

## 0.1 Particle in a conservative force-field

In last section, we examined a particle of radius  $a$  immersed in a harmonic potential  $U(x) = m\omega^2 x^2/2$ , moving through a medium with viscosity  $\eta$  and subject to thermal fluctuations of amplitude proportional to  $\sqrt{2D}$ , so that its dynamics are described by the following *stochastic differential equation*:

$$dx = -kx dt + \sqrt{2D} dB \quad k = \frac{m\omega^2}{\gamma} \quad \gamma = 6\pi\eta a$$

The solution, expressed as the *transition probability* between any two given points, is a path integral:

$$W(x_t, t|x_0, 0) = \exp\left(-\frac{x_t^2 - x_0^2}{4D}k + \frac{kt}{2}\right) \langle \exp\left(-\int_0^t V(x(\tau)) d\tau\right) \delta(x(t) - x_t) \rangle_W \quad (1)$$

with  $V(x(\tau)) = k^2 x^2(\tau)/(4D)$ . The average is computed with the Wiener measure:

$$\langle f(x(\tau)) \rangle_W \equiv \int_{\mathbb{R}^T} \left( \prod_{\tau=0^+}^t \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \right) \exp\left(-\frac{1}{4D} \int_0^t \dot{x}^2(\tau) d\tau\right) f(x(\tau))$$

with  $\mathbb{R}^T$  being the set of continuous functions  $T \rightarrow \mathbb{R}$ , and  $T = [0, t]$ .

We want now to show that, in the more general case of a particle immersed in a generic potential  $U(x)$ , a path integral similar to the highlighted term in (1) will appear. Of course, the function  $V(x(\tau))$  will be different, but it will be proportional to  $U(x)$  - as it is evident in the harmonic case.

So, let's consider a particle in a 3D space  $\mathbf{r} = (x_1, x_2, x_3)^T$ , immersed in a conservative force-field  $\mathbf{F}(\mathbf{r}) = -\nabla U(\mathbf{r})$  with potential  $U(\mathbf{r})$ , and subject to thermal noise. The Langevin equation becomes:

$$d\mathbf{r} = \mathbf{f}(\mathbf{r}) dt + \sqrt{2D} d\mathbf{B} \quad \mathbf{f}(\mathbf{r}) = \frac{\mathbf{F}(\mathbf{r})}{\gamma} \quad \gamma = 6\pi\eta a \quad (2)$$

with  $\mathbf{B} = (B_1, B_2, B_3)^T$  being a  $d = 3$  vector with gaussian components:

$$\Delta B_\alpha \sim \frac{1}{\sqrt{2\pi\Delta t}} \exp\left(-\frac{\Delta B_\alpha^2}{2\Delta t}\right) \quad \alpha = 1, 2, 3 \quad (3)$$

As different components are independent, the joint pdf for the vector  $\Delta\mathbf{B}$  is just the product of the three terms in (3):

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

As before, we introduce a time discretization  $\{t_j\}_{j=0,\dots,n}$  with  $t_0 \equiv 0$  and  $t_n \equiv t$  fixed, so that (2) becomes:

$$\Delta \mathbf{r}_i = \mathbf{r}(t_i) - \mathbf{r}(t_{i-1}) = \mathbf{f}_{i-1} \Delta t_i + \sqrt{2D} \Delta \mathbf{B}_i$$

where the force  $\mathbf{f}(\mathbf{r})$  is evaluated at the left side  $t_{i-1}$  of each discrete interval  $[t_{i-1}, t_i]$ , following Ito's prescription.

Then, starting from the joint pdf of the  $\{\Delta \mathbf{B}_i\}$ :

$$dP(\Delta \mathbf{B}_1, \dots, \Delta \mathbf{B}_n) = \prod_{i=1}^n \frac{d^3 \Delta \mathbf{B}_i}{(2\pi \Delta t)^{3/2}} \exp \left( - \sum_{i=1}^n \frac{\|\Delta \mathbf{B}_i\|^2}{2\Delta t_i} \right)$$

we perform a change of variables by inverting (2):

$$\Delta \mathbf{B}_i = \frac{\Delta \mathbf{r}_i - \mathbf{f}_{i-1} \Delta t_i}{\sqrt{2D}} \Rightarrow \left| \frac{\partial \{\Delta B_i^\alpha\}}{\partial \{\Delta r_j^\beta\}} \right| = \left| \frac{\partial \{\Delta r_j^\beta\}}{\partial \{\Delta B_i^\alpha\}} \right|^{-1} = (2D)^{3/2}$$

