Solution: The inertial time scale is controled by $\tau_{\text{inertia}} = I/\zeta$. If it is short, then we can approximation the equation of motion by

$$\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = \boldsymbol{\Gamma}_0 + \boldsymbol{\Gamma}_b \simeq \mathbf{0} \tag{26}$$

with $\boldsymbol{\Gamma}_b = -\zeta\boldsymbol{\Omega} + \boldsymbol{\xi}$. We can they write that

$$\zeta\boldsymbol{\Omega} = \boldsymbol{\Gamma}_0 + \boldsymbol{\xi} \tag{27}$$

and taking the cross product with $\mathbf{u}$ to the right leads to

$$\zeta\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \boldsymbol{\Gamma}_0 \times \mathbf{u} + \boldsymbol{\lambda} \tag{28}$$

with $\boldsymbol{\lambda} = \boldsymbol{\xi} \times \mathbf{u}$ which has correlations

$$\langle \lambda^\mu(t)\lambda^\nu(t)\rangle = C(\mathbf{u}^2\delta^{\mu\nu} - u^\mu u^\nu)\delta(t-t') \tag{29}$$

where C is the amplitude of $\boldsymbol{\xi}$.

7. Assuming one can manipulate $\mathbf{u}$ as if it were a smoothly differentiable function, does your equation respect the $\mathbf{u}^2 = 1$ constraint?

Solution:

8. We now get back to the magnetic problem of interest and consider a magnet with dipole $\mathbf{m} = m_0\mathbf{u}$ in some external field $\mathbf{B}$ (m_0 is fixed). The energy is $V_0 = -\mathbf{m}\cdot\mathbf{B}$. Translational degrees of freedom are not included in the description. Express $\boldsymbol{\Gamma}_0$ in terms of $\mathbf{m}$ and $\mathbf{B}$.

Solution: We have $\boldsymbol{\Gamma}_0 = \mathbf{m} \times \mathbf{B}$.

3 Stochastic Calculus

3.1 Differential calculus likes Stratonovich discretization

Consider a Langevin equation $\frac{\mathrm{d}x}{\mathrm{d}t} = A + B\xi$, where ξ is a Gaussian white noise with correlations $\langle\xi(t)\xi(t')\rangle = \delta(t-t')$. The multiplicative noise B is understood with the α discretization rule, namely according to

$$\Delta x = x(t+\Delta t) - x(t) = A(x(t)+\alpha\Delta x)\Delta t + B(x(t)+\alpha\Delta x)\Delta\xi,\ \Delta\xi = \int_t^{t+\Delta t}\mathrm{d}t'\xi(t') \tag{30}$$

In the above equation, in the rhs, the first term is of order Δt while the second one is of order $\sqrt{\Delta t}$.

1. Justify the above statement and show that an equivalent discretization reads

$$\Delta x = B(x(t))\Delta\xi + (A(x(t)\Delta t + \alpha B'(x(t))B(x(t))\Delta\xi^2) + \mathcal{O}(\Delta t^{3/2}) \tag{31}$$

Solution: The variance of $\Delta\xi$ is given by

$$\langle\Delta\xi^2\rangle = \int_t^{\Delta t}\int_t^{t+\Delta t} \mathrm{d}s\mathrm{d}s'\delta(s-s') = \Delta t \tag{32}$$

hence $\Delta\xi = O(\sqrt{\Delta t})$. Since x is continuous, $O(A(x(t)+\alpha\Delta x)\Delta t) = O(\Delta t)$. Let's now consider the starting point

$$\begin{aligned}\Delta x =& x(t+\Delta t) - x(t) = A(x(t)+\alpha\Delta x)\Delta t + B(x(t)+\alpha\Delta x)\Delta\xi \\ =& A(x(t))\Delta t + O(\Delta t^{3/2}) + \left(B(x(t)+\alpha\Delta x B'(x(t)+O(\Delta t)\right)\Delta\xi \\ & A(x(t))\Delta t + B(x(t))\Delta\xi + \alpha B'\Delta x\Delta\xi\end{aligned} \tag{33}$$

with

$$\Delta x\Delta\xi = B(x(t))\Delta\xi^2 + O(\Delta t^{3/2}) \tag{34}$$

so that

$$\Delta x = A(x(t))\Delta t + \alpha B'B\Delta\xi^2 + B(x(t))\Delta\xi \tag{35}$$

2. Let $x \mapsto f(x)$ be an arbitrary function. Let $F(t) = f(x(t))$. Show that $\Delta F = F(t+\Delta t) - F(t)$ can be expressed as

$$\Delta F = B\Delta\xi f'(x(t)) + (A(x(t))\Delta t + \alpha B'(x(t))B(x(t))\Delta\xi^2)f'(x(t)) + \frac{1}{2}B^2(x(t))\Delta\xi^2 f''(x(t)) \tag{36}$$

up to $\mathcal{O}(\Delta t^{3/2})$ terms.

