0.1 Introduction

(Lesson ? of 18/11/19) Compiled: November 18, 2019

We want to show that there are cases where the stochastic equation (or the resulting path integral) assume a particular form that is theoretically advantageous to be studied in an analytical way, leading to the *Feynmann-Kac* formula, useful both in stochastic processes and in quantum mechanics (note that, in the latter, it needs to be generalized to complex numbers - which isn't rigorous, but still leads to exact results).
During last lecture, when discussing the Harmonic Oscillator in the overdamped limit, we wrote that:

$$\mathrm{d}x = -kx\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}B \qquad k = \frac{m\omega^2}{\gamma}$$

Then, recall that:

$$W(x,t|x_0,0) = \exp\left(-\frac{x^2 - x_0^2}{4D}k + kt\right)\langle\exp\left(-\int_0^t V(x(\tau))\,\mathrm{d}\tau\right)\delta(x(t)-x)\rangle_W$$

where the average is intended to be computed in the Wiener measure:

$$\langle\cdots\rangle_W = \int\prod_{\tau=0}^{t}\frac{\mathrm{d}x(\tau)}{\sqrt{4\pi D}\,\mathrm{d}\tau}\exp\left[-\frac{1}{4D}\int_0^t \dot{x}^2(\tau)\,\mathrm{d}\tau\right] \qquad V(x) = \frac{k^2x^2}{4D}$$

Integrals of this kind appear quite often when a particle moves in a 3D potential. Our goal is now to consider the more general case of a particle moving in a conservative force-field, and see how the average:

$$\langle\exp\left(-\int_0^t V(x(\tau))\,\mathrm{d}\tau\right)\delta(x(t)-x)\rangle_W \equiv W_B(x,t)$$

will reappear, i.e. we will observe how general problems have a similar formulation.
Note that $V(x)$ is *proportional* to the original harmonic potential:

$$U(x) = \frac{1}{2}m\omega^2x^2$$

0.2 Particle in a conservative force-field

Let's consider a particle in a 3D space $\boldsymbol{r} = (x_1,x_2,x_3)^T$, immersed in a conservative force-field $F(\boldsymbol{r}) = -\boldsymbol{\nabla}U(\boldsymbol{r})$ with potential $U(\boldsymbol{r})$. Then:

$$\mathrm{d}\boldsymbol{r} = \boldsymbol{f}(\boldsymbol{r})\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}\boldsymbol{B}$$

with $B = (B_1,B_2,B_3)^T$ and:

$$\Delta B_\alpha \sim \frac{1}{\sqrt{2\pi\Delta t}}\exp\left(-\frac{\Delta B_\alpha^2}{2\Delta t}\right)$$

with $\boldsymbol{f} = \boldsymbol{F}/\gamma$, and $\gamma = 6\pi\eta a$. In vector notation:

$$\Delta \boldsymbol{B} \sim \exp\left(-\frac{(\Delta \boldsymbol{B})^2}{2\Delta t}\right)\frac{1}{(2\pi\Delta t)^{3/2}}$$

If we now discretize the problem:

$$\Delta \boldsymbol{r}_i = \boldsymbol{r}(t_i) - \boldsymbol{r}(t_i)$$

we can rewrite that equation as:

$$\Delta \boldsymbol{r}_i = \boldsymbol{f}_{i-1}\Delta t_i + \sqrt{2D}\Delta \boldsymbol{B}_i$$

We can then repeat all the steps we've seen in the 1D case, leading to:

$$\begin{aligned} \mathrm{d}P\left(\Delta \boldsymbol{B}_1, \dots, \Delta \boldsymbol{B}_N\right) &= \prod_{i=1}^N \frac{\mathrm{d}^3 \Delta B}{(2\pi\Delta t)^{3/2}} \exp\left(-\sum_{i=1}^N \frac{\Delta \boldsymbol{B}_i^2}{2\Delta t_i}\right) \\ \mathrm{d}P\left(\Delta \boldsymbol{r}_1, \dots, \Delta \boldsymbol{r}_N\right) &= \prod_{i=1}^N \frac{\mathrm{d}^3 \Delta \boldsymbol{r}_i}{(4\pi D\Delta t_i)^{3/2}} \exp\left[-\frac{1}{4D}\sum_{i=1}^N \frac{(\Delta \boldsymbol{r}_i - \boldsymbol{f}_{i-1}\Delta t_i)^2}{\Delta t_i}\right] \end{aligned}$$

