0.1 Harmonic overdamped oscillator

(Lesson 9 of 14/11/19) Compiled: January 2, 2020

Using the framework developed in the previous sections, we now tackle a more general setting, that of a particle moving in a *harmonic potential* and subject to thermal noise. This will be useful to model the local behaviour about the minima of *any* potential - as they are approximately harmonic.
So, consider a particle of mass m moving in one dimension through a *viscous* medium and immersed in a *harmonic* potential. To model the random collisions with the other (much smaller) particles in the fluid we add a *stochastic term* $\sqrt{2D}\gamma\xi$. The equation of motion becomes:

$$m\ddot{x} = -\gamma\dot{x} - m\omega^2 x + \sqrt{2D}\gamma\xi \tag{1}$$

As m/γ is much smaller than the timescale we are interested in, we can neglect it, reaching the *overdamped limit*:

$$\dot{x} = -\underbrace{\frac{m\omega^2}{\gamma}}_{k} x + \sqrt{2D}\xi$$

And multiplying by $\mathrm{d}t$:

$$\mathrm{d}x(t) = -kx(t)\,\mathrm{d}t + \sqrt{2D}\,\mathrm{d}B(t) \tag{2}$$

As usual, we introduce a time discretization $\{t_j\}_{j=1,\dots,n}$. Letting:

$$x(t_i) \equiv x_i; \quad \Delta x_i \equiv x_i - x_{i-1}; \qquad B(t_i) \equiv B_i; \qquad \Delta t_i = t_i - t_{i-1}$$

we arrive to:

$$\Delta x_i = -kx_{i-1}\Delta t_i + \sqrt{2D}\Delta B_i \tag{3}$$

Note that we evaluated the potential term $-kx(\tau)$ at the *left extremum* of the discretized interval $[t_{i-1}, t_i]$, following Ito's prescription.
To solve (2) the plan will be the following:

1. Use the discretization to find the *infinitesimal probability* $\mathbb{P}(\{\Delta x_i\}_{i=1,\dots,n})$ of a *discretized path*, i.e. of a path traversing all *gates* $[x_i, x_i + \mathrm{d}x_i]$ at successive instants $0 \equiv t_1 < \cdots < t_n \equiv t$.

2. Find the probability for a continuous path $\mathrm{d}P \equiv \mathbb{P}(\{x(\tau)_{\tau\in[0,t]}\})$ by taking the limit $n \to \infty$.

3. Find the transition probabilities that solve (2) by using a *path integral* to evaluate:

$$W(x_t, t; x_0, 0) = \langle \delta(x_t - x(\tau)) \rangle_W \equiv \int_{\mathbb{R}^T} \delta(x_t - x(\tau))\,\mathrm{d}P$$

In other words, this is the *fraction* of paths (from the set $\mathbb{R}^T$ of all continuous paths happening in the timeframe $[0, t]$) that start in x_0 at instant 0, and reach x_t at instant t.

To find $\mathbb{P}(\{\Delta x_i\}_{i=1,\dots,n})$ we start from the joint pdf $\mathbb{P}(\{\Delta B_i\}_{i=1,\dots,n})$ that we already know, and perform a change of random variables according to (3).
In practice, start from:

$$\mathbb{P}(\Delta B_1, \dots, \Delta B_n) = \prod_{i=1}^{n} \frac{\mathrm{d}\Delta B_i}{\sqrt{2\pi \Delta t_i}} \exp\left(-\sum_{i=1}^{n} \frac{\Delta B_i^2}{2\Delta t_i}\right)$$