Solution: We consider the difference

$$\Delta F = F(t+\Delta t) - F(t) = f(x+Deltax) - f(x) = \Delta x f'(x) + \frac{1}{2}\Delta x^2 f''(x) + O(\Delta t^{3/2}) \tag{37}$$

and we use the expression of Δx Eq. (**??**) which we substitute into Eq. (36),

$$\begin{aligned}\Delta F =& (A(x(t))\Delta t + \alpha B'B\Delta\xi^2 + B(x(t))\Delta\xi)f'(x) + \frac{1}{2}B^2\Delta\xi^2 f''(x) + O(\Delta t^{3/2}) \\ & B\Delta\xi f'(x) + A\delta t f' + \alpha B'B\Delta\xi^2 f' + \frac{1}{2}B^2\Delta\xi^2 f''(x) + O(\Delta t^{3/2})\end{aligned} \tag{38}$$

3. If regular differential calculus was allowed, one could actually write that $\frac{\mathrm{d}F}{\mathrm{d}t} = f'\frac{\mathrm{d}x}{\mathrm{d}t}$, and hence that $\frac{\mathrm{d}F}{\mathrm{d}t} = f'A + f'B\xi$. Assuming this Langevin equation is written with an α' discretization rule, show that

$$\Delta F = f'B\Delta\xi + f'A\Delta t + \alpha'(f'B)'B\Delta\xi^2 + \mathcal{O}(\Delta t^{3/2}) \tag{39}$$

where all functions are evaluated at time t.

Solution: If $\frac{\mathrm{d}F}{\mathrm{d}t} = f'A + f'B\xi$ is to be understood with some α' discretization rule then this means that

$$\Delta F = f'A(x + \alpha'\Delta x)\Delta t + \alpha' f'B(x + \alpha'\Delta x)\Delta\xi + O(\Delta t^{3/2}) \tag{40}$$

which, after expanding, leads to

$$\Delta F = f'A(x)\Delta t + \alpha'\left[f'B + \alpha'\Delta x(f'B)'\right]\Delta\xi + O(\Delta t^{3/2}) \tag{41}$$

and using again that $\Delta x\Delta\xi = B\Delta\xi^2 + O(\Delta t^{3/2})$ we arrive at

$$\Delta F = f'B\Delta\xi + f'A\Delta t + \alpha'(f'B)'B\Delta\xi^2 + \mathcal{O}(\Delta t^{3/2}) \tag{42}$$

4. What are the conditions on α and α' for the two expressions found in **2** and **3** for ΔF to match, irrespective of the function f?

Solution: For the two expressions to match we need to identify the two expressions:

$$B\Delta\xi f' + A\delta t f' + \alpha B'B\Delta\xi^2 f' + \frac{1}{2}B^2\Delta\xi^2 f'' = f'B\Delta\xi + f'A\Delta t + \alpha'(f'B)'B\Delta\xi^2 \tag{43}$$

that is

$$\alpha B'Bf' + \frac{1}{2}B^2 f'' - \alpha'(f'B)'B = 0 \tag{44}$$

which must be true for any function f. This enforces $\alpha B'Bf' - \alpha' B'B = 0$, that is $\alpha = \alpha'$, along with $\frac{1}{2}B^2 f'' - \alpha' f'' B^2 = 0$, which enforces $\alpha' = \frac{1}{2}$. Altogether we must have $\alpha = \alpha' = \frac{1}{2}$.

5. Why is it legitimate to use differential calculus when working with the Stratonovich convention?

Solution: This is exactly the translation of the previous reasoning. Regardless of the fact that none of the functions we manipulate are actually differentiable, if the $\alpha = \frac{1}{2}$ dicretization is used, the rules of differential calculus still formally hold. No other $\alpha \neq \frac{1}{2}$ discretization would work.

3.2 How "natural" is Stratonovich calculus?

In physics, a Langevin equation is always the result of a series of approximations. An obvious approximation is the existence of a diffusive limit, in which the typical length scale governing the evolution of the system is larger than the scale involved in its various changes throughout time (the size of the jump is smaller than the typical size of the process). But even before that diffusive limit, lies the Markov approximation, which is based on the separation of time scales between the (fast) ones characterizing the bath and entering the source of noise, and the (slow) ones related to the system of interest whose degrees of freedom are modeled. In the limit where memory effects induced by the time-correlations of the bath can be discarded, one gets a Markov approximation. In this exercise, we want to explore how an evolution equation with a noise displaying time correlations naturally leads, in the limit where these correlations are short-ranged, to a Langevin equation expressed in the Stratonovich discretization. This exercise echoes Sec. **IX.7** of Van Kampen's book [21].

1. Let $\Delta(t) = \frac{1}{2\tau}\mathrm{e}^{-|t|/\tau}$. Show that Δ converges to the δ distribution when $\tau \to 0$. It may be useful to consider $\int \mathrm{d}t\Delta(t)f(t)$ for an arbitrary function f in the $\tau \to 0$ limit.

Solution: Consider $\langle \Delta, f\rangle = \int \mathrm{d}t\Delta(t)f(t) = \frac{1}{2}\int \mathrm{d}y\mathrm{e}^{-|y|}f(y\tau) \to f(0)\frac{1}{2}\int \mathrm{d}y\mathrm{e}^{-|y|} = f(0)$. This shows that $\lim_{\tau\to 0}\Delta = \delta$.