This leads to the joint pdf for the increments  $\{\Delta \mathbf{r}_i\}$ :

$$dP(\Delta \mathbf{r}_1, \dots, \Delta \mathbf{r}_n) = \left( \prod_{i=1}^n \frac{d^3 \Delta \mathbf{r}_i}{(4\pi D \Delta t_i)^{3/2}} \right) \exp \left[ - \frac{1}{4D} \sum_{i=1}^n \frac{\|\Delta \mathbf{r}_i - \mathbf{f}_{i-1} \Delta t_i\|^2}{\Delta t_i} \right] \quad (4)$$

Expanding the square in the exponential:

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

allows to recognize the  $d = 3$  Wiener measure in (4):

$$\begin{aligned} dP(\{\Delta \mathbf{r}_i\}) &= \underbrace{\left( \prod_{i=1}^n \frac{d^3 \Delta \mathbf{r}_i}{(4\pi D \Delta t_i)^{3/2}} \exp \left[ - \frac{1}{4D} \sum_{i=1}^n \frac{\|\Delta \mathbf{r}_i\|^2}{\Delta t_i} \right] \right)}_{d_W^3 \mathbf{r}} \cdot \exp \left( - \frac{1}{4D} \underbrace{\sum_{i=1}^n \|\mathbf{f}_{i-1}\|^2 \Delta t_i}_{\int_0^t \|\mathbf{f}(\mathbf{r}(\tau))\|^2 d\tau} + \frac{1}{2D} \underbrace{\sum_{i=1}^n \mathbf{f}_{i-1} \cdot \Delta \mathbf{r}_i}_{\int_0^t \mathbf{f}(\mathbf{r}(\tau)) \cdot d\mathbf{r}(\tau)} \right) \quad (5) \end{aligned}$$

Let's focus on the *stochastic integral* (the one in  $d\mathbf{r}(\tau)$ ). For this we need to generalize to  $d = 3$  the integration formula we found in the previous section.

Consider a multi-variable scalar function  $h(\mathbf{r}): \mathbb{R}^3 \rightarrow \mathbb{R}$ ,  $\mathbf{r} \mapsto h(\mathbf{r})$ . As before, we start from the difference:

$$\begin{aligned} h(\mathbf{r}_n) - h(\mathbf{r}_0) &= h(\mathbf{r}_n) - h(\mathbf{r}_{n-1}) + h(\mathbf{r}_{n-1}) - h(\mathbf{r}_{n-2}) + \dots + h(\mathbf{r}_1) - h(\mathbf{r}_0) = \\ &= \sum_{i=1}^n (h(\mathbf{r}_i) - h(\mathbf{r}_{i-1})) = \sum_{i=1}^n \Delta h_i \end{aligned} \quad (6)$$

In the discretization,  $\mathbf{r}_i = \mathbf{r}_{i-1} + \Delta \mathbf{x}$ , with  $\Delta \mathbf{x} = (\Delta x_i^1, \Delta x_i^2, \Delta x_i^3)$ . Each differential  $\Delta h_i$  is then:

$$\begin{aligned} \Delta h_i &= h(\mathbf{r}_i) - h(\mathbf{r}_{i-1}) \equiv h_i - h_{i-1} = \\ &\stackrel{(a)}{=} \cancel{h(\mathbf{r}_{i-1})} + \sum_{\alpha=1}^3 \left[ \frac{\partial}{\partial x^\alpha} h(\mathbf{r}_{i-1}) \right] \Delta x_i^\alpha + \frac{1}{2} \sum_{\alpha, \beta=1}^3 \left[ \frac{\partial^2}{\partial x^\alpha \partial x^\beta} h(\mathbf{r}_{i-1}) \right] \Delta x_i^\alpha \Delta x_i^\beta + \dots - \cancel{h(\mathbf{r}_{i-1})} = \\ &\stackrel{(b)}{=} \sum_{\alpha=1}^3 \left[ \frac{\partial}{\partial x^\alpha} h(\mathbf{r}_{i-1}) \right] \Delta x_i^\alpha + D \sum_{\alpha, \beta=1}^3 \left[ \frac{\partial^2}{\partial x^\alpha \partial x^\beta} h(\mathbf{r}_{i-1}) \right] \Delta t_i \end{aligned} \quad (7)$$

