IV. APPLICATIONS OF THE FOKKER-PLANCK EQUATION

We have already encountered many examples in Sec. III of the application of the master equation to processes with discrete configuration space. In this section, we will go back to the Fokker-Planck equation for 'continuous' stochastic dynamics and use it to study a number of phenomena that are intrinsically nonequilibrium. While we will start from the general case, restricting ourselves to 1D will turn out to be very useful as it allows us to obtain exact solutions for the exit time probability and steady-state of the Fokker-Planck equation for arbitrary external potentials. We will study a variety of problems: the first-passage time for the escape of a particle from a bound state, Kramers reaction rate theory, and Brownian ratchets.

A. First-passage time and Kramers rate theory

A very important application of the Fokker-Planck (or Smoluchowski) equation is the slow dynamics of fluctuating systems in metastable states. This has many applications in chemistry and biology, essentially as a 'quasi-microscopic' model for the dynamics of chemical reactions. A typical scenario concerns a particle (temporarily) trapped in a metastable state (local minimum) *behind* a barrier of *finite* height, beyond which states of lower energy will be available. We can ask the question: *how long does it take the particle to escape this potential trap?* The particle is subject to thermal fluctuations, which for a while will keep it jittering about behind the barrier. However, an escape event will occur when one of the random kicks is strong enough to move the particle *over* the potential barrier. The time we have to wait before this happen will depend on the strength of the thermal fluctuations (noise) as well as details of the shape of the potential landscape near the trap. Note that since the barrier is of finite height, the particle will eventually escape, it is just a question of how long before it does.

1. Escape time probability

In order to base the problem in concrete setting, let us consider a particle that is confined in a region R of space, with boundary ∂R, at $t = 0$. The boundary contains a region ∂R_a from which the particle can escape, which can be represented by an *absorbing* boundary condition ($\mathcal{P} = 0$) when solving the Fokker-Planck equation. To study the exit probability, it is convenient to use the backward Fokker-Planck equation Eq. (II.54) for $\mathcal{P}(\boldsymbol{x}', t|\boldsymbol{x}, 0)$, which can be written as

$$\partial_t \mathcal{P}(\boldsymbol{x}', t|\boldsymbol{x}, 0) = \boldsymbol{v}(\boldsymbol{x}) \cdot \boldsymbol{\nabla}\mathcal{P}(\boldsymbol{x}', t|\boldsymbol{x}, 0) + D\boldsymbol{\nabla}^2\mathcal{P}(\boldsymbol{x}', t|\boldsymbol{x}, 0) \quad , \tag{IV.1}$$

since time-translation invariance gives us $\mathcal{P}(\boldsymbol{x}', t|\boldsymbol{x}, 0) = \mathcal{P}(\boldsymbol{x}', 0|\boldsymbol{x}, -t)$. We now define the probability of finding the particle somewhere within the region R at time t, knowing that it was at the position $\boldsymbol{x} \in R$ at $t = 0$, as

$$\mathcal{G}(\boldsymbol{x}, t) = \int_R \mathrm{d}^3\boldsymbol{x}'\, \mathcal{P}(\boldsymbol{x}', t|\boldsymbol{x}, 0) \quad . \tag{IV.2}$$

Since $\mathcal{G}(\boldsymbol{x}, t)$ essentially defines the probability that the exit time is larger than t, we can extract the probability that the exit time is between t and $t+\mathrm{d}t$ as $-\partial_t\mathcal{G}(\boldsymbol{x}, t)\mathrm{d}t$. From its definition, we can deduce that $\mathcal{G}(\boldsymbol{x}, t)$ satisfies the following equation

$$\partial_t\mathcal{G}(\boldsymbol{x}, t) = D\left[-\beta\boldsymbol{\nabla}U(\boldsymbol{x}) \cdot \boldsymbol{\nabla}\mathcal{G}(\boldsymbol{x}, t) + \boldsymbol{\nabla}^2\mathcal{G}(\boldsymbol{x}, t)\right] \quad , \tag{IV.3}$$