2. Determine $\int_{t_0}^{t_0+\Delta t} \mathrm{d}s\mathrm{d}s'\Delta(s-s')$ at finite τ for t_0 and $\Delta > 0$ that are fixed. Determine the asymptotic behavior of that quantity in the $\tau \to 0$ and $\Delta t \to 0$ limits. Discuss the importance of the order of limits.

Solution: We find that

$$\int_{t_0}^{t_0+\Delta t} \mathrm{d}s\mathrm{d}s'\Delta(s-s') = \Delta t - \tau\left(1-\mathrm{e}^{-\Delta t/\tau}\right) \tag{45}$$

so that

$$\lim_{\tau\to 0}\lim_{\Delta t\to 0}\int_{t_0}^{t_0+\Delta t} \mathrm{d}s\mathrm{d}s'\Delta(s-s') \simeq \frac{\Delta t^2}{2\tau},\quad \lim_{\Delta t\to 0}\lim_{\tau\to 0}\int_{t_0}^{t_0+\Delta t} \mathrm{d}s\mathrm{d}s'\Delta(s-s') \simeq \Delta t \tag{46}$$

These limits do not commute.

Let $x(t)$ be a function evolving according to the following equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = A(x(t)) + B(x(t))\eta(t) \tag{47}$$

where η is a Gaussian process with time correlations $\langle \eta(t)\eta(t')\rangle = \Delta(t-t')$. Here A and B are arbitrary smooth functions of x.

3. Let $\Delta x = x(t_0+\Delta t)-x(t_0)$ for $\Delta t > 0$, t_0 and $x(t_0) = x_0$ being given. Explain why, at fixed $\tau > 0$, the process $x(t)$ remains a smoothly differentiable function (a physicist's argument would be to show that Δx is of order Δt, instead of being of order $\sqrt{\Delta t}$ in a standard Langevin equation).

Solution: The ratio $\frac{\Delta x}{\Delta t}$ is finite as $\Delta t \to 0$, because (choosing t_0 for convenience)

$$\Delta x = \int_0^{\Delta t} A(x(t'))\mathrm{d}t' + \int_0^{\Delta t} B(x(t'))\eta(t')\mathrm{d}t' \simeq A(x(0))\Delta t + B(x(0))\int_0^{\Delta t} \mathrm{d}t'\eta(t') \tag{48}$$

and thus, taking the square and averaging, leads to $\langle \Delta x^2\rangle$ of order Δt^2 (due to the result in the previous question). Hence, the typical scale of Δx is Δt.

4. Prove that $\lim_{\Delta t\to 0}\lim_{\tau\to 0}\frac{\langle \Delta x\rangle}{\Delta t} = A(x_0) + \frac{1}{2}B'(x_0)B(x_0)$.

Solution: We have seen that Δx is at worst of order $\sqrt{\Delta t}$. We start from $\Delta x(t) = \int_0^{\Delta t} A(x(t'))\mathrm{d}t' + \int_0^{\Delta t} B(x(t'))\eta(t')\mathrm{d}t' \simeq A(x(0))\Delta t + B(x(0))\int_0^{\Delta t}\mathrm{d}t'\eta(t')$ which we expand to linear order in τ

$$\begin{aligned}
\Delta x =& \int_0^{\Delta t} A(x_0+\Delta x(t'))\mathrm{d}t' + \int_0^{\Delta t} B(x_0+\Delta x(t'))\eta(t')\mathrm{d}t' \\
\simeq& A(x(0))\Delta t \\
&+ \int_0^{\Delta t}\mathrm{d}t'\eta(t')\left[B(x_0) + \int_0^{t'}\mathrm{d}t'' B'(x(t''))(A(x(t'')) + B(x(t''))\eta(t''))\right] \\
\langle \Delta x\rangle =& A(x_0)\Delta t + B'(x_0)B'(x_0)\int_0^{\Delta t}\mathrm{d}t'\int_0^{t'}\mathrm{d}t''\langle \eta(t')\eta(t'')\rangle \\
=& (A(x_0) + B'(x_0)B'(x_0)/2)\Delta t
\end{aligned} \tag{49}$$

We have used that as $\tau \to 0$ the average $\int_0^{\Delta t}\mathrm{d}t'\int_0^{t'}\mathrm{d}t''\langle \eta(t')\eta(t'')\rangle$ behaves as $\frac{1}{2}\Delta t$. At finite τ however, the latter average is of order Δt^2.

5. Consider the α discretized Langevin equation $\dot{x} = A + B\eta$ where η is a white (delta correlated) noise. How should we choose α in order to recover the predictions of Eq. (47) in the $\tau \to 0$ limit?

3.3 Playing around with stochastic calculus

We consider a particle with position $\mathbf{r}$ evolving under the action of an external force field $\mathbf{F}(\mathbf{r})$ in contact with a thermal bath at temperature T:

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{F} + \sqrt{2T}\boldsymbol{\eta} \tag{50}$$

where the space components $\eta^\mu(t)$ of $\boldsymbol{\eta}$ are independent white noises with unit variance: $\langle \eta^\mu(t)\eta^\nu(t')\rangle = \delta^{\mu\nu}\delta(t-t')$.

1. Let $W(t) = \int_0^t \mathrm{d}t \mathbf{F}\cdot\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}$. What is the direct physical meaning of W? Explain in what sense W is the work exerted by the particle on its surrounding thermostat.

