0.1 Harmonic overdamped oscillator

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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. If we add a noise term, modelling the random collisions with the other (much smaller) particles in the fluid, 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 $\mathrm{d}t$:

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

To find a solution for $x(t)$ 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:

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

where we used Ito's prescription to choose the *mid-point* value of $x(t)$ in each discretized interval $[t_{i-1}, t_i]$ to be evaluated at the smaller extremum t_{i-1}.
Recall that the *joint* pdf of the Brownian increments ΔB_i is:

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

Then the probability of a path $x(t)$ passing "close to" a set of points $x_1, x_2, \dots, x_n$ at instants $t_1 < t_2 < \dots < t_n$ is:

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

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

and so:

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

Taking the limit $n \to \infty$:

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

Expanding the square in (2):

$$\mathrm{d}P = \prod_{i=1}^{n} \underbrace{\frac{\mathrm{d}\Delta x_i}{\sqrt{4\pi D \Delta t_i}} \exp\left(-\sum_{i=1}^{n} \frac{\Delta x_i^2}{4D\Delta t_i} \right)}_{\text{Wiener measure } (\mathrm{d}x_W)} \underbrace{\exp\left(-\frac{k}{2D} \sum_{i=1}^{n} x_{i-1} \Delta x_i \right)}_{\text{stochastic integral}} \underbrace{\exp\left(-\frac{k^2}{4D} \sum_{i=1}^{n} \Delta t_i x_{i-1}^2 \right)}_{\text{normal integral}} \tag{3}$$

Let's focus on the stochastic integral. According to Ito's rules:

$$h(x(t)) - h(x(0)) = \sum_{i=1}^{n} \Delta h_i = \sum_{i=1}^{n} (h_i' \Delta x_i + \frac{1}{2} h'' \underbrace{\Delta x_i^2}_{2D\Delta t_i}) + 0$$

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:

$$\int_0^t h' \,\mathrm{d}x(\tau) = h(x(t)) - h(x(0)) - D \int_0^t h'' \,\mathrm{d}\tau \tag{4}$$

Now, choose:

$$h(x(t)) = \frac{x(t)^2}{2}$$

So that:

$$h'(x(t)) = x(t) \qquad h''(x(t)) = 1$$

Substituting in (4) leads to:

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

Substituting this result back in (3) 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:

$$\begin{aligned} W(x_t, t|x_0, 0) &= \langle \delta(x_t - x) \rangle_W = \int_{\mathbb{R}^T} \delta(x_t - x) \, \mathrm{d}P = \\ &= \int_{\mathbb{R}^T} \mathrm{d}x_W \, \delta(x(t) - x) \exp\left(-\frac{k}{2D}\left[\frac{x_t^2 - x_0^2}{2} - Dt\right]\right) \exp\left(-\frac{k^2}{4D}\int_0^t x^2(\tau)\, \mathrm{d}\tau\right) = \\ &= \exp\left(-\frac{k}{2D}\left[\frac{x_t^2 - x_0^2}{2} - Dt\right]\right) \underbrace{\int_{\mathbb{R}^T} \mathrm{d}x_W \, \delta(x(t) - x) \exp\left(-\frac{k^2}{4D}\int_0^t x^2(\tau)\, \mathrm{d}\tau\right)}_{\text{CFR } I_4 \text{ on } 28/10} = \\ &= \exp\left(-\frac{k}{2D}\left[\frac{x_t^2 - x_0^2}{2} - Dt\right]\right) \sqrt{\frac{k}{4\pi D \sinh(kt)}} \exp\left(-\frac{k x_t^2}{4D}\coth(kt)\right) \end{aligned} \tag{5}$$

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 (5), after some algebra:

$$W(x, t|0, 0) = \sqrt{\frac{k}{2\pi D(1 - e^{-2kt})}} \exp\left(-\frac{k}{2D}\frac{x^2}{1 - e^{-2kt}}\right) \tag{6}$$

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:

$$\dot{W}(x, t|x_0, 0) = \frac{\partial}{\partial x}\left(kxW + D\frac{\partial}{\partial x}W\right) \tag{7}$$

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:

$$W(x, t|x_0, 0) = \frac{1}{Z(t)} \exp\left(-a(t)x^2 + b(t)x\right) \tag{8}$$

Where $a(t)$ and $b(t)$ are the gaussian parameters, and $Z(t)$ the normalization factor. All that's left is to substitute (8) in (7) and solve for a, b, Z.

0.1.1 Equilibrium distribution

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

$$W_{\mathrm{eq}}(x) = \frac{1}{Z}\exp(-\beta V(x)) = \frac{1}{Z}\exp\left(-\frac{m\omega^2 x^2}{2k_B T}\right) \qquad Z = \int_{\mathbb{R}} \exp(-\beta V(x)) \tag{9}$$

Starting from (6) and taking the limit $t \to \infty$:

$$\lim_{t\to\infty} W(x,t|0,0) = \sqrt{\frac{k}{2\pi D}}\exp\left(-\frac{k}{2D}x^2\right) \tag{10}$$

Comparing (9) with (10) 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:

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

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

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

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:

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