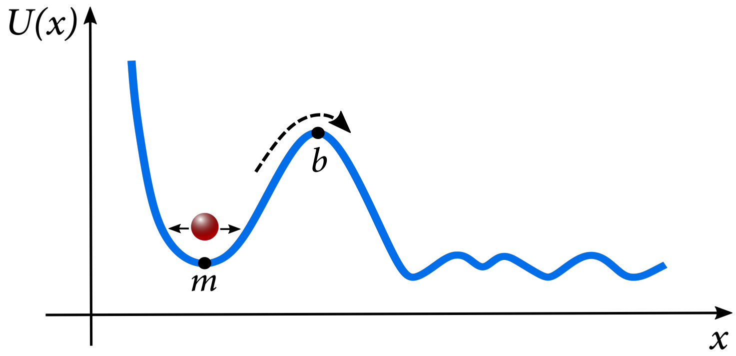

FIG. IV.1 **An activated process.** A particle trapped in a metastable state m behind a barrier b.

where we have used $\boldsymbol{v}(\boldsymbol{x}) = -\mu \boldsymbol{\nabla} U(\boldsymbol{x}) = -D\beta \boldsymbol{\nabla} U(\boldsymbol{x})$, where the Einstein-Stokes relation is used and the inverse temperature $\beta = \dfrac{1}{k_{\mathrm{B}}T}$ is introduced for simplicity. Since $\mathcal{P}(\boldsymbol{x}', 0|\boldsymbol{x}, 0) = \delta^3(\boldsymbol{x}' - \boldsymbol{x})$, the initial condition will be $\mathcal{G}(\boldsymbol{x}, 0) = 1$ for $\boldsymbol{x} \in R$ and $\mathcal{G}(\boldsymbol{x}, 0) = 0$ otherwise. Using the probability, we can calculate the mean exit time, or the *mean first-passage time* as

$$\mathcal{T}(\boldsymbol{x}) = -\int_0^\infty \mathrm{d}t\, t\, \partial_t \mathcal{G}(\boldsymbol{x}, t) = \int_0^\infty \mathrm{d}t\, \mathcal{G}(\boldsymbol{x}, t) \quad , \tag{IV.4}$$

and show that it inherits the following equation

$$-\beta \boldsymbol{\nabla} U(\boldsymbol{x}) \cdot \boldsymbol{\nabla} \mathcal{T}(\boldsymbol{x}) + \boldsymbol{\nabla}^2 \mathcal{T}(\boldsymbol{x}) = -\frac{1}{D} \quad . \tag{IV.5}$$

We have used $\mathcal{G}(\boldsymbol{x}, \infty) = 0$ in the derivation of Eq. (IV.5), since the escape will eventually happen. Equations (IV.3) and (IV.5) will need to be solved with the relevant boundary conditions, namely the vanishing of the fields ($\mathcal{G}$ and $\mathcal{T}$) on ∂R_a and the vanishing of the normal flux on the *reflecting* (impenetrable) parts of ∂R.

In 1D, the problem is considerably simplified as Eq. (IV.5) can be directly integrated for any arbitrary potential. To this end, we start from

$$-\frac{\mathrm{d}}{\mathrm{d}x}(\beta U)\frac{\mathrm{d}\mathcal{T}}{\mathrm{d}x} + \frac{\mathrm{d}^2\mathcal{T}}{\mathrm{d}x^2} = -\frac{1}{D} \quad , \tag{IV.6}$$

and rewrite it as

$$e^{\beta U(x)} \frac{\mathrm{d}}{\mathrm{d}x}\left[e^{-\beta U(x)} \frac{\mathrm{d}\mathcal{T}}{\mathrm{d}x}\right] = -\frac{1}{D} \quad , \tag{IV.7}$$

which can easily be integrated to yield

$$e^{-\beta U(x)} \frac{\mathrm{d}\mathcal{T}}{\mathrm{d}x} - e^{-\beta U(x_0)} \left.\frac{\mathrm{d}\mathcal{T}}{\mathrm{d}x}\right|_{x_0} = -\frac{1}{D}\int_{x_0}^{x} \mathrm{d}x'\, e^{-\beta U(x')} \quad . \tag{IV.8}$$