where in (a) we expanded the first term in Taylor series about  $\mathbf{r}_{i-1}$ , and in (b) we used Ito's rules, and in particular the fact that:

$$\Delta x_i^\alpha \Delta x_i^\beta = \Delta t_i 2D \delta_{\alpha\beta}$$

Substituting (7) back in (6) leads to:

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

and then, in the continuum limit:

$$h(\mathbf{r}(t)) - h(\mathbf{r}(0)) = \int_0^t \nabla h(\mathbf{r}) \cdot d^3 \mathbf{r} + D \int_0^t \nabla^2 h(\mathbf{r}(\tau)) d\tau$$

Rearranging we arrive at the desired formula for integration:

$$\int_0^t \nabla h(\mathbf{r}) \cdot d^3 \mathbf{r} = h(\mathbf{r}(t)) - h(\mathbf{r}(0)) - D \int_0^t \nabla^2 h(\mathbf{r}(\tau)) d\tau \quad (8)$$

Thanks to (8) we can solve the stochastic integral in (5):

$$\int_0^t \mathbf{f}(\mathbf{r}(\tau)) \cdot d^3 \mathbf{r}(\tau)$$

Inserting  $\mathbf{f}(\mathbf{r}) = -\nabla U(\mathbf{r})/\gamma$  and applying the formula leads to:

$$\int_0^t \mathbf{f}(\mathbf{r}(\tau)) \cdot d^3 \mathbf{r}(\tau) = -\frac{1}{\gamma} \int_0^t \nabla U(\mathbf{r}(\tau)) \cdot d^3 \mathbf{r}(\tau) = -\frac{1}{\gamma} \left[ U(\mathbf{r}(t)) - U(\mathbf{r}(0)) - D \int_0^t \nabla^2 U(\mathbf{r}(\tau)) d\tau \right]$$

Substituting back in (5):

$$\begin{aligned} dP &= d_W^3 \mathbf{r} \exp \left( -\frac{1}{4D} \int_0^t \|\mathbf{f}\|^2 d\tau + \frac{1}{2D} \left[ -\frac{1}{\gamma} [U(\mathbf{r}(t)) - U(\mathbf{r}(0))] + \frac{D}{\gamma} \int_0^t \nabla^2 U(\mathbf{r}(\tau)) d\tau \right] \right) = \\ &= d_W^3 \mathbf{r} \exp \left( -\frac{1}{4D} \int_0^t d\tau \underbrace{\left[ \|\mathbf{f}\|^2 - \frac{2D}{\gamma} \nabla^2 U \right]}_{V(\mathbf{r})} \right) \exp \left( -\frac{1}{2D\gamma} [U(\mathbf{r}(t)) - U(\mathbf{r}(0))] \right) \end{aligned}$$

where:

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

Using the just found measure  $dP$  we can compute path integrals, and in particular *transition probabilities*:

$$\begin{aligned} W(\mathbf{r}, t | \mathbf{r}_0, 0) &= \int_{\mathbb{R}^T} dP \delta(\mathbf{r}(t) - \mathbf{r}) \equiv \langle \delta(\mathbf{r}(t) - \mathbf{r}(0)) \rangle_W = \\ &= \int_{\mathbb{R}^T} d^3_W \mathbf{r} \exp \left( -\frac{1}{4D} \int_0^t V(\mathbf{r}(\tau)) d\tau \right) \delta(\mathbf{r}(t) - \mathbf{r}) \exp \left( -\frac{1}{2D\gamma} (U(\mathbf{r}) - U(\mathbf{r}_0)) \right) = \\ &= \langle \exp \left( -\frac{1}{4D} \int_0^t V(\mathbf{r}(\tau)) d\tau \right) \delta(\mathbf{r}(t) - \mathbf{r}) \rangle_W \exp \left( -\frac{1}{2D\gamma} (U(\mathbf{r}) - U(\mathbf{r}_0)) \right) \end{aligned}$$

This expression is indeed similar to that derived in the specific case of the harmonic oscillator (1), meaning that the techniques we used to evaluate previous path integrals can be useful in much more general cases.