   Solution: The Langevin equation expresses a balance betwwen the external force field $\mathbf{F}$ and the force exerted by the bath on the particle, which is $-\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}+\sqrt{2T}\boldsymbol{\eta}$ (after setting the mobility to unity), so that $-(-\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}+\sqrt{2T}\boldsymbol{\eta}) = \mathbf{F}$ is the force of the particle on the bath, hence the interpretation of W being the work exerted by the particle on its surrounding thermostat.

2. Write a stochastic evolution for W (aka Langevin equation) that couples to $\mathbf{r}$. If you did it right, this equation features a multiplicative noise. Write the equation in both the Ito and the Stratonovich forms.

   Solution: We know that the rules of differential calculus only apply if Langevin equations are understood in a Stratonovich sense. Hence we start from $\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{F}+\sqrt{2T}\boldsymbol{\eta}$ Stratonovich-discretized (of course, at he level of this equation, it does not really matter, all discretizations are equivalent). Then we write that

   $$\frac{\mathrm{d}W}{\mathrm{d}t} = \mathbf{F}\cdot\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{F}^2+\sqrt{2T}\mathbf{F}\cdot\boldsymbol{\eta} \tag{51}$$

   which is Stratonovich-discretized. We may now determine the first moment of $\Delta W = W(t+\Delta t)-W(t)$:

   $$\begin{aligned}\Delta W =&[\mathbf{F}(\mathbf{r}+\Delta\mathbf{r}/2)]^2\Delta t+\sqrt{2T}\mathbf{F}(\mathbf{r}+\Delta\mathbf{r}/2)\cdot\Delta\boldsymbol{\eta}\\ =&[\mathbf{F}(\mathbf{r})]^2\Delta t+\sqrt{2T}\mathbf{F}(\mathbf{r})\cdot\Delta\boldsymbol{\eta}+\sqrt{2T}\frac{1}{2}\partial_\mu F^\nu(\mathbf{r})\Delta r^\mu\Delta\eta^\nu+O(\Delta t^{3/2}\\ =&[\mathbf{F}(\mathbf{r})]^2\Delta t+\sqrt{2T}\mathbf{F}(\mathbf{r})\cdot\Delta\boldsymbol{\eta}+\sqrt{2T}\frac{1}{2}\partial_\mu F^\nu(\mathbf{r})(F^\mu\Delta t+\sqrt{2T}\Delta\eta^\mu)\Delta\eta^\nu+O(\Delta t^{3/2}\end{aligned} \tag{52}$$

   so that we arrive at $\lim_{\Delta t\to 0}\frac{\langle\Delta W\rangle}{\Delta t} = \mathbf{F}^2+T\boldsymbol{\nabla}\cdot\mathbf{F}$. Hence, in its Itō form, the Langevin equation for W reads

   $$\frac{\mathrm{d}W}{\mathrm{d}t} = \mathbf{F}^2+T\boldsymbol{\nabla}\cdot\mathbf{F}+\sqrt{2T}\mathbf{F}\cdot\boldsymbol{\eta} \tag{53}$$

3. Let $\mathscr{V} = \frac{\mathbf{r}^2}{2}$. Write a stochastic evolution for $\mathscr{V}$ that couples to $\mathbf{r}$. Write the equation in both the Itō and the Stratonovich forms. From this equation deduce that the pressure of an ideal gas of N identical Langevin particles is $P = NT/V$. (Hint: Think of the

particle being trapped in a closed box of volume V and of $\mathbf{F}$ as being the force exerted by the wall.

Solution: It may not appear at first sight, but the quantity $\mathscr{V}$ is the stochastic overdamped analog of the virial $\mathbf{r}\cdot\mathbf{p}$ in Hamiltonian or underdamped dynamics. We proceed just as before to obtain a Stratonovich discretized equation,

$$\frac{\mathrm{d}\mathscr{V}}{\mathrm{d}t}=\mathbf{F}\cdot\mathbf{r}+\sqrt{2T}\mathbf{r}\cdot\boldsymbol{\eta} \tag{54}$$

and in the Itō-discretized version this becomes

$$\frac{\mathrm{d}\mathscr{V}}{\mathrm{d}t}=\mathbf{F}\cdot\mathbf{r}+dT+\sqrt{2T}\mathbf{r}\cdot\boldsymbol{\eta} \tag{55}$$

Indeed,

$$\begin{aligned}\Delta\mathscr{V}=&\mathbf{F}(\mathbf{r}+\Delta\mathbf{r}/2)\cdot(\mathbf{r}+\Delta\mathbf{r}/2)\Delta t+\sqrt{2T}(\mathbf{r}(t)+\Delta\mathbf{r}/2)\cdot\Delta\boldsymbol{\eta}\\ =&\mathbf{F}(\mathbf{r})\cdot\mathbf{r}\Delta t+\sqrt{2T}\mathbf{r}\cdot\boldsymbol{\eta}+\frac{1}{2}\sqrt{2T}\Delta\mathbf{r}\cdot\Delta\boldsymbol{\eta}+O(\Delta t^{3/2})\\ =&\mathbf{F}(\mathbf{r})\cdot\mathbf{r}\Delta t+\sqrt{2T}\mathbf{r}\cdot\boldsymbol{\eta}+\frac{1}{2}\sqrt{2T}(\mathbf{F}\Delta t+\sqrt{2T}\Delta\boldsymbol{\eta})\cdot\Delta\boldsymbol{\eta}+O(\Delta t^{3/2})\end{aligned} \tag{56}$$