Now, consider a potential profile $U(x)$ of the form shown in Figure IV.1. that diverges as $x \to -\infty$ (forming an impenetrable barrier to the left), and has a *metastable* state m with (minimum) potential energy $U(m)$ which is 'confined' by a barrier b of height $U(b) - U(m)$ (the potential energy at the top of the barrier is $U(b)$). We can solve Eq. (IV.8) for such a profile to calculate $\mathcal{T}(m)$, using the boundary

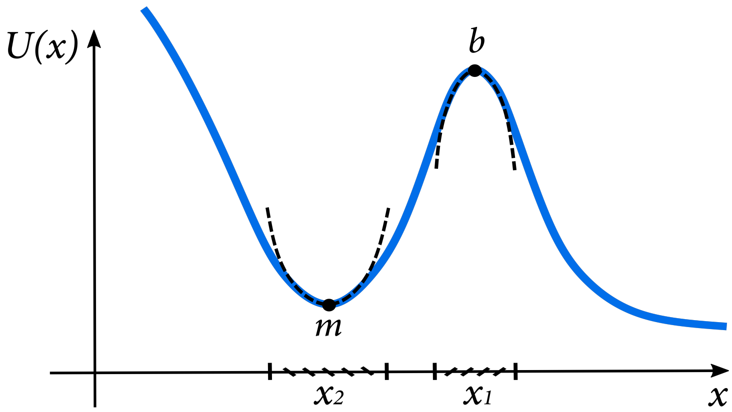

FIG. IV.2 **Kramers theory.** The potential well and the barrier are approximated by parabolas.

conditions

$$\left.\frac{\mathrm{d}\mathcal{T}}{\mathrm{d}x}\right|_{x\to-\infty} = 0 \quad [\text{not necessary since } U|_{x\to-\infty}\to\infty] \quad , \qquad\qquad \mathcal{T}(f) = 0 \quad , \tag{IV.9}$$

where f is a point beyond the barrier b where we can consider the particle to be completely absorbed by the right-hand-side lower energy states. This gives us the mean first-passage (mfp) time for the escape of a particle located initially at $x = m$, as

$$\mathcal{T}_{\mathrm{mfp}} = \mathcal{T}(m) = \frac{1}{D}\int_m^f \mathrm{d}x_1\, e^{\beta U(x_1)} \int_{-\infty}^{x_1} \mathrm{d}x_2\, e^{-\beta U(x_2)} \quad . \tag{IV.10}$$

Other boundary conditions, for example a metastable state with finite barriers on both sides, can be treated similarly.

2. The Kramers rate theory

The result we found for the mean first passage time [Eq. (IV.10)] can be further simplified if the potential barrier is a sharp peak.

Following Kramers, we note that if the variation of the potential $U(x)$ in the region of the barrier is large compared to $k_{\mathrm{B}}T$, then $e^{\beta U(x_1)}$ is sharply peaked around $x_1 = b$ while $e^{-\beta U(x_2)}$ is very small near $x_2 = b$. Hence, the integral $\int_{-\infty}^{x_1} \mathrm{d}x_2\, e^{-\beta U(x_2)}$ is a slowly varying function of x_1 around $x_1 = b$, which means that its value will be nearly constant in the region where $e^{\beta U(x_1)}$ is significantly different from zero. Therefore, we can set the upper limit of the x_2 integral in Eq. (IV.10) to b rather than x_1. Conversely, $e^{-\beta U(x_2)}$ is sharply peaked near $x = m$.