Then insert ΔB_i in terms of Δx_i from (3):

$$\Delta B_i = \frac{\Delta x_i + k x_{i-1} \Delta t_i}{\sqrt{2D}}$$

and then multiply by the determinant J of the jacobian of the change of variables to find the desired new pdf:

$$\begin{aligned}\mathbb{P}(x_1, x_2, \dots, x_n) &= \mathbb{P}(\Delta x_1)\mathbb{P}(\Delta x_2|\Delta x_1)\mathbb{P}(\Delta x_3|\Delta x_1, \Delta x_2)\cdots = \\ &= \prod_{i=1}^{n} \frac{\mathrm{d}\Delta x_i}{\sqrt{2\pi\Delta t_i}} \exp\left(-\sum_{i=1}^{n} \frac{1}{2\Delta t_i}\left(\frac{\Delta x_i + k x_{i-1}\Delta t_i}{\sqrt{2D}}\right)^2\right) J\end{aligned}$$

$$J = \det\left|\frac{\partial(\Delta B_1, \dots, \Delta B_n)}{\partial(\Delta x_1, \dots, \Delta x_n)}\right| = \det\left|\frac{\partial(\Delta x_1, \dots, \Delta x_n)}{\partial(\Delta B_1, \dots, \Delta B_n)}\right|^{-1} = \begin{vmatrix} \sqrt{2D} & 0 & \cdots & 0 \\ 0 & \sqrt{2D} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \sqrt{2D} \end{vmatrix}_{n\times n}^{-1} = (2D)^{-n/2}$$

And so:

$$\mathbb{P}(\Delta x_1, \dots, \Delta x_n) = \prod_{i=1}^{n}\left(\frac{\mathrm{d}\Delta x_i}{\sqrt{4\pi D \Delta t_i}}\right) \exp\left(-\sum_{i=1}^{n}\frac{1}{2\Delta t_i}\left(\frac{\Delta x_i + k x_{i-1}\Delta t_i}{\sqrt{2D}}\right)^2\right) \quad (4)$$

Taking the limit $n \to \infty$:

$$\mathrm{d}P \equiv \mathbb{P}(x(\tau)) = \prod_{\tau=0^+}^{t} \frac{\mathrm{d}x(\tau)}{\sqrt{4\pi D\,\mathrm{d}\tau}} \exp\left(-\frac{1}{4D}\int_0^t (\dot{x} + kx)^2\,\mathrm{d}\tau\right)$$

where we used:

$$\frac{1}{\Delta t_i}(\Delta x_i + k x_{i-1}\Delta t_i)^2 = \frac{\Delta t_i^2}{\Delta t_i}\left(\frac{\Delta x_i}{\Delta t_i} + k x_{i-1}\frac{\Delta t_i}{\Delta t_i}\right)^2 \xrightarrow[n\to\infty]{} (\dot{x} + kx)^2\,\mathrm{d}t$$

Expanding the square in (4):

$$\mathrm{d}P = \prod_{i=1}^{n} \underbrace{\frac{\mathrm{d}\Delta x_i}{\sqrt{4\pi D\Delta t_i}} \exp\left(-\sum_{i=1}^{n}\frac{\Delta x_i^2}{4D\Delta t_i}\right)}_{\text{Wiener measure } (\mathrm{d}x_W)} \underbrace{\exp\left(-\frac{k}{2D}\sum_{i=1}^{n} x_{i-1}\Delta x_i\right)}_{\text{stochastic integral}} \underbrace{\exp\left(-\frac{k^2}{4D}\sum_{i=1}^{n}\Delta t_i x_{i-1}^2\right)}_{\text{normal integral}} \quad (5)$$

Let's focus on the stochastic integral. We already know that, for Ito's integrals, the usual rules of calculus do not apply. In particular, we can't just do:

$$\sum_{i=1}^{n} x_{i-1}\Delta x_i \xrightarrow[n\to\infty]{} \int_0^t x(\tau)\,\mathrm{d}x(\tau) \neq \frac{x^2(t)-x^2(0)}{2}$$

So, more in general for a differentiable function $h(x)$:

$$\int_0^t h'(\tau)\,\mathrm{d}x(\tau) \neq h(x(t)) - h(x(0)) \tag{6}$$

The idea is now to start from the right side and use Ito's rules to *correct* the left side, so to have a usable identity for integration. As always, we start by discretizing time $\{t_i\}_{i=1,\dots,n}$:

$$h(x(t)) - h(x(0)) = \sum_{i=1}^{n}[h(x(t_i)) - h(x(t_{i-1}))] \equiv \sum_{i=1}^{n}\Delta h_i$$