so that

$$\lim_{\Delta t\to 0}\frac{\langle\Delta\mathscr{V}\rangle}{\Delta t}=\frac{1}{2}\sqrt{2T}^2\frac{\langle\Delta\boldsymbol{\eta}\cdot\Delta\boldsymbol{\eta}\rangle}{\Delta t}=dT \tag{57}$$

where d is the number of space dimensions. In the steady-state, we thus have that

$$\langle\mathbf{F}\cdot\mathbf{r}\rangle=-dT \tag{58}$$

One way to proceed is to write a bit loosely that

$$\langle\mathbf{F}\cdot\mathbf{r}\rangle=\int(-P\mathrm{d}^2\mathbf{S}\cdot\mathbf{r})=\int\boldsymbol{\nabla}\cdot(P\mathbf{r})\mathrm{d}^3r=dPV \tag{59}$$

and then we have that $PV=T$, where V is the volume occupied by one particle. For N particles, this becomes $PV=NT$. More rigorously, if $\mathbf{F}=\mathbf{F}_w=-\boldsymbol{\nabla}U_w$, where U_w is the repulsive potential exerted by the wall on the particle, then

$$\langle\mathbf{F}_w\cdot\mathbf{r}\rangle=-\int\mathrm{d}^3r\boldsymbol{\nabla}U_w\cdot\mathbf{r}p(\mathbf{r}) \tag{60}$$

where $p(\mathbf{r})$ is the probability to find the particle at location $\mathbf{r}$. Suppose there is a wall à $x=0$ and another one at $x=L$, then $U_w(\mathbf{r})$, where U_w is a steeply repulsive potential with range σ small (with respect to any other relevant length scale, U_w acts in a region of size σ at eachh wall). Then we must have that

$$\begin{aligned}\langle\mathbf{F}\cdot\mathbf{r}\rangle=&-S\int_{-\sigma-L/2}^{-L/2}\mathrm{d}x\frac{\mathrm{d}U}{\mathrm{d}x}xp(x)-S\int_{L/2}^{L/2+\sigma}\mathrm{d}x\frac{\mathrm{d}U}{\mathrm{d}x}xp(x)\\ =&-\int_{-\sigma}^{0}\mathrm{d}x\left(\frac{L}{2}+x\right)\frac{\mathrm{d}U}{\mathrm{d}x}p(x)-\int_0^{\sigma}\mathrm{d}\left(\frac{L}{2}+x\right)\frac{\mathrm{d}U}{\mathrm{d}x}p(x)\\ \simeq&\frac{L}{2}PS\times 2\end{aligned} \tag{61}$$

where $PS = \int \frac{\mathrm{d}U}{\mathrm{d}x} p(x)\mathrm{d}x$ is total the force exerted by the particle on the wall (we have used $L \gg \sigma$). When interactions are taken into account, namely when the force on particle i is $\mathbf{F}_i = \mathbf{F}_{i,w} + \sum_{j\neq i} \mathbf{f}_{j\to i}$ then

$$\begin{aligned} \langle \mathbf{F}_i \cdot \mathbf{r}_i \rangle =& dPV + \sum_{j\neq i} \langle \mathbf{f}_{j\to i} \cdot \mathbf{r}_i \rangle \\ =& dPV + \frac{1}{2} \sum_{j\neq i} \langle \mathbf{f}_{j\to i} \cdot (\mathbf{r}_i - \mathbf{r}_j) \rangle \end{aligned} \tag{62}$$

which is the known as the virial formula for the equation of state (and this can be derived, in equilibrium, directly from the partition function). Here, we have not assumed equilibrium to hold.

4. First consider the conservative case where we have $\mathbf{F} = -\nabla V$ (here V depends on $\mathbf{r}$ only). Write a stochastic evolution for V that couples to $\mathbf{r}$. Write the equation in both the Itō and the Stratonovich forms.

Solution: We find that

$$\frac{\mathrm{d}V}{\mathrm{d}t} \stackrel{\text{Strato}}{=} -(\nabla V)^2 + \sqrt{2T}\nabla V \cdot \boldsymbol{\eta} \stackrel{\text{Itō}}{=} -(\nabla V)^2 + +T\Delta V + \sqrt{2T}\nabla V \cdot \boldsymbol{\eta} \tag{63}$$

and in equilibrium, $\langle (\nabla V)^2 \rangle = T\langle \Delta V \rangle$ can be verified directly from he Boltzmann distribution.

5. Second, consider $\mathbf{F} = -\nabla V + \mathbf{f}$, where the force $\mathbf{f}$ stands for a (possibly time dependent) additional force (like that of an operator performing some action on the system). Between t and $t+\mathrm{d}t$, V varies by $\mathrm{d}V = V(\mathbf{r}(t+\mathrm{d}t)) - V(\mathbf{r}(t))$. Show that it is possible to write $\mathrm{d}V = \delta W + \delta Q$, where $\delta W = \mathbf{f} \cdot \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\mathrm{d}t$. What is the microscopic mechanical meaning of δQ? Does this relationship ring any bell?