From these observations, we infer that the integral $\int_m^f \mathrm{d}x_1\, e^{\beta U(x_1)}$ will be dominated by the region close to $x_1 = b$ where it is strongly varying, while the integral $\int_{-\infty}^b \mathrm{d}x_2\, e^{-\beta U(x_2)}$ will be dominated by the region close to $x_2 = m$ where it is varying strongly. We can thus approximate the potential by its behaviour around its dominant parts: the maximum b where $\left.\frac{\mathrm{d}U}{\mathrm{d}x}\right|_b = 0$ and the minimum m, where

$\left.\frac{\mathrm{d}U}{\mathrm{d}x}\right|_m = 0$ as Fig. IV.2 demonstrates. We have

$$U(x_2) \;\approx\; U(m) + \frac{1}{2}U''(m)(x_2-m)^2 \quad ; \quad U''(m) = \left.\frac{\mathrm{d}^2U}{\mathrm{d}x^2}\right|_m > 0\,, \tag{IV.11}$$

$$U(x_1) \;\approx\; U(b) - \frac{1}{2}|U''(b)|(x_1-b)^2 \quad ; \quad U''(b) = \left.\frac{\mathrm{d}^2U}{\mathrm{d}x^2}\right|_b < 0\,. \tag{IV.12}$$

We can now write the mean first-passage time as

$$\mathcal{T}_{\mathrm{mfp}} \simeq \frac{1}{D}\,\lambda_1\,\lambda_2 \quad , \tag{IV.13}$$

where

$$\lambda_2 \;=\; \int_{-\infty}^{b} \mathrm{d}x_2\; e^{-\beta U(x_2)} \;\simeq\; e^{-\beta U(m)} \int_{-\infty}^{\infty} \mathrm{d}x_2\; e^{-\frac{1}{2}\beta U''(m)(x_2-m)^2} \tag{IV.14}$$

$$\Rightarrow \quad \lambda_2 \;\simeq\; \sqrt{\frac{2\pi}{\beta U''(m)}}\; e^{-\beta U(m)} \quad , \tag{IV.15}$$

and

$$\lambda_1 \;=\; \int_{m}^{f} \mathrm{d}x_1\; e^{\beta U(x_1)} \;\simeq\; e^{\beta U(b)} \int_{-\infty}^{\infty} \mathrm{d}x_1\; e^{-\frac{1}{2}\beta |U''(b)|(x_1-b)^2} \tag{IV.16}$$

$$\Rightarrow \quad \lambda_1 \;\simeq\; \sqrt{\frac{2\pi}{\beta |U''(b)|}}\; e^{\beta U(b)} \quad . \tag{IV.17}$$

Putting them altogether, we obtain the *Kramers escape time*:

$$\mathcal{T}_{\mathrm{K}} = \mathcal{T}_{\mathrm{mfp}} = \frac{2\pi\zeta}{\sqrt{U''(m)|U''(b)|}}\; e^{\beta[U(b)-U(m)]} \quad , \tag{IV.18}$$

where we have used the Einstein-Stokes relation. We see the familiar Arrhenius form of the exponential dependence of the escape time on the height of the potential barrier multiplied by a prefactor called *the inverse attempt frequency*, which takes account of the number of states around the metastable minimum from which the particle will begin and the width of the barrier over which it has to jump.

Kramers theory can be used to calculate reaction rates from a more 'microscopic picture' where x corresponds to an approximate one dimensional *reaction coordinate* as discussed earlier. The reaction rate is simply the inverse of the Kramers escape time. Since the one dimensional trajectory is an approximation, it is not really a microscopic description. A complete description of such a truly microscopic model, which will correspond to random motion in a potential in a very high dimensional space, is an active area of current research.

B. Brownian ratchets and rectification of stochastic motion

The nonequilibrium dynamics of particles moving in a periodic potential is a very important class of stochastic dynamical systems, which can be used to model the dynamics of a variety of physical systems. For example, we can consider the dynamics of molecular motors on a protein filament track that provides a periodic template (which can be approximately modelled as a potential) on which the motor moves. As in the previous section, restricting ourselves to 1D will allow us to have an in-depth study of these problems, due to the existence of exact results.