In the limit, $t_i = t_{i-1} + \mathrm{d}t$, and so the Δh_i are *differentials* of h:

$$\Delta h_i = \frac{\mathrm{d}h}{\mathrm{d}x_i}\Delta x_i + \frac{1}{2}\frac{\mathrm{d}^2 h}{\mathrm{d}x_i^2}\Delta x_i^2 + O(\Delta x_i^3)$$

Now:

$$\Delta x_i = \frac{\mathrm{d}\Delta B_i}{\mathrm{d}\Delta x_i}\Delta B_i + O(\Delta B_i^2) \approx \sqrt{2D}\Delta B_i$$

And by Ito's rules, $\Delta B_i^2 = \Delta t_i$ and $\Delta B_i^n = 0$ for $n \geq 3$. So:

$$\Delta h_i = h'\Delta x_i + \frac{1}{2}h''\underbrace{\Delta x_i^2}_{2D\Delta t_i}$$

And substituting back in (6) leads to:

$$h(x(t)) - h(x(0)) = \sum_{i=1}^{n}(h_i'\Delta x_i + h''D\Delta t_i)$$

Rearranging:

$$\sum_{i=1}^{n} h_i'\Delta x_i = h(x(t)) - h(x(0)) - D\sum_{i=1}^{n} h''\Delta t_i$$

In the limit $n \to \infty$, the sums become integrals:

$$\int_0^t h'\,\mathrm{d}x(\tau) = h(x(t)) - h(x(0)) - D\int_0^t h''\,\mathrm{d}\tau \tag{7}$$

We can finally apply the result (7) to our case, by setting $h'(x(\tau)) = x(\tau)$, so that:

$$h(x(t)) = \int x(\tau) = \frac{x(t)^2}{2}; \qquad h''(x(\tau)) = 1$$

Substituting in (7) leads to:

$$\sum_{i=1}^{n} x_{i-1}\Delta x_i \xrightarrow[n\to\infty]{} \int_0^t x(\tau)\,\mathrm{d}x(\tau) = \frac{x^2(t)-x^2(0)}{2} - D\underbrace{\int_0^t \mathrm{d}\tau}_{t} = \frac{x^2(t)-x^2(0)}{2} - Dt$$

And substituting this result back in (5) leads to:

$$\mathrm{d}P \underset{n\to\infty}{=} \mathrm{d}x_W \exp\left(-\frac{k}{2D}\left[\frac{x_t^2-x_0^2}{2} - Dt\right]\right)\exp\left(-\frac{k^2}{4D}\int_0^t x^2(\tau)\,\mathrm{d}\tau\right)$$

From this expression we can compute *transition probabilities*. Let $T=[0,t]$ and $\mathbb{R}^T$ be the space of continuous functions $T\to\mathbb{R}$, then:

$$\begin{aligned}
W(x_t,t|x_0,0) &= \langle\delta(x_t-x)\rangle_W = \int_{\mathbb{R}^T}\delta(x_t-x)\,\mathrm{d}P = \\
&= \int_{\mathbb{R}^T}\mathrm{d}x_W\,\delta(x(t)-x)\exp\left(-\frac{k}{2D}\left[\frac{x_t^2-x_0^2}{2}-Dt\right]\right)\exp\left(-\frac{k^2}{4D}\int_0^t x^2(\tau)\,\mathrm{d}\tau\right) = \\
&= \exp\left(-\frac{k}{2D}\left[\frac{x_t^2-x_0^2}{2}-Dt\right]\right)\underbrace{\int_{\mathbb{R}^T}\mathrm{d}x_W\,\delta(x(t)-x)\exp\left(-\frac{k^2}{4D}\int_0^t x^2(\tau)\,\mathrm{d}\tau\right)}_{\text{CFR } I_4 \text{ on } 28/10} = \\
&= \exp\left(-\frac{k}{2D}\left[\frac{x_t^2-x_0^2}{2}-Dt\right]\right)\sqrt{\frac{k}{4\pi D\sinh(kt)}}\exp\left(-\frac{kx_t^2}{4D}\coth(kt)\right)
\end{aligned} \tag{8}$$