(Note that, in the textbook, instead of $\boldsymbol{f}_{i-1}$ they are using the Stratonovich prescription $(\boldsymbol{f}_i + \boldsymbol{f}_{i-1})/2$, complicating the jacobian for a change of variables, while we are using Ito's. In the end, however, the final result will not depend on this choice - at least for this case).
Expanding the exponential:

$$-\frac{1}{4D}\sum_{i=1}^N\left[\frac{\Delta \boldsymbol{r}_i^2}{\Delta t_i} + \boldsymbol{f}_{i-1}^2\Delta t_i - 2\Delta \boldsymbol{r}_{\boldsymbol{i}} \cdot \boldsymbol{f}_{i-1}\right]$$

and substituting back:

$$\mathrm{d}P\left(\{\Delta \boldsymbol{r}_i\}\right) = \underbrace{\prod_{i=1}^N \frac{\mathrm{d}^3 \Delta r_i}{(4\pi D\Delta t_i)^{3/2}} \exp\left[-\frac{1}{4D}\sum_{i=1}^N \frac{\Delta \boldsymbol{r}_i^2}{\Delta t_i}\right]}_{\mathrm{d}_W r} \exp\left(-\frac{1}{4D}\underbrace{\sum_{i=1}^N \boldsymbol{f}_{i-1}^2\Delta t_i}_{\int_0^t \boldsymbol{f}^2(\boldsymbol{r}(\tau))\,\mathrm{d}\tau} + \frac{1}{2D}\underbrace{\sum_{i=1}^N \boldsymbol{f}_{i-1}\cdot\Delta \boldsymbol{r}_i}_{\int_0^t \boldsymbol{f}(\boldsymbol{r}(\tau))\,\mathrm{d}_J\boldsymbol{r}(\tau)}\right)$$

Note that, for a vector function $h(\boldsymbol{r})$, letting $\boldsymbol{r}_i = \boldsymbol{r}_{i-1} + \Delta \boldsymbol{r}_i \Rightarrow \Delta \boldsymbol{r}_i = (\Delta x_i^1, \Delta x_i^2, \Delta x_i^3)^T$ leads to the following expansion:

$$\Delta h_i = h(\boldsymbol{r}_i) - h(\boldsymbol{r}_{i-1}) = \sum_{\alpha=1}^3 \Delta x_i^\alpha \frac{\partial}{\partial x^\alpha}h(\boldsymbol{r}_{i-1}) + \frac{1}{2}\sum_{\alpha,\beta=1}^3 \Delta x_i^\alpha \cdot \Delta x_i^\beta \frac{\partial^2}{\partial x^\alpha \partial x^\beta}h(\boldsymbol{r}_{i-1}) + \dots$$

Taking the continuum limit we make the following substitution:

$$\Delta x_i^\alpha \Delta x_i^\beta \to \Delta t_i 2D\delta^{\alpha\beta}$$

Then, summing all the increments:

$$h(\boldsymbol{r}_N) - h(\boldsymbol{r}_0) = \sum_{i=1}^{N} \Delta h_i = \sum_{\alpha=1}^{3} \sum_i \frac{\partial}{\partial x^\alpha} h_{i-1} \Delta x_i^\alpha + D \sum_{\alpha=1}^{3} \frac{\partial^2}{\partial x^{\alpha 2}} h_{i-1} \Delta t_i$$

and then, in the continuum limit:

$$h(\boldsymbol{r}(t)) - h(\boldsymbol{r}(0)) = \int_0^t \boldsymbol{\nabla} h \cdot \mathrm{d}_J \boldsymbol{r} + D \int_0^t \nabla^2 h \,\mathrm{d}t$$

