Exercise 0.1:

Prove that:

$$\int_{t_0}^{t} \mathrm{d}\tau \, \langle V(x(\tau),\tau) \exp\left(-\int_{t_0}^{\tau} \mathrm{d}s \, V(x(s),s)\right) \delta(x-x(t))\rangle_W = \\ = \int_{t_0}^{t} \mathrm{d}\tau \int_{\mathbb{R}} \mathrm{d}x' \, W_B(x',\tau|x_0,t_0) V(x',\tau) W(x,t|x',\tau)$$

where:

$$W_B(x,t|x_0,t_0) = \langle \delta(x-x(t)) \exp\left(-\int_{t_0}^{t} \mathrm{d}\tau \, V(x(\tau),\tau)\right)\rangle_W$$

and $V(x(\tau),\tau)$ is a potential.

Here the $\langle \cdot \rangle_W$ notation denotes the average over paths from $x(t_0) = x_0$ to x at t, with *unconstrained* end-point, which corresponds to $\langle \cdot \rangle_w$ in Maritan's notes. For the *fixed end-point* case, $\langle \cdots \delta(x - x(t))\rangle_W$ in these notes is equivalent to $\langle \cdots \rangle_W$ in Maritan's notes.

Solution. The equality follows if the integrands are equal, i.e. if:

$$\langle V(x(\tau),\tau) \exp\left(-\int_{t_0}^{\tau} \mathrm{d}s \, V(x(s),s)\right) \delta(x-x(t))\rangle_W = \\ = \int_{\mathbb{R}} \mathrm{d}x' \, W_B(x',\tau|x_0,t_0) V(x',\tau) W(x,t|x',\tau)$$

Expanding the average:

$$I \equiv \langle V(x(\tau),\tau) \exp\left(-\int_{t_0}^{\tau} \mathrm{d}s \, V(x(s),s)\right) \delta(x-x(t))\rangle_W = \\ = \int_{\mathcal{C}\{x_0,t_0;t\}} \mathrm{d}_W x V(x(\tau),\tau) \exp\left(-\int_{t_0}^{\tau} \mathrm{d}s \, V(x(s),s)\right) \delta(x-x(t))$$

where the integral is over all paths starting at $x(t_0) = x_0$ and reaching an arbitrary end-point at t. The presence of the δ fixes the *end-point*, leading to:

$$= \int_{\mathcal{C}\{x_0,t_0;x,t\}} \mathrm{d}_W x \, V(x(\tau),\tau) \exp\left(-\int_{t_0}^{\tau} \mathrm{d}s \, V(x(s),s)\right)$$

Now the integral is over all paths from $x(t_0) = x_0$ to $x(t) = x$. Note that τ is fixed, and so is $V(x(\tau),\tau)$ depends on the position $x(\tau)$ reached by a path after τ. We can then rewrite:

$$= \int_{\mathbb{R}} \mathrm{d}x' \int_{\mathcal{C}\{x_0,t_0;x,t\}} \mathrm{d}_W x \, V(x',\tau) \delta(x'-x(\tau)) \exp\left(-\int_{t_0}^{\tau} \mathrm{d}s \, V(x(s),s)\right)$$

In this way, $V(x', \tau)$ can be brought out of the path integral:

$$= \int_{\mathbb{R}} \mathrm{d}x'\, V(x', \tau) \int_{\mathcal{C}\{x_0, t_0; x, t\}} \mathrm{d}_W x\, \delta(x' - x(\tau)) \exp\left(-\int_{t_0}^{\tau} \mathrm{d}s\, V(x(s), s)\right)$$

Note how the integrand depends only on $x(s)$ with $s \leq \tau$. In other words, the paths starting at $x(\tau)$ and arriving at $x(t)$ have an *unit weight*:

$$= \int_{\mathbb{R}} \mathrm{d}x'\, V(x', \tau) \underbrace{\int_{\mathcal{C}\{x_0, t_0; x', \tau\}} \mathrm{d}_W x \exp\left(-\int_{t_0}^{\tau} \mathrm{d}s\, V(x(s), s)\right)}_{W_B(x', \tau | x_0, t_0)} \underbrace{\int_{\mathcal{C}\{x', \tau; x, t\}} \mathrm{d}_W x}_{W(x, t | x', \tau)}$$

$\boxed{\textbf{Exercise 0.2:}}$

Prove the *backward Fokker-Planck* equation:

$$\partial_{t_0} W_B(x, t | x_0, t_0) = -D(\partial_{x_0}^2 - V(x_0, t_0)) W_B(x, t | x_0, t_0)$$

in two ways:

1. Using the Bloch equation:

$$\partial_t W_B(x, t | x_0, t_0) = (D\partial_x^2 - V(x, t)) W_B(x, t | x_0, t_0) \tag{1}$$

   and defining a $\mathcal{L}_t$ operator so that $\partial_t W_B(t) = \mathcal{L}_t W_B(t)$ and repeated integrations over intermediate times.

2. Using the path integral formulation

Solution.