Exercise 0.1.1 (Some more integrals)**:**

> Check that:
>
> $$W(x,0|x_0,0) = \delta(x-x_0)$$
>
> **Hint**. Start from the case $x_0=0$. Using (8), after some algebra:
>
> $$W(x,t|0,0) = \sqrt{\frac{k}{2\pi D(1-e^{-2kt})}}\exp\left(-\frac{k}{2D}\frac{x^2}{1-e^{-2kt}}\right) \tag{9}$$
>
> And then show $W(x,t|0,0)\xrightarrow[t\to 0]{}\delta(x)$. The general case follows by translating that solution.

Alternative derivation The same result for the transition probabilities $W(x,t|x_0,0)$ can be found solving the Fokker-Planck equation:

$$\dot{W}(x,t|x_0,0) = \frac{\partial}{\partial x}\left(kxW + D\frac{\partial}{\partial x}W\right) \tag{10}$$

A quick way to solve this differential equation is to note that $\{\Delta B_i\}$ are all i.i.d. gaussian variables, and so x, which is a sum of ΔB_i must have a *gaussian* pdf. So we can make an *ansatz* for the solution:

$$W(x,t|x_0,0) = \frac{1}{Z(t)} \exp\left(-a(t)x^2 + b(t)x\right) \tag{11}$$

Where $a(t)$ and $b(t)$ are the gaussian parameters, and $Z(t)$ the normalization factor. All that's left is to substitute (11) in (10) and solve for a, b, Z.

0.1.1 Equilibrium distribution

As before, we expect the equilibrium distribution to follow Maxwell-Boltzmann formula:

$$W_{\text{eq}}(x) = \frac{1}{Z} \exp(-\beta V(x)) = \frac{1}{Z} \exp\left(-\frac{m\omega^2 x^2}{2k_B T}\right) \qquad Z = \int_{\mathbb{R}} \exp(-\beta V(x)) \tag{12}$$

Starting from (9) and taking the limit $t \to \infty$:

$$\lim_{t\to\infty} W(x,t|0,0) = \sqrt{\frac{k}{2\pi D}} \exp\left(-\frac{k}{2D} x^2\right) \tag{13}$$

Comparing (12) with (13) we find:

$$\frac{m\omega^2}{2k_B T} = \frac{k}{2D} = \frac{m\omega^2}{2\gamma D} \Rightarrow k_B T = \gamma D$$

So we obtain the same relation between D and T that we found in the general case.

0.1.2 High dimensional generalization

We can generalize the previous results to the case where $\boldsymbol{\Delta B_i} = (\Delta B_i^1, \dots, \Delta B_i^d)^T$ are d-dimensional vectors, following a *multivariate gaussian distribution*:

$$\mathbb{P}(\boldsymbol{\Delta B_1}, \dots, \boldsymbol{\Delta B_n}) = \prod_{i=1}^n \prod_{\alpha=1}^d \frac{\mathrm{d}B_i^\alpha}{\sqrt{2\pi \Delta t_i}} \exp\left(-\frac{\Delta B_i^\alpha}{2\Delta t_i}\right)$$

As different components of the same $\boldsymbol{\Delta B_i}$ are independent, by Ito's rules of integration:

$$\mathrm{d}B_i^\alpha \, \mathrm{d}B_i^\beta = \delta_{\alpha\beta} \, \mathrm{d}t_i \qquad \mathrm{d}B_i^\alpha \, \mathrm{d}B_i^\beta \, \mathrm{d}B_i^\gamma = 0$$

We then need to write d different Langevin equations, one for each component:

$$\mathrm{d}x^\alpha(t) = f^\alpha(x(t), t) \, \mathrm{d}t + \sqrt{2D_\alpha(x(t), t)} \, \mathrm{d}B^\alpha(t)$$

More in general, the stochastic term could be:

$$\sum_{\beta=1}^d g_{\alpha\beta}(x(t), t) \, \mathrm{d}B^\beta(t)$$

and in our case $g_{\alpha\beta} = 2\sqrt{2D_\alpha}\delta_{\alpha\beta}$.