Note that now, by rearranging, we find a formula for the integral we needed:

$$\int_0^t \boldsymbol{\nabla} h \cdot \mathrm{d}_J \boldsymbol{r} = h(\boldsymbol{r}(t)) - h(\boldsymbol{r}(0)) - D \int_0^t \nabla^2 h \,\mathrm{d}t$$

In fact, we can use it for solving:

$$\int_0^t \boldsymbol{f}(\boldsymbol{r}(\tau)) \,\mathrm{d}_J \boldsymbol{r}(\tau)$$

as we know that the force $\boldsymbol{f}$ comes from a potential:

$$\int_0^t \boldsymbol{f} \cdot \mathrm{d}_J \boldsymbol{r} = -\frac{1}{\gamma} \int \boldsymbol{\nabla} U \cdot \mathrm{d}_I \, \boldsymbol{r} = -\frac{1}{\gamma} \left[U(\boldsymbol{r}(t)) - U(\boldsymbol{r}(0)) - D \int_0^t \nabla^2 U \cdot \mathrm{d}\tau \right]$$

Substituting back in the first formula:

$$\mathrm{d}P\left(\{\boldsymbol{\Delta r}_i\}\right) \to \mathrm{d}_W \, \boldsymbol{r} \exp\left(-\frac{1}{4D} \int_0^t V(\boldsymbol{r}(\tau)) \,\mathrm{d}\tau \right) \exp\left(-\frac{1}{2D\gamma} [U(\boldsymbol{r}(t)) - U(\boldsymbol{r}(0))] \right)$$

where:

There may be missing factors

$$V = \boldsymbol{f}^2 - \frac{2D}{\gamma} \nabla^2 U = \boldsymbol{f}^2 - 2D \boldsymbol{\nabla} \cdot \boldsymbol{f}$$

(recalling that $\boldsymbol{\nabla} U/\gamma = -\boldsymbol{f}$).
Now:

$$\begin{aligned} W(\boldsymbol{r}, t | \boldsymbol{r}_0, 0) &= \int \mathrm{d}P \, \delta(\boldsymbol{r}(t) - \boldsymbol{r}) = \langle \delta(\boldsymbol{r}(t) - \boldsymbol{r}(0)) \rangle = \\ &= \int \mathrm{d}_W \boldsymbol{r} \exp\left(-\frac{1}{4D} \int_0^t V(\boldsymbol{r}(\tau)) \,\mathrm{d}\tau \right) \delta(\boldsymbol{r}(t) - \boldsymbol{r}) \exp\left(-\frac{1}{2D\gamma} (U(\boldsymbol{r}) - U(\boldsymbol{r}_0)) \right) = \\ &= \langle \exp\left(-\frac{1}{4D} \int_0^t V \,\mathrm{d}\tau \right) \delta(\boldsymbol{r}(t) - \boldsymbol{r}) \rangle_W \exp\left(-\frac{1}{2D\gamma} (U(\boldsymbol{r}) - U(\boldsymbol{r}_0)) \right) \end{aligned}$$

which is the general expression we were searching for.

0.2.1 Correspondence with Quantum Mechanics

An important result (here stated for the 1D case, for notational simplicity) is the following. Define:

$$W_B(x, t) \equiv \langle \exp\left(-\int_0^t V(x(\tau)) \,\mathrm{d}\tau \right) \delta(x(t) - x) \rangle_W \tag{1}$$

(the $4D$ constant has been absorbed by V). Then the following holds:

$$\partial_t W_B(x,t) = D\partial_x^2 W_B(x,t) - V(x)W_B(x,t) \tag{2}$$

Recall the Schrödinger equation:

