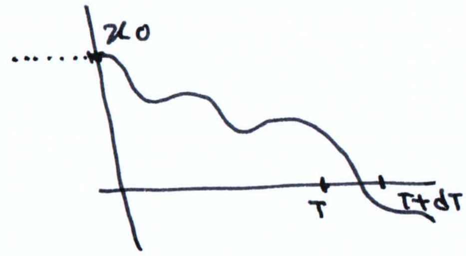
$$\boxed{S_T(x_0) = \int_0^\infty dx_T\, G_T(x_T|x_0) = \mathrm{Erf}\left(\frac{x_0}{\sqrt{4DT}}\right)}$$

The survival probability

* First passage probability density $f_{x_0}(T)$:

The probability that a Brownian particle starting at $x_0 > 0$, crosses the origin for the first time between time window T and $T+dT$ is given by $f_{x_0}(T)\, dT$.

Convince yourself that



$$f_{x_0}(T) = -\frac{d S_T(x_0)}{dT}$$

no of paths that crossed origin betwee T to T+dT firsttime

= no of paths survived up to T

− no. of path survived up to T+dT

$$\Rightarrow \quad f_{x_0}(T)\, dT = S_T(x_0) - S_{T+dT}(x_0)$$

Gives the well known result

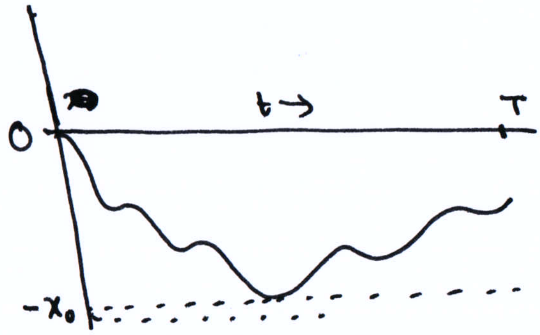
$$\boxed{f_{x_0}(T) = \frac{x_0}{\sqrt{4\pi D}} \cdot \frac{e^{-\frac{x_0^2}{4DT}}}{T^{3/2}} \sim \frac{1}{T^{3/2}}}$$

Remember the exponent!

<u>Remark</u> : notice that it is the Lévy distribution ($\alpha = \frac{1}{2}$) for which mean first passage time is infinite, although the probability that the particle will eventually cross is $\int_0^\infty dT\, f_{x_0}(T) = 1$ (certainly cross!).

This mean in 1 dimension a Brownian motion is recurrent, This is a version of Polya's theorem. [see Assignment problem]

* Probability of maximum/minimum



Let $\mathcal{P}_T(-x_0)$ be the prob for a Brownian particle to have minimum position $(-x_0)$, with $x_0 > 0$, in time T. (By symmetry it is also the probability for maximum ~~val~~ position x_0).

Following a similar arguement as for the first passage prob, convince yourself that

$$\mathcal{P}_T(-x_0) = \frac{d S_T(x_0)}{dx_0}$$

$$= \frac{e^{-\frac{x_0^2}{4Ddt}}}{\sqrt{\pi D dt}}$$

~~Rem~~