1. We rewrite the Bloch equation in operator form:

$$\partial_t W_B(t) = \mathcal{L}_t W_B(t) \tag{2}$$

   where $W_B(t) \equiv W_B(x, t | x_0, t_0)$ for simplicity. $\mathcal{L}_t$ is a matrix with *infinite elements*, that can act over any function $h(x)$ replicating the rhs of (1):

$$(\mathcal{L}_t h)(x) = \int_{\mathbb{R}} \mathrm{d}y\, \mathcal{L}_t(x, y) h(y) = (D\partial_x^2 - V(x, t)) h(x) \tag{3}$$

   where $\mathcal{L}_t(x, y)$ are the *matrix elements* of $\mathcal{L}_t$. From (3) we can see that $\mathcal{L}_t$ must be diagonal:

$$\mathcal{L}_t(x, y) = (D\partial_x^2 - V(x, t)) \delta(x - y) \tag{4}$$

Now we integrate (2) over $[t_0, t]$, with the initial condition $W_B(0) = W_0$:

$$\int_{t_0}^{t} \partial_t W_B(t) = W_B(t) - W_0 = \int_{t_0}^{t} \mathrm{d}t_1 \, \mathcal{L}_{t_1} W_B(t_1)$$

And rearranging:

$$W_B(t) = W_0 + \int_{t_0}^{t} \mathrm{d}t_1 \, \mathcal{L}_{t_1} W_B(t_1) \tag{5}$$

We can use (5) to evaluate $W_B(t_1)$:

$$W_B(t_1) = W_0 + \int_{t_0}^{t_1} \mathrm{d}t_2 \, \mathcal{L}_{t_2} W_B(t_2) \tag{6}$$

And substituting (6) in (5) we get:

$$W_B(t) = W_0 + \int_{t_0}^{t} \mathrm{d}t_1 \, \mathcal{L}_{t_1} \left(W_0 + \int_{t_0}^{t_1} \mathrm{d}t_2 \, \mathcal{L}_{t_2} W_B(t_2) \right)$$

We can reiterate this procedure an *infinite* number of times, reaching a **formal solution** of (2):

$$\begin{aligned} W_B(t) = W_0 + \int_{t_0}^{t} \mathrm{d}t_1 \, \mathcal{L}_{t_1} W_0 + \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \, \mathcal{L}_{t_1} \mathcal{L}_{t_2} W_0 + \\ + \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \, \mathcal{L}_{t_1} \mathcal{L}_{t_2} \mathcal{L}_{t_3} W_0 + \dots \end{aligned} \tag{7}$$

Note that each integral appearing in $W(t)$ can be interpreted as a sum over *univariate paths*. For example, consider the second one:

$$\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \, \mathcal{L}_{t_1} \mathcal{L}_{t_2} W_0 \tag{8}$$

Here we are summing over all values of t_1, t_2 in the domain $[t_0, t]$ such that $t_2 < t_1$. To see this explicitly, consider the integration extrema:

$$t_0 < t_1 < t \qquad t_0 < t_2 < t_1$$

In other words: evaluate $\mathcal{L}_{t_1} \mathcal{L}_{t_2} W_0$ over all possible choices of two *consecutive* points t_1, t_2 in the segment $[t_0, t]$, and then sum all the results.

Written like (8), the procedure is as follows:

- Start by choosing $t_1 \in [t_0, t]$. This will be the *last* point in the segment.
- Choose the second point in the *preceding region*, i.e. $t_2 \in [t_0, t_1]$.
- Compute the integrand.

Note that here we are starting *from the end*, and proceeding backwards. A more natural way would be to choose a *starting point* and proceed *forwards*. That is:

- Choose $t_2 \in [t_0, t]$. This will be the *first* point in the segment.
- Choose t_1 in the *consecutive region*, i.e. $t_1 \in [t_2, t]$.

This amounts to the rewriting:

$$\int_{t_0}^{t} \mathrm{d}t_2 \int_{t_2}^{t} \mathrm{d}t_1 \, \mathcal{L}_{t_1} \mathcal{L}_{t_2} W_0$$

This procedure can be generalized to n points, and so we can rewrite (7) as follows:

$$\begin{aligned} W_B(t) = W_0 + \int_{t_0}^{t} \mathrm{d}t_1 \, \mathcal{L}_{t_1} W_0 + \int_{t_0}^{t} \mathrm{d}t_2 \int_{t_2}^{t} \mathrm{d}t_1 \, \mathcal{L}_{t_1} \mathcal{L}_{t_2} W_0 + \\ + \int_{t_0}^{t} \mathrm{d}t_3 \int_{t_3}^{t} \mathrm{d}t_2 \int_{t_2}^{t} \mathrm{d}t_1 \, \mathcal{L}_{t_1} \mathcal{L}_{t_2} \mathcal{L}_{t_3} W_0 + \dots \end{aligned} \tag{9}$$

Now it would be really nice to make all *integrand extrema* equal, i.e. write, for example:

$$\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t} \mathrm{d}t_2 \, \mathcal{L}_{t_1} \mathcal{L}_{t_2} W_0$$

However, in order not to break causality, $\mathcal{L}_{t_1} \mathcal{L}_{t_2} W_0$ must be evaluated only with $t_2 < t_1$. This can be solved by *reordering* the operators as needed. That is:

- If $t_2 < t_1$, evaluate $\mathcal{L}_{t_1} \mathcal{L}_{t_2} W_0$ as usual.
- If $t_1 < t_2$, evaluate $\mathcal{L}_{t_2} \mathcal{L}_{t_1} W_0$ instead.

To *automatically* reorder the operators as needed we define the **time ordering** (meta)**operator**:

$$\mathcal{T}[\mathcal{L}_{t_1} \cdots \mathcal{L}_{t_n}] = \mathcal{L}_{p_1} \cdots \mathcal{L}_{p_n} \text{ such that } t_{p_1} > t_{p_2} > \cdots > t_{p_n}$$

So we consider:

$$\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t} \mathrm{d}t_2 \, \mathcal{T}[\mathcal{L}_{t_1} \mathcal{L}_{t_2}] W_0$$

Now the operators are in order, but we are computing *twice* the integral in (8)! In fact, for any choice of $t_1, t_2 \in [t_0, t]$, there are *two possible orderings*, and here we are counting both of them (by properly rearranging the operators). We can correct this by dividing by 2, or - in the general case involving the reordering of n operators, by $n!$.