The Fokker-Planck equation then becomes:

$$\dot{W}(\boldsymbol{x},t) = \sum_{\alpha=1}^{d} \frac{\partial}{\partial x^\alpha} \left(-f_\alpha(\boldsymbol{x},t)W(\boldsymbol{x},t) + \frac{\partial}{\partial x^\alpha} D_\alpha(\boldsymbol{x},t)W(\boldsymbol{x},t) \right)$$

And the joint probability for a *discretized* path:

$$\mathbb{P}(\boldsymbol{\Delta x_1},\dots,\boldsymbol{\Delta x_n}) = \prod_{i=1}^{n}\prod_{\alpha=1}^{d} \frac{\mathrm{d}\Delta x_i^\alpha}{\sqrt{4\pi D_\alpha \Delta t_i}} \exp\left(-\sum_{i=1}^{n}\sum_{\alpha=1}^{d} \frac{(\Delta x_i^\alpha - f_{i-1}^\alpha \Delta t_i)^2}{4D_\alpha \Delta t_i} \right)$$

And taking the limit $n \to \infty$:

$$\mathbb{P}(\boldsymbol{x}(\tau)) = \prod_{\tau=0^+}^{t} \left(\frac{\mathrm{d}^d \boldsymbol{x}(\tau)}{\sqrt{4\pi\,\mathrm{d}\tau}\prod_{\alpha=1}^{d}\sqrt{D_\alpha}} \right) \exp\left(-\sum_{\alpha=1}^{d} \frac{1}{4D_\alpha} \int_0^t (\dot{x}^\alpha - f^\alpha)^2 \,\mathrm{d}\tau \right)$$

0.1.3 Underdamped Harmonic Oscillator

If we do not ignore the inertia term in (1) we are left with:

$$m\ddot{\boldsymbol{x}} = m\dot{\boldsymbol{v}} = -\gamma\dot{\boldsymbol{x}} + \boldsymbol{F}(\boldsymbol{x}) + \sqrt{2D}\boldsymbol{\xi}$$

This second order (stochastic) differential equation can be written as a system of two first order equations:

$$\begin{cases} \mathrm{d}\boldsymbol{x} = \boldsymbol{v}\,\mathrm{d}t \\ \mathrm{d}\boldsymbol{v} = \left(-\dfrac{\gamma}{m}\boldsymbol{v} + \dfrac{\boldsymbol{F}(\boldsymbol{x})}{m} \right)\mathrm{d}t + \dfrac{\sqrt{2D}}{m}\,\mathrm{d}\boldsymbol{B} \end{cases}$$

This leads to a *generalization* of the Fokker-Planck equation, named **Kramer equation**:

$$\dot{W}(\boldsymbol{x},\boldsymbol{v},t) = \boldsymbol{\nabla_v}\left[\left(\frac{\gamma\boldsymbol{v}}{m} - \frac{\boldsymbol{F}}{m} \right) W(\boldsymbol{x},\boldsymbol{v},t) + \frac{\gamma^2 D}{m^2}\boldsymbol{\nabla_v} W(\boldsymbol{x},\boldsymbol{v},t) \right] + \boldsymbol{\nabla_x}(-\boldsymbol{v}W(\boldsymbol{x},\boldsymbol{v},t))$$

In the limit $t \to \infty$, the distribution at equilibrium will be:

$$W(\boldsymbol{x},\boldsymbol{v}) = \frac{1}{Z}\exp\left(-\beta\left[\frac{m\|\boldsymbol{v}\|^2}{2} + V(\boldsymbol{x}) \right] \right) \qquad D = \frac{k_B T}{\gamma}$$