## 0.2 Feynman-Kac formula

It is possible to use the machinery of stochastic processes and path integrals to solve certain partial differential equations, which - as we will see - are of fundamental importance in Quantum Mechanics.

In this regard, a very important result is offered by the **Feynman-Kac formula**. The main idea is to use a Brownian process to *simulate many paths*, and express the solution of the differential equation as the *average* of a certain functional computed over all these paths.

More precisely, consider the following *partial differential equation* (Bloch's equation):

$$\partial_t W_B(x, t) = D \partial_x^2 W_B(x, t) - V(x) W_B(x, t) \quad D \in \mathbb{R}, V: \mathbb{R} \rightarrow \mathbb{R} \quad (9)$$

The **Feynman-Kac** formula states that the function  $W_B(x, t)$  that solves (9) can be found by computing a Wiener path integral:

$$W_B(x, t) \equiv \langle \exp \left( - \int_0^t V(x(\tau)) d\tau \right) \delta(x(t) - x) \rangle_W \quad (10)$$

Note that this result can be generalized to more dimensions - but we will limit ourselves to the  $d = 1$  case for simplicity.

**Proof.** We now show that (10) indeed satisfies (9). As usual, we start by defining a time discretization,  $\{t_i\}_{i=0, \dots, n+1}$ , so that  $t_0 \equiv 0$  and  $t_{n+1} \equiv \bar{t}$  is the instant at which we wish to evaluate the solution  $W_B(x, t)$ . Then (10) at that instant will be obtained by the *continuum limit* of the discretized average  $\psi_{n+1}(x)$ :

$$\begin{aligned} W_B(x, \bar{t}) &= \lim_{n \rightarrow \infty} \psi_{n+1}(x) \\ \psi_{n+1}(x) &= \int_{\mathbb{R}^{n+1}} \left( \prod_{i=1}^{n+1} \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \right) \exp \left( - \sum_{i=1}^{n+1} \frac{(x_i - x_{i-1})^2}{4D \Delta t_i} - \sum_{i=1}^{n+1} \Delta t_i V(x_i) \right) \delta(x_{n+1} - x) \end{aligned} \quad (11)$$

Note that  $\psi_{n+1}(x)$  is the average of a functional over *all paths* that arrive in  $x$  at the instant  $\bar{t}$ , making exactly  $n + 1$  steps from their starting point 0. In the

following, the intuition is to see these paths as *being generated*, i.e. evolving *step* after *step* from 0 to  $x$ . For example, suppose we want to approximate (11). We would start by choosing an *ensemble* of paths arriving to  $x$  after  $n + 1$  timesteps, compute the functional on each of them, and average the results. However, we could also do it in another - a bit stranger - way. Consider the same ensemble of paths we already (supposedly) generated. From each of them, remove the last step. We now have a set of paths that arrive *close* to  $x$ , and will arrive exactly there if we let another timestep pass. However, we decide to compute the functional on each of these paths and then average the results, before letting them arrive at their destination. So, in a certain sense, we will estimate the value of the functional “a timestep in the past”. Of course, we can repeat this process, removing more and more timesteps at every iteration. At the end, we will have a sequence of numbers detailing the “evolution” of the functional from the start to the end. Turns out that the *rule* for such an evolution is exactly (9). So, to prove Feynman-Kac, we just have to find that rule - meaning how to relate  $\psi_{n+1}$  to its “past”  $\psi_n$  (in the continuum limit  $n \rightarrow \infty$ ).

This is just an informal intuition, that will only be useful as a guide for the rest of the proof. So, let's go on.