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x,t) + v(x)\psi(x,t)$$

So by mapping $t \to -it$ (passing to "imaginary time"), and $\psi(-it,x) \equiv \hat{\psi}(t,x)$ we can cancel the i the Schrödinger equation, leading to:

$$\hbar\frac{\partial}{\partial t}\hat{\psi} = \underbrace{\frac{\hbar^2}{2m}}_{D}\partial_x^2\hat{\psi} - \underbrace{\frac{v(x)}{\hbar}}_{V}\hat{\psi}$$

which is equivalent to the Bloch equation.
We want now to prove that (1) satisfies (2). To do this, we discretize once again:

$$\psi_{N+1}(x) = \int\prod_{i=1}^{N+1}\frac{\mathrm{d}x_i}{\sqrt{4\pi D\Delta t_i}}\exp\left(-\sum_{i=1}^{N+1}\frac{(x_i - x_{i-1})^2}{4D\Delta t_i} - \sum_{i=1}^{N+1}\Delta t_i V(x_i)\right)\delta(x_{N+1} - x) \tag{3}$$

Choose $\Delta t_i \equiv \epsilon$, such that $t_{N+1} = (N+1)\epsilon = t \Rightarrow \epsilon = t/(N+1)$. Then:

$$W_B(x,t) = \lim_{N\to\infty}\psi_{N+1}(x)$$

Integrating over x_{N+1}:

$$(3) = \frac{1}{\sqrt{4\pi D\epsilon}}\int\prod_{i=1}^{N}\frac{\mathrm{d}x_i}{\sqrt{4\pi D\epsilon}}\exp\left(-\sum_{i=1}^{N}\frac{(x_i - x_{i-1}^2)}{4D\epsilon} - \sum_{i=1}^{N}\epsilon V(x_i)\right)\exp\left(\frac{-(x_{N+1} - x_N)^2}{4D\epsilon} - \epsilon V(x_{N+1})\right) =$$

Then $x_{N+1} \equiv x$ and:

$$= \int\frac{\mathrm{d}x_N}{\sqrt{4\pi D\epsilon}}\exp\left(-\frac{(x - x_N)^2}{4D\epsilon} - \epsilon V(x)\right)\boxed{\frac{1}{\sqrt{4\pi D\epsilon}}\int\prod_{i=1}^{N-1}\frac{\mathrm{d}x_i}{\sqrt{4\pi D\epsilon}}\exp\left(-\sum_{i=1}^{N}\frac{(x_i - x_{i-1})^2}{4D\epsilon} - \epsilon\sum_{i=1}^{N}V(x_i)\right)}$$

The highlighted part is equal to:

$$= \int\prod_{i=1}^{N}\frac{\mathrm{d}y_i}{\sqrt{4\pi D\epsilon}}\exp\left(-\sum_{i=1}^{N}\left[\frac{(y_i - y_{i-1})^2}{4D\epsilon} + \epsilon V(y_i)\right]\right)\delta(y_N - x_N) = \psi_N(x_N)$$

and so:

$$\psi_{N+1}(x) = e^{-\epsilon V(x)}\int\frac{\mathrm{d}x_N}{\sqrt{4\pi D\epsilon}}\exp\left(-\frac{(x - x_N)^2}{4D\epsilon}\right)\psi_N(x_N)$$

which looks like an evolution equation for ψ.

If we now change variables:

$$z \equiv \frac{x - x_N}{\sqrt{2D\epsilon}}$$

we arrive at:

$$\psi_{N+1}(x) = e^{-\epsilon V(x)} \int \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \psi_N(x - z\sqrt{2D\epsilon})$$

z is small, and so we can Taylor expand:

$$= e^{-\epsilon V(x)} \int \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \left[\psi_N(x) - z\sqrt{2D\epsilon}\psi'_N(x) + z^2 D\epsilon\psi''_N(x) + O(z^3\epsilon^{3/2})\right] =$$
$$= e^{-\epsilon V(x)}[\psi_N(x) + D\epsilon\psi''_N(x) + O(\epsilon^2)]$$

expanding also the exponential:

$$e^{-\epsilon V(x)} = \left(1 - \epsilon V(x) + \frac{\epsilon^2 V(x)^2}{2} + \dots\right)$$