1. Stationary solution of 1D Fokker-Planck equation

We start with the Fokker-Planck equation for a particle moving in a potential $U(\boldsymbol{x})$, namely

$$\partial_t \mathcal{P}(\boldsymbol{x},t) + \boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x},t) = 0 \quad , \tag{IV.19}$$

where the probability flux is given by

$$\boldsymbol{J}(\boldsymbol{x},t) = -D\beta\boldsymbol{\nabla}U(\boldsymbol{x})\,\mathcal{P}(\boldsymbol{x},t) - D\boldsymbol{\nabla}\mathcal{P}(\boldsymbol{x},t) \qquad . \tag{IV.20}$$

In the stationary state, the Fokker-Planck equation simplifies to

$$\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x}) = 0 \quad , \tag{IV.21}$$

which in one dimension reduces to

$$\frac{\mathrm{d}}{\mathrm{d}x}J(x) = 0 \quad \Rightarrow \quad J(x) = \text{constant} \quad . \tag{IV.22}$$

Consequently, we can write Eq. (IV.20) as

$$J = -D\left[\frac{\mathrm{d}}{\mathrm{d}x}(\beta U)\,\mathcal{P}(x) + \frac{\mathrm{d}\mathcal{P}}{\mathrm{d}x}\right] = -D\,e^{-\beta U(x)}\,\frac{\mathrm{d}}{\mathrm{d}x}\left[e^{\beta U(x)}\,\mathcal{P}(x)\right] \quad , \tag{IV.23}$$

which can easily be integrated to yield

$$-\frac{J}{D}\int_{x_0}^{x}\mathrm{d}x'\;e^{\beta U(x')} = e^{\beta U(x)}\;\mathcal{P}(x) - e^{\beta U(x_0)}\mathcal{P}(x_0) \quad . \tag{IV.24}$$

This is a general (exact) stationary solution to the Fokker-Planck equation for a particle in an arbitrary potential $U(x)$. It can be rearranged to obtain an explicit expression for the steady-state probability density at an arbitrary position x as

$$\mathcal{P}(x) = \mathcal{P}(x_0)\,e^{-\beta[U(x)-U(x_0)]} - \frac{J}{D}\,e^{-\beta U(x)}\int_{x_0}^{x}\mathrm{d}x'\;e^{\beta U(x')} \quad . \tag{IV.25}$$

The solution is characterized by two constants: the steady-state current J, and the probability density at one particular position $\mathcal{P}(x_0)$. They will be specified by the boundary conditions of the particular problem being studied. The equilibrium solution corresponds to the special case $J = 0$.

2. The tilting ratchet

Let us now consider a periodic potential $W(x)$ with a repeat distance L (as shown in Figure IV.3) such that

$$W(x+L) = W(x) \quad . \tag{IV.26}$$

In the stationary state we can use the general solution Eq. (IV.25) to obtain the probability density profile under the influence of the periodic potential $U(x) = W(x)$. The periodicity of the potential necessarily implies that in the stationary state of the probability profile will also be periodic, i.e.

$$\mathcal{P}(x+L) = \mathcal{P}(x) \quad . \tag{IV.27}$$

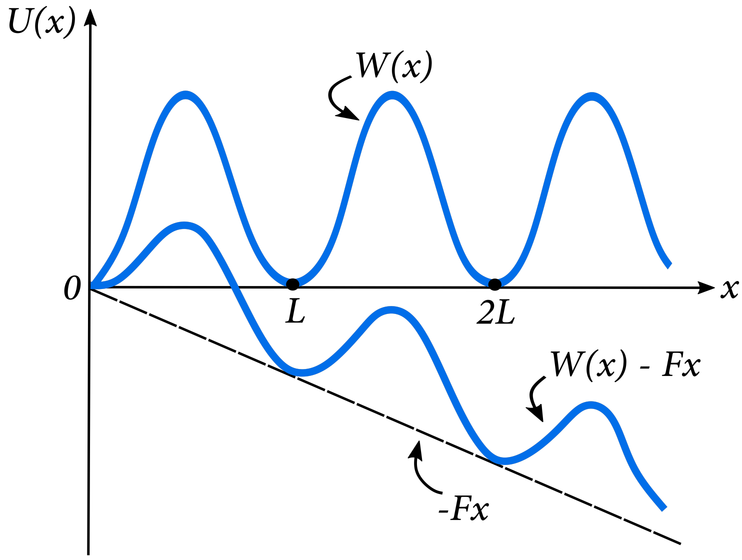

FIG. IV.3 **Tilted potential.** (a) A periodic potential $W(x)$ with repeat period L. (b) The periodic potential tilted by an external force F.