At the end of this long journey, we can rewrite the formal solution (9) as follows:

$$W_B(t) = W_0 + \int_{t_0}^{t} \mathcal{L}_{t_1} W_0 + \frac{1}{2!}\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t} \mathrm{d}t_2\, \mathcal{T}[\mathcal{L}_{t_1}\mathcal{L}_{t_2}]W_0 + \tag{10}$$

$$+ \frac{1}{3!}\int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t} \mathrm{d}t_2 \int_{t_0}^{t} \mathrm{d}t_3\, \mathcal{T}[\mathcal{L}_{t_1}\mathcal{L}_{t_2}\mathcal{L}_{t_3}]W_0 + \cdots =$$

$$= \sum_{n=0}^{+\infty} \frac{1}{n!}\mathcal{T}\left[\prod_{i=1}^{n} \int_{t_0}^{t} \mathcal{L}_{t_i}\,\mathrm{d}t_i\right] W_0 \equiv \mathcal{T}\left[\exp\left(\int_{t_0}^{t} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\right] \tag{11}$$

We are finally arrived at a point when we can *differentiate*! So, without further ado:

$$\partial_{t_0} W_B(t) = \partial_{t_0}\mathcal{T}\left[\exp\left(\int_{t_0}^{t} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\right] W_0 = \mathcal{T}\left[\partial_{t_0}\exp\left(-\int_{t}^{t_0} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\right] W_0 =$$

$$= \mathcal{T}\left[-\exp\left(-\int_{t}^{t_0} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\partial_{t_0}\int_{t}^{t_0} \mathcal{L}_\tau\,\mathrm{d}\tau\right] W_0 =$$

$$= -\mathcal{T}\left[\exp\left(\int_{t_0}^{t} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\mathcal{L}_{t_0}\right] W_0$$

Let $W_0 = \delta(x - x_0)$ and let's compute explicitly the matrix product:

$$\partial_{t_0} W_B(t|t_0) = -\int_{\mathbb{R}} \mathrm{d}y\, \underbrace{\mathcal{T}\left[\exp\left(\int_{t_0}^{t} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\mathcal{L}_{t_0}\right](x,y)}_{\text{Matrix element}}\,\delta(y - x_0) =$$

$$= -\mathcal{T}\left[\exp\left(\int_{t_0}^{t} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\mathcal{L}_{t_0}\right](x, x_0)$$

Now note that $\mathcal{L}_{t_0}$ is before all the others $\mathcal{L}_\tau$, so it is already ordered - meaning that we can bring it out the $\mathcal{T}$ operator:

$$= -\left(\mathcal{T}\left[\exp\left(\int_{t_0}^{t} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\right]\mathcal{L}_{t_0}\right)(x, x_0)$$

Then we write explicitly the matrix product between the $\mathcal{T}$ block and the $\mathcal{L}_{t_0}$:

$$= -\int_{\mathbb{R}} \mathrm{d}y\, \underbrace{\left(\mathcal{T}\left[\exp\left(\int_{t_0}^{t} \mathcal{L}_\tau\,\mathrm{d}\tau\right)\right]\right)(x,y)}_{W(x,t|y,t_0)}\,\mathcal{L}_{t_0}(y, x_0) =$$

$$= -\int_{\mathbb{R}} \mathrm{d}y\, W_B(x,t|y,t_0)\mathcal{L}_{t_0}(y, x_0)$$

Finally, use (4) to evaluate $\mathcal{L}_{t_0}(y, x_0)$:

$$\partial_{t_0} W_B(x,t|x_0,t_0) = -\int_{\mathbb{R}} \mathrm{d}y\, W_B(x,t|y,t_0)(D\partial_y^2 - V(y,t_0))\delta(x_0 - y) =$$

$$= -(D\partial_{x_0}^2 - V(x_0,t_0))W_B(x,t|x_0,t_0)$$

which is the *backward* Fokker-Planck equation.

2. Recall that:

$$W_B(x,t|x_0,t_0) = \langle \delta(x - x(t)) \exp\left(-\int_{t_0}^{t} \mathrm{d}\tau\, V(x(\tau),\tau)\right)\rangle_W$$

Let's introduce a **uniform** discretization $\{t_j\}_{j=1,\dots,n+1}$ with fixed t_0 and $t_{n+1} \equiv t$. Then we can write $W_B(x,t|x_0,t_0)$ as the continuum limit of the discretized integral:

$$\psi_0 = W_B^{(\epsilon)}(x,t_{n+1}|x_0,t_0) = \int_{\mathbb{R}^{n+1}} \left(\prod_{i=1}^{n+1} \frac{\mathrm{d}x_i}{\sqrt{4\pi D\epsilon}}\right) \cdot \\ \cdot \exp\left(-\sum_{i=1}^{n+1} \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \epsilon \sum_{i=1}^{n+1} V_i\right) \delta(x_{n+1} - x)$$

We add a *previous* timestep t_{-1} to the discretization, and consider the paths that started in x_{-1} at t_{-1}:

$$\psi_{-1} = W_B^{(\epsilon)}(x,t_{n+1}|x_{-1},t_{-1}) = \int_{\mathbb{R}^{n+2}} \left(\prod_{i=0}^{n+1} \frac{\mathrm{d}x_i}{\sqrt{4\pi D\epsilon}}\right) \cdot \\ \cdot \exp\left(-\sum_{i=0}^{n+1} \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \epsilon \sum_{i=0}^{n+1} V_i\right) \delta(x_{n+1} - x)$$

We interpret ψ_0 as the *evolution one timestep later* of ψ_{-1}, in the sense that the starting point "moves by one step forward". This is analogy to what we did for the forward Bloch equation, when we considered ψ_{n+1} as the evolution of ψ_n, in the sense that in the former the *arrival point* was *one timestep forward* with respect to the latter. So, while considering the *arrival point* leads to the forward equation, considering the *starting point* - as we are doing now - leads to the *backward* one.