we arrive at:

$$= \psi_N(x) + D\epsilon\psi''_N(x) - \epsilon V(x)\psi_N(x) + O(\epsilon^2)$$

Rearranging:

$$\frac{\psi_{N+1} - \psi_N}{\epsilon} = D\psi''_N - V\psi_N$$

And when $\epsilon \to 0$:

$$\partial_t W_B(x,t) = D\partial_x^2 W_B(x,t) - V(x)W_B(x,t)$$

which is Bloch's equation.
So we can *solve* this partial differential equation by simply generating random *paths* going from x_0 at time 0 to x at time t, computing the exponential of the integral $\int_0^t V(x(\tau))\,\mathrm{d}\tau$ and averaging the results:

$$W_B(x,t) \equiv \langle \exp\left(-\int_0^t V(x(\tau))\,\mathrm{d}\tau\right) \delta(x(t) - x)\rangle_W$$

0.3 Variational methods

One powerful technique to solve Wiener integral is through *variational methods*.
Consider a symmetric $N \times N$ matrix A ($A = A^T$) and the following gaussian integral:

$$\int \prod_{i=1}^N \exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x} + \boldsymbol{b}^T\boldsymbol{x}\right) = \frac{(2\pi)^{N/2}}{|A|^{1/2}} \exp\left(\frac{1}{2}\boldsymbol{b}^T A^{-1}\boldsymbol{b}\right) = \frac{(2\pi)^{N/2}}{|A|^{1/2}} \exp\left(\mathrm{Stat}_{\boldsymbol{x}}\left[-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x} + \boldsymbol{b}\cdot\boldsymbol{x}\right]\right)$$

where:

$$\mathrm{Stat}_{\boldsymbol{x}}\, F(\boldsymbol{x}) = F(\boldsymbol{x}_c); \qquad \boldsymbol{x_c} \text{ such that } \forall i \frac{\partial F(\boldsymbol{x})}{\partial x_i}\bigg|_{\boldsymbol{x}=\boldsymbol{x}_c} = 0$$

In this case:

$$\boldsymbol{F} = -\frac{\boldsymbol{x}^T A \boldsymbol{x}}{2} + \boldsymbol{b}^T \boldsymbol{x} \Rightarrow \partial_i F = -\sum_j A_{ij} x_j + b_i = -A\boldsymbol{x} + \boldsymbol{b} \overset{!}{=} 0 \Rightarrow \boldsymbol{x}_c = A^{-1}\boldsymbol{b}$$

Then, substituting in the original expression:

$$F(\boldsymbol{x}_c) = -\boldsymbol{x}_c^T A \boldsymbol{x}_c + \boldsymbol{b} \cdot \boldsymbol{x}_c = \frac{1}{2} \boldsymbol{b}^T A^{-1} \boldsymbol{b}$$

gives back the correct exponent for the integral's result.
This interesting idea can be applied also to Wiener integrals:

$$\begin{aligned} W(x, t|x_0, 0) &= \int \prod_{\tau=0}^{t} \frac{\mathrm{d}x(\tau)}{\sqrt{4\pi D \,\mathrm{d}\tau}} \exp\left(-\frac{1}{4D}\int_0^t \dot{x}^2(\tau)\,\mathrm{d}\tau\right) \delta(x - x(t)) = \\ &= \text{''} \lim_{N\to\infty} \text{''} \int \prod_{i=1}^{N} \frac{\mathrm{d}x_i}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\sum_{i=1}^{N} \frac{(x_i - x_{i-1})^2}{4D\Delta t_i}\right) \delta(x - x_N) \end{aligned}$$