Solution: Using the Stratononich discretization, we find that

$$\mathrm{d}V = \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} \cdot \nabla V \mathrm{d}t = (-\mathbf{F} + \mathbf{f}) \cdot \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\mathrm{d}t = \delta Q + \delta W \tag{64}$$

where $\delta Q = -\mathbf{F} \cdot \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\mathrm{d}t$ is the heat received by the system from the thermostat.

3.4 Particle in contact with a thermostat

Our interest goes to a particle with unit mass in contact with a thermostat at temperature T and with friction coefficient γ. The velocity v of the particle evolves according to a Langevin equation

$$\frac{\mathrm{d}v}{\mathrm{d}t} = F \tag{65}$$

where the force F reads $F = -\gamma v + \sqrt{2\gamma T}\xi$, with ξ a Gaussian white noise with correlations $\langle \xi(t)\xi(t')\rangle = \delta(t-t')$. Let $E(t) = \frac{1}{2}v^2(t)$ be the particle's kinetic energy.

1. Write the evolution equation for the probability $p(v,t)$ that the particle has velocity v at time t.

Solution: Fokker-Planck equation for the process :

$$\partial_t p(v,t) = \gamma\partial_v(v(t)p(v,t)) + \gamma T\partial_v^2 p(v,t) \tag{66}$$

2. Write a Langevin equation for $E(t)$ that couples to ξ.

Solution: One possibility is to resort to Ito's lemma:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}E &= v\dot{v} + \gamma T \\ &= -\gamma v^2 + \gamma T + \sqrt{2\gamma T}\xi v\end{aligned} \tag{67}$$

An alternative, which is of course fully equivalent, is to view the Langevin equation

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -\gamma v + \sqrt{2\gamma T}\xi \tag{68}$$

as being Stratonovich discretized (actually, we do not need to specify anything because this is an additive Langevin equation: whether Itō or Stratonovich, the Fokker-Planck equation would be the same). Then, we can use standard differential calculus and thus

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}E &= v\dot{v} \\ &= -\gamma v^2 + \gamma T + \sqrt{2\gamma T}\xi v \\ &= -2\gamma E + 2\sqrt{\gamma T}\sqrt{E}\xi\end{aligned} \tag{69}$$

which is Stratonovich-discretized. This is just as good as the Itō-discretized Langevin equation, in the sense that it has the same physics, in spite of a different vidual appearance.

3. Let t_0 be a given time at which the energy is $E(t_0)$ and let Δt be an infinistesimal time duration. Find $\frac{\langle E(t_0+\Delta t)-E(t_0)\rangle}{\Delta t}$ as a function of γ and of T.

Solution: Given that the mean is linear, one immediately get from the Itō-discretized equation, that

$$\lim_{\Delta t\to 0}\frac{\langle E(t_0+\Delta t)-E(t_0)\rangle}{\Delta t} = \langle\frac{\mathrm{d}}{\mathrm{d}t}E(t)\rangle = -\gamma\langle v^2\rangle + \gamma T \tag{70}$$

If one would have started from the Stratonovich-discretized one, which means in practice that

$$E(t+\Delta t)-E(t) = -2\gamma(E(t)+\frac{1}{2}\Delta E)\Delta t+2\sqrt{\gamma T}(E(t)+\frac{1}{2}\Delta E)^{1/2}\int_t^{t+\Delta t}\xi(s)\mathrm{d}s \tag{71}$$

then we would have found that

$$\begin{aligned}\lim_{\Delta t\to 0}\frac{\langle\Delta E\rangle}{\Delta t} &= -2\gamma E + 2\sqrt{\gamma T}\frac{1}{2}\langle\frac{1}{2\sqrt{E}}\Delta E\int_t^{t+\Delta t}\xi(s)\mathrm{d}s\rangle/\Delta t \\ &= -2\gamma E + 2\sqrt{\gamma T}\frac{1}{2}\sqrt{\gamma T} \\ &= -2\gamma E + \gamma T\end{aligned} \tag{72}$$

This result is of course consistent with the one obtained by a direct application of Itō's lemma (because it basically amounts to re-deriving the formula).

4. What's the stationary value of $\langle v^2\rangle = T$? Was that expected?

Solution: In a stationary equilibrium state, $\frac{\mathrm{d}}{\mathrm{d}t}E(t) = 0$, hence :

$$\langle v^2\rangle = T \tag{73}$$

This was of course expected since this is a statement of the equipartition theorem (when using a unit Boltzmann constant $k_B = 1$).

5. We define $W(t) = \int_0^t \mathrm{d}t\sqrt{2\gamma T}\xi v$. Can you endow W with some physical meaning? In the evolution equation for E found in **2**, not only does $\frac{\mathrm{d}W}{\mathrm{d}t}$ appear, but also some additional contribution the physical meaning of which will be given.