The idea is now to highlight a ψ_0 inside of ψ_{-1}. As ψ_0 starts from x_0, we highlight the term with x_0:

$$\psi_{-1} = \int_{\mathbb{R}^{n+2}} \left(\prod_{i=0}^{n+1} \frac{\mathrm{d}x_i}{\sqrt{4\pi D\epsilon}}\right) \exp\left(-\frac{(x_0 - x_{-1})^2}{4D\epsilon} - \epsilon V_0\right) \cdot \\ \cdot \exp\left(-\sum_{i=1}^{n+1} \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \epsilon \sum_{i=1}^{n+1} V_i\right) \delta(x_{n+1} - x)$$

We wish to *free* that term from the path integral. To do this, we *rename*

x_0 to x' with a δ, so that:

$$\psi_{-1} = \frac{1}{\sqrt{4\pi D\epsilon}} \int_{\mathbb{R}} \mathrm{d}x' \exp\left(-\frac{(x'-x_{-1})^2}{4D\epsilon} - \epsilon V(x', t_0) \right) \int_{\mathbb{R}^{n+1}} \left(\prod_{i=1}^{n+1} \frac{\mathrm{d}x_i}{\sqrt{4\pi D\epsilon}} \right) \cdot$$
$$\cdot \exp\left(-\sum_{i=1}^{n+1} \frac{(x_i - x_{i-1})^2}{4D\epsilon} - \epsilon \sum_{i=1}^{n+1} V_i \right) \delta(x_{n+1} - x) \delta(x' - x_0) =$$
$$= \frac{1}{\sqrt{4\pi D\epsilon}} \int_{\mathbb{R}} \mathrm{d}x' \exp\left(-\underbrace{\frac{(x'-x_{-1})^2}{4D\epsilon}}_{z^2/2} - \epsilon V(x', t_0) \right) W_B^{(\epsilon)}(x, t_{n+1}|x', t_0)$$

To simplify the gaussian we change variables:

$$\frac{z^2}{2} = \frac{(x'-x_{-1})^2}{4D\epsilon} \Rightarrow z = \frac{x'-x_{-1}}{\sqrt{2D\epsilon}} \Rightarrow \mathrm{d}x' = \sqrt{2D\epsilon}\,\mathrm{d}z\,;\; x' = x_{-1} + z\sqrt{2D\epsilon}$$

leading to:

$$\psi_{-1} = \frac{\sqrt{2D\epsilon}}{\sqrt{4\pi D\epsilon}} \int_{\mathbb{R}} \mathrm{d}x' \exp\left[-z^2 - \epsilon V(x_{-1} + z\sqrt{2D\epsilon}) \right] \cdot$$
$$\cdot W_B^{(\epsilon)}(x, t_{n+1}|x_{-1} + z\sqrt{2D\epsilon}, t_0)$$

Then we perform a Taylor expansion about $z\sqrt{2D\epsilon} \sim 0$ of both the potential and the solution:

$$\exp\left(-\epsilon V(x_{-1} + z\sqrt{2D\epsilon}) \right) \approx \exp\left(-\epsilon [V x_{-1} + O(\epsilon^{1/2})] \right) \approx 1 - \epsilon V(x_{-1}) + O(\epsilon^{3/2})$$

Let $W_B^{(\epsilon)}(x, t_{n+1}|x_{-1}, t_0)$ be ψ:

$$W_B^{(\epsilon)}(x, t_{n+1}|x_{-1} + z\sqrt{2D\epsilon}, t_0) = \psi + \psi' z\sqrt{2D\epsilon} + \psi'' z^2 2D\epsilon$$

Substituting back in the integral, and ignoring higher order terms:

$$\psi_{-1} = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}x' \exp\left(-\frac{z^2}{2} \right) [1 - \epsilon V(x_{-1})](\psi + \psi' z\sqrt{2D\epsilon} + \psi'' z^2 2D\epsilon) =$$
$$= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}x' \exp\left(-\frac{z^2}{2} \right) \left[\psi(1 - \epsilon V(x_{-1})) + z\psi'\sqrt{2D\epsilon} + z^2 \psi'' 2D\epsilon) \right]$$

Note that:

$$f(z) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{z^2}{2} \right)$$

is a normalized gaussian with 0 mean and unit variance. So the first moment is null, and the second is 1, leading to:

$$\begin{gathered}\psi_{-1} = W_B(x,t|x_{-1},t_{-1}) = \\ = (1-\epsilon V(x_{-1}))W_B(x,t|x_{-1},t_0) + 2D\epsilon\partial^2_{x_{-1}} W_B(x,t|x_{-1},t_0)\end{gathered}$$

Rearranging:

$$\begin{gathered}W_B(x,t|x_{-1},t_0) - W_B(x,t|x_{-1},t_{-1}) = \\ = \epsilon V(x_{-1})W_B(x,t|x_{-1},t_0) - 2D\epsilon\partial^2_{x_{-1}} W_B(x,t|x_{-1},t_0)\end{gathered}$$

Dividing by ϵ and taking the continuum limit $\epsilon \to 0^+$:

$$\begin{aligned}&\lim_{\epsilon\to 0^+} \frac{W_B(x,t|x_{-1},t_0) - W_B(x,t|x_{-1},t_{-1})}{\epsilon} = \partial_{t_0} W(x,t|x_{-1},t_0) = \\ &= V(x_{-1},t_0)W_B(x,t|x_{-1},t_0)) - 2D\partial^2_{x_{-1}} W(x,t|x_{-1},t_0)\end{aligned}$$

And renaming $x_{-1} \to x_0$ leads to the desired result.