For simplicity, we choose the time discretization as **uniform**, so that  $\Delta t_i \equiv \epsilon \forall i$ , and:

$$t_{n+1} = (n + 1)\epsilon \equiv \bar{t} \Rightarrow \epsilon = \frac{\bar{t}}{n + 1}$$

We then rewrite (11), highlight the last term (the one with the  $x_{n+1}$ ) and integrate to remove the  $\delta$ :

$$\begin{aligned} \psi_{n+1}(x) &= \int_{\mathbb{R}^n} \left( \prod_{i=1}^n \frac{dx_i}{\sqrt{4\pi D\epsilon}} \right) \exp \left( - \sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \sum_{i=1}^n \epsilon V(x_i) \right) \cdot \\ &\quad \cdot \int_{\mathbb{R}} \frac{dx_{n+1}}{\sqrt{4\pi D\epsilon}} \exp \left( - \frac{(x_{n+1} - x_n)^2}{4D\epsilon} - \epsilon V(x_{n+1}) \right) \delta(x_{n+1} - x) = \\ &= \int_{\mathbb{R}^n} \left( \prod_{i=1}^n \frac{dx_i}{\sqrt{4\pi D\epsilon}} \right) \exp \left( - \sum_{i=1}^n \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \sum_{i=1}^n \epsilon V(x_i) \right) \cdot \\ &\quad \cdot \frac{1}{\sqrt{4\pi D\epsilon}} \exp \left( - \frac{(x - x_n)^2}{4D\epsilon} - \epsilon V(x) \right) \end{aligned} \quad (12)$$

Now, with some algebra, we recognize in these integrals a term  $\psi_n(x_n)$ , indicating the expected value of the functional over all paths reaching  $x_n$  (which is close to the end-point  $x$ ) at timestep  $t_n = t - \epsilon$ . We start by rearranging, putting the integration over  $dx_n$  at the front:

$$\begin{aligned} (12) &= \int_{\mathbb{R}} \frac{dx_n}{\sqrt{4\pi D\epsilon}} \exp \left( - \frac{(x - x_n)^2}{4D\epsilon} - \epsilon V(x) \right) \cdot \\ &\quad \cdot \frac{1}{\sqrt{4\pi D\epsilon}} \int_{\mathbb{R}^{n-1}} \left( \prod_{i=1}^{n-1} \frac{dx_i}{\sqrt{4\pi D\epsilon}} \right) \exp \left( - \sum_{i=1}^{\textcolor{red}{n}} \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \epsilon \sum_{i=1}^{\textcolor{red}{n}} V(x_i) \right) \end{aligned} \quad (13)$$

Now we *change* all the  $x_i$  in the second line to  $y_i$ , and then add a  $\delta$  (with its integral) to *connect*  $y_n$  to  $x_n$ , which appears in the integral in the first line. In this way we will highlight the desired  $\psi_n(x_n)$ :

$$(13) = \int_{\mathbb{R}} \frac{dx_n}{\sqrt{4\pi D\epsilon}} \exp\left(-\frac{(x-x_n)^2}{4D\epsilon} - \epsilon V(x)\right) \cdot \underbrace{\int_{\mathbb{R}^n} \left(\prod_{i=1}^n \frac{dy_i}{\sqrt{4\pi D\epsilon}}\right) \exp\left(-\sum_{i=1}^n \frac{(y_i - y_{i-1})^2}{4D\epsilon} - \epsilon \sum_{i=1}^n V(y_i)\right) \delta(x_n - y_n)}_{\psi_n(x_n)} \quad (14)$$

And so:

$$\psi_{n+1}(x) = e^{-\epsilon V(x)} \int_{\mathbb{R}} \frac{dx_n}{\sqrt{4\pi D\epsilon}} \exp\left(-\frac{(x-x_n)^2}{4D\epsilon}\right) \psi_n(x_n) \quad (15)$$

This is relation between  $\psi_{n+1}(x)$  and its “past”  $\psi_n(x)$  that we were searching for. Now, to retrieve (9), all that’s left is to put (15) in differential form.

We start by simplifying the integral, making it similar to a gaussian with a change of variables:

$$-\frac{(x-x_n)^2}{4D\epsilon} \stackrel{!}{=} -\frac{z^2}{2} \Rightarrow z = -\frac{x-x_n}{\sqrt{2D\epsilon}}; \quad x_n = x + \sqrt{2D\epsilon}z; \quad dx_n = \sqrt{2D\epsilon}dz$$

which leads to:

$$\psi_{n+1}(x) = e^{-\epsilon V(x)} \int_{-\infty}^{+\infty} \frac{dz}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right) \psi_n(x_n + z\sqrt{2D\epsilon}) \quad (16)$$

As  $n \rightarrow \infty$ ,  $z \rightarrow 0$ . We will not prove this, but note that:

$$z = -\frac{x-x_n}{\epsilon} \frac{\sqrt{\epsilon}}{\sqrt{2D}}$$

where the first factor is a *velocity*, which must be physically limited, and so  $n \rightarrow \infty \Rightarrow \epsilon \rightarrow 0 \Rightarrow z \rightarrow 0$ .