Solution:

The quantity $W(t)$ is the work done by the fluctuating part of the force on the particle by the path throughout its trajectory from time $t=0$ to t. This is the energy injected by the thermostat that balances out the viscous dissipation loss $\int \mathrm{d}t\,(-\gamma v)v$. In an energy balance equation, in the absence of a potential energy contribution, we have that $\mathrm{d}E = \delta Q$, where

$$\delta Q = \int \mathrm{d}t \left(-\gamma v + \sqrt{2\gamma T}\xi\right) v \tag{74}$$

is the work of the force $F_{\mathrm{th}} = -\gamma v + \sqrt{2\gamma T}\xi$ exerted by the thermostat on the particle (which is also the heat received by the particle from the thermostat). In the presence of an external potential $V(x,h)$ that possibly depends on a parameter h, the equation of motion reads

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -\partial_x V + F_{\mathrm{th}} \tag{75}$$

so that, in a Stratonovich-discretized form, $E = \frac{1}{2}v^2 + V$ evolves according to

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \dot{h}\partial_h V + F_{\mathrm{th}}.v \tag{76}$$

when h is time-dependent. The quantity $\delta W = \dot{h}\partial_h V \mathrm{d}t$ is the work exerted by the external operator while $\delta Q = F_{\mathrm{th}}.v\mathrm{d}t$ is the heat exchanged with the thermostat. The first principle of thermodynamics survives down to this stochastic level.

6. We set out to determine the large time behavior of the pdf of W. Write an evolution equation for the probability $p(v,W,t)$ that the particle has velocity v at time t, and that $W(t) = W$.

Solution: As a reminder: if the x_i are random variables evolving according to n coupled Langevin equations, then, denoting by

$$M_1^{(1)} = \lim_{\Delta t\to 0} \frac{\langle \Delta x_i\rangle}{\Delta t},\ M_2^{(ij)} = \frac{1}{2}\lim_{\Delta t\to 0}\frac{\langle \Delta x_i \Delta x_j\rangle}{\Delta t} \tag{77}$$

the corresponding Fokker-Planck equation reads

$$\partial_t p(x_1,\ldots,x_n,t) = -\sum_i \partial_{x_i}(M_1^{(i)}p) + \sum_{i,j}\partial^2_{x_i,x_j}(M_2^{(ij)}p) \tag{78}$$

Hence we only need to determine the average of Δv an ΔW, and of their correlations.

Given

$$\frac{\mathrm{d}}{\mathrm{d}t}W(t) = \sqrt{2\gamma T}v(t)\xi(t) \tag{79}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}v(t) = -\gamma v(t) + \sqrt{2\gamma T}\xi(t) \tag{80}$$

The Kramers-Moyal expansion is :

$$\partial_t p = -\partial_v[M_1^{(v)}p] + \partial_v^2[M_2^{(vv)}p] - \partial_w[M_1^{(w)}p] + \partial_w^2[M_2^{(ww)}p] + 2\partial_v\partial_w[M_2^{(vw)}p] \tag{81}$$

Discretizing :

$$\Delta v = -\gamma v(t)\Delta t + \sqrt{2\gamma T} \underbrace{B_{\Delta t}}_{\sim\mathcal{N}(0,\Delta t)} \tag{82}$$

$$\begin{aligned} \Delta W &= \sqrt{2\gamma T}B_{\Delta t}(v + \frac{\Delta v}{2}) \\ &= \sqrt{2\gamma T}B_{\Delta t}v - \frac{1}{2}\sqrt{2\gamma T}B_{\Delta t}\gamma v\Delta t + \gamma T B_{\Delta t}^2 \end{aligned} \tag{83}$$

Therefore, keeping in mind that $\langle B_{\Delta t}\rangle = 0$ and that $\langle B_{\Delta t}^2\rangle = \Delta t$, we get :

$$M_1^{(w)} = \lim_{\Delta t \to 0} \frac{\langle \Delta W\rangle}{\Delta t} = \gamma T \tag{84}$$

$$M_2^{(ww)} = \lim_{\Delta t \to 0} \frac{1}{2}\frac{\langle \Delta W^2\rangle}{\Delta t} = \gamma T v^2 \tag{85}$$

Moreover :

$$\begin{aligned} \Delta W \Delta v = &-\gamma v \Delta t\sqrt{2\gamma T}B_{\Delta t} + \underbrace{2\gamma T B_{\Delta t}^2 v}_{\mathcal{O}(\Delta t)} + \frac{\gamma v^2 \Delta t^2}{2}\sqrt{2\gamma T}B_{\Delta t} \\ &-\gamma T B_{\Delta t}^2 v\Delta t - \gamma^2 T v \Delta t B_{\Delta t}^2 + \gamma T\sqrt{2\gamma T}B_{\Delta t}^3 \end{aligned} \tag{86}$$

$$M_2^{(vw)} = \lim_{\Delta t \to 0} \frac{1}{2}\frac{\langle \Delta W \Delta v\rangle}{\Delta t} = \gamma T v \tag{87}$$

The Fokker-Planck equation is :

$$\partial_t p = \gamma\partial_v(vp) + \gamma T\partial_v^2 p - \gamma T\partial_w p + 2\gamma T\partial_w\partial_v(vp) + \gamma T\partial_w^2(v^2 p) \tag{88}$$