Exercise 0.3:

Prove that:

$$W_B(\boldsymbol{x},t|\boldsymbol{x_0},t_0) = \langle \exp\left(-\int_{t_0}^t V(\boldsymbol{x}(s),s)\,\mathrm{d}s\right)\delta^k(\boldsymbol{x}(t)-\boldsymbol{x})\rangle$$

satisfies the backward Bloch equation:

$$\begin{gathered}\partial_{t_0} W_B(\boldsymbol{x},t|\boldsymbol{x_0},t_0) = \\ -\left[\sum_{\omega=1}^k \left(f(\boldsymbol{x_0},t_0)\frac{\partial}{\partial x_{0,\omega}} + \sum_{\nu=1}^k D^{\omega\nu}(\boldsymbol{x_0},t_0)\frac{\partial^2}{\partial x^2_{0,\nu}}\right) - V(\boldsymbol{x_0},t_0)\right] W_B(\boldsymbol{x},t|\boldsymbol{x_0},t_0)\end{gathered} \tag{12}$$

for the simplest case $k = d = 1$ and $D(x,t) > 0$ generic.

Hint: use the discrete measure for $d = 1$:

$$\begin{gathered}\mathrm{d}\mathbb{P}_{t_1,\ldots,t_n}(\boldsymbol{x_1},\ldots,\boldsymbol{x_n}|\boldsymbol{x_0},t_0) = \\ \prod_{i=1}^n \prod_{\alpha=1}^d \frac{\mathrm{d}x_i^\alpha}{\sqrt{4\pi D^\alpha_{i-1}\Delta t_i}} \exp\left(-\sum_{i=1}^n\sum_{\alpha=1}^d \frac{(\Delta x_i^\alpha - f^\alpha_{i-1}\Delta t_i)^2}{4D^\alpha_{i-1}\Delta t_i}\right)\end{gathered} \tag{13}$$

Notice that it is easier to prove the backward Bloch (12) rather than the *forward one* since a change of variable involved in the derivation does not need complicated derivations).

Equation (12) is different from the one referenced in Maritan's notes, as the derivatives should be wrt the *starting point* and not the *arrival*.

Solution. The procedure is really similar to that used in ex. 6.2 part 2, but we now consider the dependence of D on x and t, and an added force $f(x,t)$. First we rewrite everything in the $d=1$ case. We start from:

$$W_B(x,t|x_0,t_0) = \langle \exp\left(-\int_{t_0}^{t} V(x(s),s)\,\mathrm{d}s\right)\delta(x(t)-x)\rangle \tag{14}$$

and we want to prove that:

$$\partial_{t_0} W_B(x,t|x_0,t_0) = -\left[\left(f(x_0,t_0)\frac{\partial}{\partial x_0} + D(x_0,t_0)\frac{\partial^2}{\partial x_0^2}\right) - V(x_0,t_0)\right] W_B(x,t|x_0,t_0)$$

Introduce a uniform time discretization $\{t_j\}_{j=0,\dots,n}$, with fixed end-points and $\Delta t_i = t_i - t_{i-1} \equiv \epsilon$. Then, following (13) and adding the term $-\epsilon V_i$ for the exponential of the integral from (14), we get:

$$\begin{aligned} W_B(x,t|x_0,t_0) &= \lim_{\epsilon\to 0^+} W_B^{(\epsilon)}(x,t|x_0,t_0) \equiv \psi_0 \\ \psi_0 &= \int_{\mathbb{R}^n}\left(\prod_{i=1}^{n}\frac{\mathrm{d}x_i}{\sqrt{4\pi D_{i-1}\epsilon}}\right)\cdot \\ &\quad\cdot \exp\left(-\sum_{i=1}^{n}\frac{(x_i - x_{i-1} - f_{i-1}\epsilon)^2}{4D_{i-1}\epsilon} - \sum_{i=1}^{n}\epsilon V_i\right)\delta(x_n - x) \end{aligned}$$

Note that we have f_{i-1} and D_{i-1}, but V_i. This is because the first two come from a change of random variables from the Ito SDE, for which Ito's prescription applies. On the other hand, V comes from the functional that we are averaging.

As in the previous exercise, we consider the solution with the starting point *a timestep in the past*, that is:

$$\begin{aligned} \psi_{-1} &= \int_{\mathbb{R}^{n+1}}\left(\prod_{i=0}^{n}\frac{\mathrm{d}x_i}{\sqrt{4\pi D_{i-1}\epsilon}}\right)\cdot \\ &\quad\cdot \exp\left(-\sum_{i=0}^{n}\frac{(x_i - x_{i-1} - f_{i-1}\epsilon)^2}{4D_{i-1}\epsilon} - \sum_{i=0}^{n}\epsilon V_i\right)\delta(x_n - x) \end{aligned}$$

Then we highlight the first term (the one in x_0):

$$\psi_{-1} = \int_{\mathbb{R}^{n+1}} \left(\prod_{i=0}^{n} \frac{\mathrm{d}x_i}{\sqrt{4\pi D_{i-1}\epsilon}} \right) \cdot \\ \cdot \exp\left(-\frac{(x_0 - x_{-1} - f_{-1}\epsilon)^2}{4D_{-1}\epsilon} - \epsilon V_0 \right) \cdot \\ \cdot \exp\left(-\sum_{i=1}^{n} \frac{(x_i - x_{i-1} - f_{i-1}\epsilon)^2}{4D_{i-1}\epsilon} - \sum_{i=1}^{n} \epsilon V_i \right) \delta(x_n - x)$$