It is easy to see that putting in Eqs. (IV.26) and (IV.27) in the general solution Eq. (IV.25), and choosing $x - x_0 = L$, leads to the conclusion that $J = 0$. This means that for a periodic potential, the stationary state is the equilibrium state where

$$\mathcal{P}(x) = \mathcal{P}_{\rm eq}(x) \propto e^{-\beta W(x)} \quad . \tag{IV.28}$$

However by applying a bias on the system, such as an external force, we can drive it away from equilibrium. A constant applied force F which changes the potential to

$$U(x) = W(x) - F\,x \quad , \tag{IV.29}$$

tilts the energy landscape and puts a bias on the diffusion of the particles in the direction of the applied force.

Now the bias in the in the energy landscape does not change the periodicity of the problem so that the steady-state profile, $\mathcal{P}_F(x)$, in the tilted problem will necessarily remain periodic, i.e.

$$\mathcal{P}_F(x+L) = \mathcal{P}_F(x) \quad . \tag{IV.30}$$

Now, it is straightforward to show that Eq. (IV.25) necessitates a nonzero current.

To calculate the probability profile $\mathcal{P}_F(x)$, we evaluate Eq. (IV.25) for two points separated by L, e.g x and $x + L$:

$$\begin{aligned} \mathcal{P}_F(x+L) &= \mathcal{P}_F(x)\, e^{-\beta[W(x+L)-F\,x-F\,L-W(x)+F\,x]} \\ &\quad -\frac{J}{D}\, e^{-\beta[W(x+L)-F\,x-F\,L]} \int_x^{x+L} \mathrm{d}x_1\; e^{\beta[W(x_1)-F\,x_1]} \quad . \end{aligned} \tag{IV.31}$$

Now using Eqs. (IV.30), (IV.29), and (IV.26), this can be simplified to give

$$\mathcal{P}_F(x) = \frac{J}{D}\, \frac{e^{-\beta[W(x)-F\,x]}}{(1-e^{-\beta F\,L})} \int_x^{x+L} \mathrm{d}x_1\; e^{\beta[W(x_1)-F\,x_1]} \quad . \tag{IV.32}$$

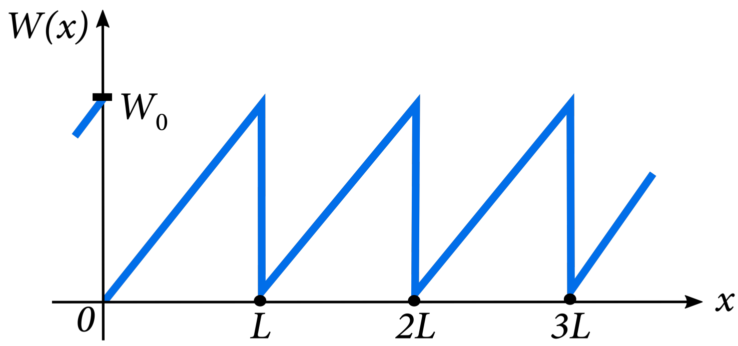

FIG. IV.4 **Sawtooth potential.** A piece-wise constant-slope periodic potential with repeat period L.

This can be used to calculate the average escape time of a particle from one well to the next.

Without loss of generality we consider the mean escape time $T_{\rm esc}$ from the region $[0,L)$ to the region $[L,2L)$. First, we note that in order to calculate that we must initially have the particle in the region $x\in[0,L)$. To ensure that, we assume that on average there is one particles per period, such that

$$\int_0^L \mathrm{d}x\,\mathcal{P}_F(x)=1 \quad\Rightarrow\quad T_{\rm esc}\equiv\frac{1}{J}=\frac{1}{D}\int_0^L \mathrm{d}x\;\frac{e^{-\beta[W(x)-F\,x]}}{(1-e^{-\beta F\,L})}\int_x^{x+L}\mathrm{d}x_1\;e^{\beta[W(x_1)-F\,x_1]}\quad . \tag{IV.33}$$