7. Fourier transform the equation found in **6** with respect to W, and prove that $\hat{p}(v, \lambda, t) =$

$\int \mathrm{d}W \mathrm{e}^{-\lambda W} p(v, W, t)$ evolves according to

$$\partial_t \hat{p} = \text{part with no explicit dependence in } \lambda + \gamma T(\lambda^2 v^2 - \lambda)\hat{p} + 2\gamma T \lambda \partial_v (v\hat{p}) \quad (89)$$

Solution: For $f : w \to f(w)$ locally integrable and for which the integral defining the Laplace transform converges, we have :

$$\mathcal{L}\{f''(w)\} = \lambda^2 \hat{f}(\lambda) - \lambda f(0) - f'(0)$$

Discarding boundary terms, we get :

$$\partial_t \hat{p} = \gamma \partial_v (v\hat{p}) + \gamma T \partial_v^2 \hat{p} - \gamma T \lambda \hat{p} + 2\gamma T \partial_v (v\hat{p}) + \gamma T \lambda^2 v^2 \hat{p} \quad (90)$$

$$\partial_t \hat{p} = \underbrace{\gamma \partial_v (v\hat{p}) + \gamma T \partial_v^2 \hat{p}}_{\text{no explicit dependence in } \lambda} + \gamma T(\lambda^2 v^2 - \lambda)\hat{p} + 2\gamma T \lambda \partial_v (v\hat{p}) \quad (91)$$

8. Prove that $\hat{p}(v, \lambda, t) = \mathrm{e}^{t\psi(\lambda)} \mathrm{e}^{-av^2}$ is a solution. Express both a and ψ in terms of T, γ and λ.

Solution: In this case :

$$\partial_t \hat{p} = \psi(\lambda)\hat{p} \quad (92)$$

$$\partial_v (v\hat{p}) = \hat{p} - 2av^2 \hat{p} \quad (93)$$

$$\partial_v^2 \hat{p} = \partial_v(-2av\hat{p}) = -2a\hat{p} + 4a^2 v^2 \hat{p} \quad (94)$$

$$\psi(\lambda)\hat{p} = [\gamma - 2av\gamma - 2a\gamma T + 4a^2 v^2 \gamma T + \gamma T(\lambda^2 v^2 - \lambda) + 2\gamma T \lambda - 4av\lambda\gamma T]\hat{p} \quad (95)$$

Therefore by identification:

$$\psi(\lambda) = \gamma(1 + 4a^2 T v^2 + T\lambda(1 + v^2 \lambda) - 2a(T + v^2 + 2Tv^2 \lambda)) \quad (96)$$

which is possible only if the v-dependent terms vanish, which in turn enforces that:

$$0 = 4a^2 T + T\lambda^2 - a(2 + 4T\lambda) \quad (97)$$

There are two solutions $a_\pm = \frac{1+2T\lambda \pm \sqrt{1+4T\lambda}}{4T}$, with $\psi_\pm = 1 - 2a_\pm T + T\lambda$. But since $\psi(0) = 0$ we select a_+, and we arrive at:

$$\psi(\lambda) = \frac{1}{2}\left[1 - \sqrt{1 + 4T\lambda}\right] \quad (98)$$

This derivation does not explain why ψ is indeed the largest eigenvalue of the linear operator governing the evolution of $\hat{p}$.

9. Justify that the probability to get a value W at large times behaves as $P(W,t) \simeq \mathrm{e}^{t\pi(W/t)}$, where the function $\pi(w)$ will be related to $\psi(\lambda)$.

Solution: We know that $\hat{p}(v,\lambda,t) = \int dW e^{-\lambda W} p(v,W,t) \sim e^{\psi t - av^2}$ at large times, so that:

$$p(v,W,t) = \int \frac{\mathrm{d}\lambda}{2\pi i} e^{\lambda W} e^{\psi t - av^2} \tag{99}$$

and thus, up to some time-independent prefactor,

$$p(W,t) = \int \frac{\mathrm{d}\lambda}{2\pi i} e^{\lambda W} e^{\psi t} \tag{100}$$

Writing $W = wt$:

$$p(wt,t) = \int \frac{\mathrm{d}\lambda}{2\pi i} e^{t(\lambda w + \psi(\lambda))} \tag{101}$$

and realizing that the λ integral is dominated by λ such that $\lambda w + \psi(\lambda)$ is the largest. The saddle-point approximation then immediately tells us that:

$$p(wt,t) \sim e^{t\pi(w)},\ \pi(w) = \sup_{\lambda}\{\lambda w + \psi(\lambda)\} \tag{102}$$

By solving $\frac{\mathrm{d}}{\mathrm{d}\lambda}[\lambda w + \psi(\lambda)] = 0$, we obtain:

$$\lambda^* = \frac{T}{2w^2} - \frac{1}{4T} \tag{103}$$

So that:

$$\pi(w) = -\frac{(w-T)^2}{4Tw}\Theta(w) \tag{104}$$

10. Qualitatively plot $\pi(w)$ as a function of w. Does this function possess any remarkable symmetry property? Comment on your finding.

Solution:

There is no reason to have any remarkable property for $\pi(w)$, as has been discussed by J. Farago in J. Stat. Phys. **107**, 781 (2002), *Injected Power Fluctuations in Langevin Equation*. We know what the general appearance of π is because it has to be zero at the optimal value of w, which is $\langle w \rangle = -\psi'(0) = T$.

4 The Fokker-Planck Equation