This means that we can expand  $\psi_n$  in Taylor series about  $x$ :

$$\psi_n(x_n + z\sqrt{2D\epsilon}) = \psi_n(x) + z\sqrt{2D\epsilon}\psi'_n(x) + z^2 D\epsilon \psi''_n(x) + O(z^3 \epsilon^{3/2})$$

Substituting back in (16):

$$\begin{aligned} \psi_{n+1}(x) = e^{-\epsilon V(x)} & \left[ \underbrace{\psi_n(x) \int_{\mathbb{R}} \frac{dz}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2}\right)}_1 + \underbrace{\sqrt{2D\epsilon}\psi'_n(x) \int_{\mathbb{R}} \frac{dz}{\sqrt{2\pi}} z \exp\left(-\frac{z^2}{2}\right)}_0 + \right. \\ & \left. + D\epsilon \psi''_n(x) \underbrace{\int_{\mathbb{R}} \frac{dz}{\sqrt{2\pi}} z^2 \exp\left(-\frac{z^2}{2}\right)}_1 + O(\epsilon^2) \right] \quad (17) \end{aligned}$$

as the integrand is just a standard gaussian ( $\mu = 0, \sigma = 1$ ). Note how the error term is of order  $\epsilon^2$ , as the first non-null integral in the series will be that with  $z^4$ :

$$\int_{\mathbb{R}} \frac{dz}{\sqrt{2\pi}} z^k \frac{(2D\epsilon)^{k/2}}{k!} \psi_n^{(k)} = \begin{cases} 0 & k \text{ odd} \\ 1^k (k-1)!! & k \text{ even} \end{cases}$$

Expanding also the  $e^{-\epsilon V(x)}$  term:

$$e^{-\epsilon V(x)} = 1 - \epsilon V(x) + \frac{\epsilon^2 V^2(x)}{2} + O(\epsilon^3)$$

Finally, substituting back in (17), expanding the product and ignoring all terms of order 2 or higher in  $\epsilon$ :

$$\psi_{n+1}(x) = \psi_n(x) + D\epsilon \psi_n''(x) - \epsilon V(x) \psi_n(x) + O(\epsilon^2)$$

Rearranging:

$$\frac{\psi_{n+1} - \psi_n}{\epsilon} = D\psi_n'' - V\psi_n$$

And when  $\epsilon \rightarrow 0$  the first term becomes a time derivative, leading to Bloch's equation, and proving Feynman-Kac formula:

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

### 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:

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

where:

$$\text{Stat}_{\mathbf{x}} F(\mathbf{x}) = F(\mathbf{x}_c); \quad \mathbf{x}_c \text{ such that } \forall_i \frac{\partial F(\mathbf{x})}{\partial x_i} \Big|_{\mathbf{x}=\mathbf{x}_c} = 0$$

In this case:

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

Then, substituting in the original expression:

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

gives back the correct exponent for the integral's result.

This interesting idea can be applied also to Wiener integrals:

$$\begin{aligned} W(x, t | x_0, 0) &= \int \prod_{\tau=0}^t \frac{dx(\tau)}{\sqrt{4\pi D d\tau}} \exp\left(-\frac{1}{4D} \int_0^t \dot{x}^2(\tau) d\tau\right) \delta(x - x(t)) = \\ &= " \lim_{N \rightarrow \infty} " \int \prod_{i=1}^N \frac{dx_i}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\sum_{i=1}^N \frac{(x_i - x_{i-1})^2}{4D \Delta t_i}\right) \delta(x - x_N) \end{aligned}$$

Integrating over  $x_N$ :

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

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

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

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

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

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

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

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

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

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

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

Integrating by parts leads to:

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

then  $\mathbf{X}(\tau) = 0$  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:

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

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

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