Note that now the last term looks like ψ_0, which is what we want. We just need to bring the first term *outside* the path integral - and we do this by renaming x_0 to x' with another δ:

$$\psi_{-1} = \int_{\mathbb{R}} \frac{\mathrm{d}x'}{\sqrt{4\pi D_{-1}\epsilon}} \exp\left(-\frac{(x' - x_{-1} - f_{-1}\epsilon)^2}{4D_{-1}\epsilon} - \epsilon V(x', t_0) \right) \cdot \\ \cdot \int_{\mathbb{R}^n} \left(\prod_{i=1}^{n} \frac{\mathrm{d}x_i}{\sqrt{4\pi D_{i-1}\epsilon}} \right) \exp\left(-\sum_{i=1}^{n} \frac{(x_i - x_{i-1} - f_{i-1}\epsilon)^2}{4D_{i-1}\epsilon} - \sum_{i=1}^{n} \epsilon V_i \right) \cdot \\ \cdot \delta(x_n - x)\delta(x_0 - x') = \\ = \int_{\mathbb{R}} \frac{\mathrm{d}x'}{\sqrt{4\pi D_{-1}\epsilon}} \exp\left(-\underbrace{\frac{(x' - x_{-1} - f_{-1}\epsilon)^2}{4D_{-1}\epsilon}}_{z^2/2} - \epsilon V(x', t_0) \right) W_B^{(\epsilon)}(x, t | x', t_0)$$

We then perform a change of variables:

$$z = \frac{x' - x_{-1} - f_{-1}\epsilon}{\sqrt{2D_{-1}\epsilon}} \Rightarrow x' = x_{-1} + f_{-1}\epsilon + z\sqrt{4D_{-1}\epsilon}$$

leading to:

$$W_B^{(\epsilon)}(x, t | x_{-1}, t_{-1}) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}z \exp\left(-\frac{z^2}{2} \right) \exp\left(-\epsilon V(x_{-1} + f_{-1}\epsilon + z\sqrt{4D_{-1}\epsilon}) \right) \cdot \\ \cdot W_B(x, t | x_{-1} + f_{-1}\epsilon + z\sqrt{4D_{-1}\epsilon}, t_0)$$

Finally, we perform some Taylor expansions for $f_{-1}\epsilon + z\sqrt{4D_{-1}\epsilon} \sim 0$:

$$\exp\left(-\epsilon V(x_{-1} + f_{-1}\epsilon + z\sqrt{4D_{-1}\epsilon}) \right) = \exp\left(-\epsilon V(x_{-1}) + O(\epsilon\sqrt{\epsilon}) \right) = \\ = 1 - \epsilon V(x_{-1}) + O(\epsilon^2)$$

Let $W_B^{(\epsilon)}(x, t | x_{-1}, t_0) = \psi$, and denote with ψ' the first derivative wrt x_{-1} (and so on). Then:

$$W_B^{(\epsilon)}(x, t | x_{-1} + f_{-1}\epsilon + z\sqrt{4D_{-1}\epsilon}, t_0) = \psi + (f_{-1}\epsilon + z\sqrt{4D_{-1}\epsilon})\psi' + \\ + \frac{1}{2}(f_{-1}\epsilon + z\sqrt{4D_{-1}\epsilon})^2\psi''$$

Substituting back in the integrand, and neglecting everything of order > 1 in ϵ:

$$W_B^{(\epsilon)}(x,t|x_{-1},t_{-1}) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}z \exp\left(-\frac{z^2}{2}\right)\Bigg[\psi(1-\epsilon V(x_{-1})) + f_{-1}\epsilon\psi' + \\ + z\psi'\sqrt{4D_{-1}\epsilon} + \frac{1}{2}z^2 4D_{-1}\epsilon\psi''\Bigg]$$

These are all gaussian integrals involving the moments of a standard gaussian (with 0 mean and 1 standard deviation), and so:

$$W_B^{(\epsilon)}(x,t|x_{-1},t_{-1}) = W_B^{(\epsilon)}(x,t|x_{-1},t_0)(1-\epsilon V(x_{-1},t_0)) + f_{-1}\epsilon\partial_{x_{-1}}W_B^{(\epsilon)}(x,t|x_{-1},t_0) + \\ + 2D_{-1}\epsilon\partial^2_{x_{-1}}W_B^{(\epsilon)}(x,t|x_{-1},t_0)$$

Rearranging, dividing by ϵ and taking the continuum limit $\epsilon \to 0^+$ finally leads to:

$$\partial_{t_0}W_B(x,t|x_0,t_0) = -[f(x_0)\partial_{x_0} + 2D(x_0)\partial^2_{x_0} - V(x_0)]W(x,t|x_0,t_0)$$

Exercise 0.5:

Derive the analogous of the Bloch equation and of the backward Bloch equation for the Master Equation of exercise 5.7.
Hint: The trajectory $i(t)$ stays constant and suddenly jumps at random times. Thus $\int_{t_0}^t V_{i(s)}\,\mathrm{d}s$ is well defined. When evaluating the average:

$$W_B(i,t|i_0,t_0) = \langle \exp\left(-\int_{t_0}^t V_{i(s)}\,\mathrm{d}s\right)\delta_{i(t),i}\rangle \qquad (15)$$

where $W_B(i,t_0|i_0,t_0) = \delta_{i,i_0}$ and δ_{i,i_0} is the Kronecker delta, at time $t + \mathrm{d}t$ one has to consider two contributions: one from no change of state and the other from the change of state.