Integrating over x_N:

$$= \frac{1}{\sqrt{4\pi D\Delta t_i}} \int \prod_{i=1}^{N-1} \frac{\mathrm{d}x_i}{\sqrt{4\pi D\Delta t_i}} \exp\left(-\sum_{i=1}^{N} \frac{(x_i - x_{i-1})^2}{4D\Delta t_i}\right)\bigg|_{x_N = x}$$

and now the *constraint* $\delta(x - x(t))$ is *inducing* a *linear term* in the exponential:

$$\sum_{i=1}^{N-1} \frac{(x_i - x_{i-1})^2}{4D\Delta t_i} - \underbrace{\frac{1}{4D\Delta t_N}(x - x_{N-1})^2}_{\frac{1}{4D\Delta t_N}(x^2 - 2x x_{N-1} + x_{N-1}^2)}$$

Passing to the continuum limit, we substitute the finite vector $\{x_i\}$ with the infinite one $\{x(\tau)\}$, so that:

$$W(x, t|x_0, 0) = N \exp\left(\mathrm{Stat}_{\{x(\tau)\}} -\frac{1}{4D}\int \dot{x}^2(\tau)\,\mathrm{d}\tau\right)$$

where $x(0) = x_0$ and $x(t) = x$. Recall that:

$$F(\boldsymbol{x}) = F(\boldsymbol{x}_c) + \sum_{i=1}^{N} X_i \frac{\partial}{\partial x_i} F(\boldsymbol{x}_c) + \dots \qquad \boldsymbol{x} = \boldsymbol{x}_c + \boldsymbol{X}$$

and the stationarity conditions are $\partial_i F(\boldsymbol{x}_c) = 0$. Differentiating:

$$\dot{x}(\tau) = \dot{x}_c(\tau) + \dot{X}(\tau) \qquad x_c(\tau) = \begin{cases} x_0 & \tau = 0 \\ x & \tau = t \end{cases}$$

Then, computing the integral $\dot{\boldsymbol{x}}^2$ with these coordinates "centered" on $\boldsymbol{x}_c$:

$$\int_0^t (\dot{\boldsymbol{x}}_c + \dot{\boldsymbol{X}})^2 \,\mathrm{d}\tau = \int_0^t \dot{\boldsymbol{x}}_c{}^2 \,\mathrm{d}\tau + 2\int_0^t \dot{\boldsymbol{x}}_c \dot{\boldsymbol{X}} \,\mathrm{d}\tau + \int_0^t \dot{\boldsymbol{X}}^2(\tau)\,\mathrm{d}\tau$$

Integrating by parts leads to:

$$= \dot{\boldsymbol{x}}_c(\tau)\boldsymbol{X}(\tau)\Big|_0^t - \int_0^t \ddot{\boldsymbol{x}}_c(\tau)\boldsymbol{X}(\tau)\,\mathrm{d}\tau$$

then $X(\tau) = 0$ both at $\tau = 0, t$, and with the boundary conditions $\ddot{x}_c = 0$, $x_c(0) = x_0$ and $x_c(t) = x$ leads to the *line solution*:

$$x_c(\tau) = x_0 + \frac{\tau}{t}(x - x_0) \quad \dot{x}_c(\tau) = \frac{x - x_0}{t}$$

Note that X does not depend on the boundary conditions, and so:

$$\begin{aligned}
W(x, t|x_0, 0) &= \mathcal{N}(t) \exp\left(\mathrm{Stat}_{\{x(\tau)\}} - \frac{1}{4D}\int \dot{x}^2(\tau)\,\mathrm{d}\tau\right) = \\
&= \mathcal{N}(t)\exp\left(-\frac{1}{4D}\int_0^t \dot{x}_c{}^2(\tau)\,\mathrm{d}\tau\right) = \mathcal{N}(t)\exp\left(-\frac{1}{4D}\int_0^t \left(\frac{x - x_0}{t}\right)^2 \mathrm{d}\tau\right) = \\
&= \mathcal{N}(t)\exp\left(-\frac{1}{4D}\frac{(x - x_0)^2}{t}\right)
\end{aligned}$$

and $\mathcal{N}(t)$ is just a normalization constant that can be determined by integration:

$$\mathcal{N}(t) = \frac{1}{\sqrt{4D\pi t}}$$