Consequently, the average drift velocity of the particles is found as

$$v_{\rm drift}\equiv\frac{L}{T_{\rm esc}}=J\,L\quad , \tag{IV.34}$$

which reads

$$v_{\rm drift}(F)=\frac{DL\left(1-e^{-\beta F\,L}\right)}{\displaystyle\int_0^L \mathrm{d}x\;e^{-\beta[W(x)-F\,x]}\int_x^{x+L}\mathrm{d}x_1\;e^{\beta[W(x_1)-F\,x_1]}}\quad . \tag{IV.35}$$

This general result applies to any arbitrary periodic potential $W(x)$, tilted by a force F. Note that the drift velocity in Eq. (IV.35) vanishes for $F=0$ as required by the equilibrium condition of zero current. The sign of the drift velocity is also determined by the sign of the external force F. However, $v_{\rm drift}(F)$ is a highly nonlinear function of F. It is of particular interest (there are many applications as we will see later) when the the underlying periodic potential $W(x)$ is *asymmetric*.

It is instructive to analyze the problem for a simple and computationally tractable *asymmetric* potential. A particularly nice example is the *sawtooth* periodic potential :

$$W(x)=\frac{W_0}{L}\,(x-n\,L)\quad ;\quad nL\le x<(n+1)L\quad , \tag{IV.36}$$

where n is any integer.

To be concrete we can calculate the probability profile for $n=0$, i.e. for $x\in[0,L)$.

$$\mathcal{P}_F(x)=\frac{JL}{D\beta(W_0-FL)}\left[\left(\frac{1-e^{-\beta W_0}}{1-e^{-\beta FL}}\right)e^{\beta(W_0/L-F)(L-x)}-1\right]\quad , \tag{IV.37}$$

for $(0\le x<L)$, with the same probability density profile repeated for $x\in[L,2L)$ (with $x\to x-L$), and similarly for every subsequent period (domain) L.