Solution. Recall that in ex. 5.7 we considered a system evolving through states $i \in J$, according to the following rule:

$$\dot{P}_i(t) = (H(t)P(t))_i \qquad H_{ij}(t) = W_{ij}(t) - \delta_{ij}\sum_{k\in J}W_{ki}(t)$$

Let's consider a *uniform* time discretization $\{t_j\}_{j=0,\dots,n}$ with $t_n \equiv t$ and $\Delta t_j = t_j - t_{j-1} \equiv \epsilon$. Introduce a potential $V\colon J \to \mathbb{R}$ and denote with V_i the potential at the state i. We then consider a *path* through states as a vector $\{i_j\}_{j=0,\dots,n}$, where $i_j \in J$ is the state explored at time t_j.

Then we discretize (15):

$$
\begin{aligned}
W_B(i,t|i_0,t_0) &= \lim_{\epsilon\to 0^+} W_B^{(\epsilon)}(i,t_n|i_0,t_0)\\
W_B^{(\epsilon)}(i,t_n|i_0,t_0) &= \langle \exp\left(-\sum_{s=1}^n V_{i_s}\epsilon\right)\delta_{i_n,i}\rangle =\\
&= \underbrace{\sum_{i_1\in J}\cdots\sum_{i_n\in J}}_{\text{Sum over all paths}} \underbrace{\epsilon W_{i_n,i_{n-1}}\cdots\epsilon W_{i_1,i_0}}_{\text{Probability for a path}} \exp\left(-\sum_{s=1}^n V_{i_s}\epsilon\right) \underbrace{\delta_{i_n,i}}_{\text{Fix endpoint}}
\end{aligned}
\tag{16}
$$

The average is over all *discrete* paths connecting i_0 at t_0 to i at t (it can't be written as an integral in the Wiener measure, as the states J are discrete too).

For the **forward** Bloch equation we *evolve* the destination by one time-step:

$$
W_B^{(\epsilon)}(i,t_{n+1}|i_0,t_0) = \psi_{n+1} = \sum_{i_1\in J}\cdots\sum_{i_{n+1}\in J}\epsilon W_{i_{n+1},i_n}\cdots\epsilon W_{i_1,i_0}\exp\left(-\sum_{s=1}^{n+1}V_{i_s}\epsilon\right)\delta_{i_{n+1},i}
$$

The sum over i_{n+1} can be computed to remove the δ:

$$
\psi_{n+1} = \exp\left(-V_i\epsilon\right)\sum_{i_1\in J}\cdots\sum_{i_n\in J}\epsilon W_{i,i_n}\cdots\epsilon W_{i_1,i_0}\exp\left(-\sum_{s=1}^n V_{i_s}\epsilon\right)
$$

Then we highlight the i_n term:

$$
\psi_{n+1} = \exp\left(-V_i\epsilon\right)\sum_{i_1\in J}\cdots\sum_{i_n\in J}\epsilon W_{i,i_n}\cdots\epsilon W_{i_1,i_0}\exp\left(-\sum_{s=1}^n V_{i_s}\epsilon\right)
$$

To bring it out of the *sum over paths* we insert a δ:

$$
\begin{aligned}
\psi_{n+1} &= \exp(-V_i\epsilon)\sum_{i'\in J}\epsilon W_{i,i'}\cdot\\
&\quad\cdot\underbrace{\sum_{i_1\in J}\cdots\sum_{i_n\in J}\epsilon W_{i_n,i_{n-1}}\cdots\epsilon W_{i_1,i_0}\exp\left(-\sum_{s=1}^n V_{i_s}\epsilon\right)\delta_{i_n,i'}}_{(16):\ W_B(i',t|i_0,t_0)} =\\
&= \exp(-V_i\epsilon)\sum_{i'\in J}\epsilon W_{i,i'}W_B(i',t|i_0,t_0)
\end{aligned}
$$

We now split the transition probability $W_{i',i}$ over the case $i'=i$ and $i'\neq i$, using the same trick of ex. 5.7 to express everything with the off-diagonal terms:

$$
\psi_{n+1} = \exp(-V_i\epsilon)\Big(\sum_{i'\in J\setminus\{i\}}\epsilon W_{i,i'}W_B(i',t|i_0,t_0) + \Big[1-\sum_{i'\in J\setminus\{i\}}\epsilon W_{i',i}\Big]W_B(i,t|i_0,t_0)\Big)
$$

Note that we can extend the sums over the entire $i' \in J$, as the $i = i'$ terms cancel out.
We then expand the exponential:

$$\exp(-V_i\epsilon) = 1 - V_1\epsilon + O(\epsilon^2)$$

Substituting back and neglecting higher order terms in ϵ:

$$\begin{aligned} W_B^{(\epsilon)}(i, t_{n+1}|i_0, t_0) = (1 - V_i\epsilon)\Bigg[& W_B(i, t|i_0, t_0) + \\ & + \epsilon \sum_{i' \in J} \Big(W_{i,i'} W_B^{(\epsilon)}(i', t|i_0, t_0) - W_{i',i} W_B^{(\epsilon)}(i, t|i_0, t_0) \Big) \Bigg] \end{aligned}$$

Rearranging, dividing by ϵ and taking the continuum limit leads to:

$$\begin{aligned} \partial_t W_B(i, t|i_0, t_0) &= \lim_{\epsilon \to 0} \frac{W_B^{(\epsilon)}(i, t_{n+1}|i_0, t_0) - W_B^{(\epsilon)}(i, t|i_0, t_0)}{\epsilon} = \\ &= -V_i W_B(i, t|i_0, t_0) + \sum_{i' \in J} \Big(W_{i,i'} W_B(i', t|i_0, t_0) - W_{i',i} W_B(i, t|i_0, t_0) \Big) \end{aligned}$$

For the **backward** Bloch equation we start from:

$$\frac{\partial}{\partial t_0} W_B(i, t|i_0, t_0) = \lim_{\epsilon \to 0^+} \frac{W_B(i, t|i_0, t_0) - W_B(i, t|i_0, t_{-1})}{\epsilon}$$

Applying the ESCK relation:

$$W_B(i, t|i_0, t_{-1}) = \sum_{i' \in J} W_B(i, t|i', t_0) W_B(i', t_0|i_0, t_{-1})$$

The last term is the average over only one step:

$$W_B(i', t_0|i_0, t_{-1}) = \exp\big(-V_{i'}\epsilon\big) W_{i',i_0}\epsilon$$

And so:

$$\begin{aligned} W_B(i, t|i_0, t_{-1}) &= \sum_{i' \in J} W_B(i, t|i', t_0) \exp\big(-V_{i'}\epsilon\big) W_{i',i_0}\epsilon = \\ &= \sum_{i' \neq i_0} W_B(i, t|i', t_0) W_{i',i_0} \exp\big(-V_{i'}\epsilon\big) + \\ &\quad + W_B(i, t|i_0, t_0) \exp\big(-V_{i_0}\epsilon\big) \left[1 - \sum_{k \neq i_0} W_{k,i_0}\epsilon \right] \end{aligned}$$

Then we compute the difference:

$$\begin{aligned} W_B(i, t|i_0, t_0) - W_B(i, t|i_0, t_{-1}) = &- \sum_{i' \neq i_0} W_B(i, t|i', t_0) W_{i',i_0} \exp\big(-V_{i'}\epsilon\big) + \\ &+ W_B(i, t|i_0, t_0) \exp\big(-V_{i_0}\epsilon\big) \sum_{k \neq i_0} W_{k,i_0}\epsilon \end{aligned}$$

We then add a δ to merge the two sums, and extend them to include the diagonal terms (without adding anything, because the two terms cancel out in that case):

$$= -\sum_{i'} W_B(i,t|i',t_0) W_{i',i_0}\epsilon \exp\bigl(-V_{i'}\epsilon\bigr) + \sum_{i} \delta_{i',i_0} W_B(i,t|i',t_0) \exp\bigl(-V_{i'}\epsilon\bigr) \sum_{k\neq i_0} W_{ki_0}\epsilon =$$
$$= -\sum_{i'} W_B(i,t|i',t_0) \exp\bigl(-V_{i'}\epsilon\bigr)\epsilon[W_{i' i_0} - \delta_{i',i_0} \sum_{k\neq i_0} W_{k,i_0}]$$

Dividing by ϵ and taking the continuum limit leads to:

$$\partial_{t_0} W_B(i,t|i_0,t_0) =$$

$$\begin{aligned}
W_B^{(\epsilon)}(i,t_n|i_0,t_{-1}) = \psi_{-1} &= \sum_{i'_0\in J}\sum_{i_1\in J}\cdots\sum_{i_n\in J} \epsilon W_{i_n,i_{n-1}}\cdots \epsilon W_{i_1,i'_0}\epsilon W_{i'_0,i_0}\cdot \\
&\cdot \exp\bigl(-V_{i'_0}\epsilon\bigr)\exp\left(-\sum_{s=1}^{n} V_{i_s}\epsilon\right)\delta_{i_n,i} = \\
&= \sum_{i'\in J} \exp\bigl(-V_{i'}\epsilon\bigr)\epsilon W_{i',i_0} W_B^{(\epsilon)}(i,t|i'_0,t_0) = \\
&= \sum_{i'\in J\setminus\{i_0\}} \exp\bigl(-V_{i'}\epsilon\bigr)\epsilon W_{i',i_0} W_B^{(\epsilon)}(i,t|i'_0,t_0) + \\
&+ \exp\bigl(-V_{i_0}\epsilon\bigr)\Bigl(1 - \sum_{i'\in J\setminus\{i\}} \epsilon W_{i',i_0}\Bigr) W_B^{(\epsilon)}(i,t|i_0,t_0)
\end{aligned}$$

$$W_B^{(\epsilon)}(i,t_n|i_0,t_0) - W_B^{(\epsilon)}(i,t_n|i_0,t_{-1}) =$$

Highlight the term with i'_0:

$$\psi_{-1} = \sum_{i_0\in J}\cdots\sum_{i_n\in J} \exp\bigl(-V_{i_0}\epsilon\bigr)\epsilon W_{i_0,i_{-1}}\left[\epsilon W_{i_n,i_{n-1}}\cdots\epsilon W_{i_1,i_0}\right]\exp\left(-\sum_{s=1}^{n} V_{i_s}\epsilon\right)\delta_{i_n,i}$$

And we extract it out the paths sum by inserting a δ:

$$\begin{aligned}
\psi_{-1} = &\sum_{i'\in J} \epsilon W_{i',i_{-1}}\cdot \\
&\cdot \sum_{i_0\in J}\cdots\sum_{i_n\in J} \epsilon W_{i_n,i_{n-1}}\cdots\epsilon W_{i_1,i_0}\exp\left(-\sum_{s=1}^{n} V_{i_s}\epsilon\right)\exp\bigl(-V_{i'}\epsilon\bigr)\delta_{i_n,i}\delta_{i_0,i'}
\end{aligned}$$

Now the sum over i_0 can be computed, eliminating a δ:

$$\begin{aligned}
\psi_{-1} = &\sum_{i'\in J} \epsilon W_{i',i_{-1}}\cdot \\
&\cdot \exp\bigl(-V_{i_0}\epsilon\bigr)\sum_{i_1\in J}\cdots\sum_{i_n\in J} \epsilon W_{i_n,i_{n-1}}\cdots\epsilon W_{i_1,i'}\exp\left(-\sum_{s=1}^{n} V_{i_s}\epsilon\right)
\end{aligned}$$