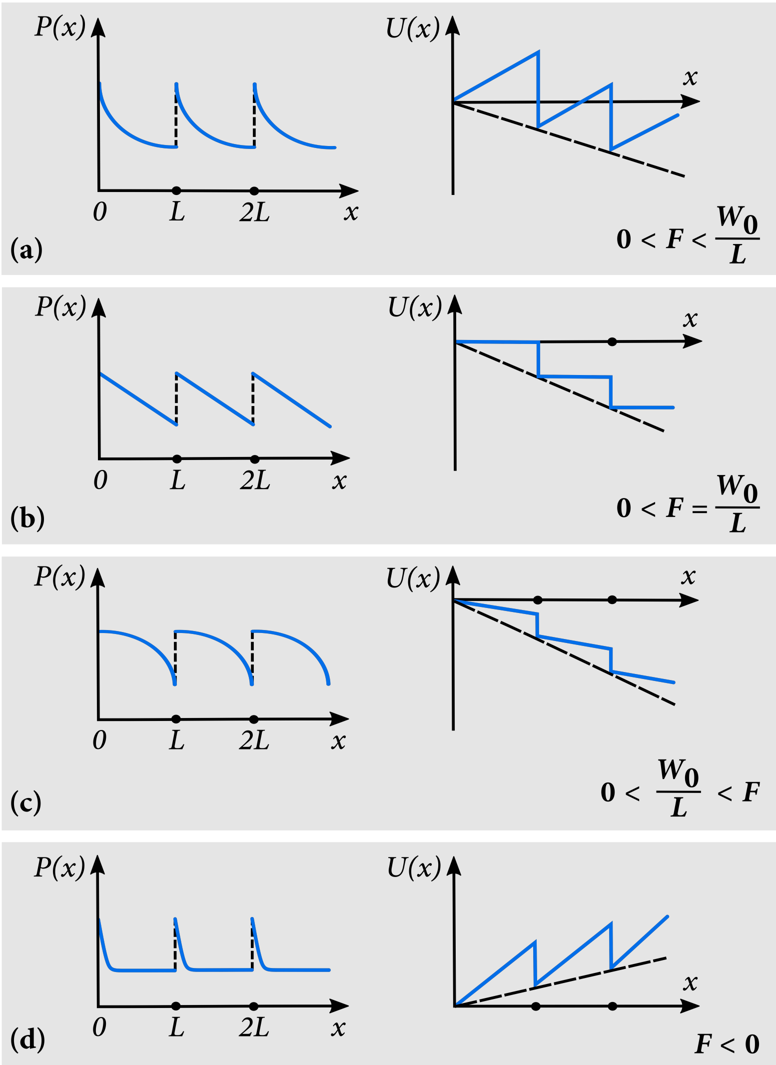

FIG. IV.5 **Stationary probability profiles.** The probability density profile for a particle diffusing in a tilted (by force F) sawtooth periodic potential with repeat period L for varying values of F. (a) $0 < F < W_0/L$, (b) $F = W_0/L$, (c) $0 < W_0/L < F$, and (d) $F = -|F| < 0$.

Depending on the value of the force, we can classify four different regimes of behaviour.

(a) When $0 < F < W_0/L \Rightarrow W_0 - FL > 0$, and $e^{-\beta W_0} < e^{-\beta FL}$ then

$$\mathcal{P}_F(x) = \frac{JL}{D\beta(W_0 - FL)} \left[\underbrace{\left(\frac{1 - e^{-\beta W_0}}{1 - e^{-\beta FL}}\right)}_{>1} \underbrace{e^{\beta(W_0 - FL)}}_{>1} e^{-\beta(W_0 - FL)x/L} - 1 \right] \quad ,$$

showing exponential decay. Since $F > 0$ the particles are biased to move towards the right but have to jump over the energy barriers in order to do this. The probability density profile shows an accumulation of particles at the potential minima with an exponential decay (i.e. curving upwards, $\mathcal{P}_F''(x) > 0$) towards the next period (domain).

(b) There is a critical force $F = W_0/L$ when the barrier disappears and the decay of the probability from the potential minima becomes linear so

$$\mathcal{P}_F(x) = \frac{JL}{D} \left(1 - \frac{x}{L}\right) \quad ,$$

(c) For even larger forces $0 < W_0/L < F$, the effect of the barrier is much weaker and the particles can much more easily diffuse around the whole potential landscape. Here $W_0 - FL < 0$, and $e^{-\beta W_0} > e^{-\beta FL}$ and

$$\mathcal{P}_F(x) = \frac{JL}{D\beta(FL - W_0)}\left[1 - \underbrace{\left(\frac{1-e^{-\beta W_0}}{1-e^{-\beta FL}}\right)}_{<1}\underbrace{e^{\beta(W_0 - FL)}}_{<1}e^{\beta(F-W_0/L)x}\right] \quad ,$$

the probability density profile is initially flat and then curves downwards ($\mathcal{P}_F''(x) < 0$) from the maximum near the potential minima.

(d) Finally, we note that negative forces, $F = -|F| < 0$ bias the particles to go to the left (change the sign of J) so

$$\mathcal{P}_F(x) = \frac{JL}{D\beta(W_0 + |F|L)}\left[\underbrace{\left(\frac{e^{\beta W_0}-1}{e^{-\beta|F|L}-1}\right)}_{<0}e^{-\beta(W_0+|F|L)x/L} - 1\right] \quad ,$$

since $\mathcal{P}_F(x) \geq 0$ this requires that $J < 0$. The particles get jammed behind the barriers for small $|F|$ and the profile becomes flat as $|F|$ increases.

We can similarly calculate the drift velocity of the particles by evaluating Eq. (IV.35) for this potential, $V_{\text{drift}}(F) = JL$:

$$V_{\text{drift}}(F) = \frac{D\beta(W_0/L - F)}{\left(\frac{1-e^{-\beta W_0}}{1-e^{-\beta FL}}\right)\frac{\left[e^{\beta(W_0-FL)}-1\right]}{\beta(W_0-FL)} - 1} \quad . \tag{IV.38}$$

This result shows many interesting features, which we highlight below.

For $W_0 \ll k_{\text{B}}T$, Eq. (IV.38) gives

$$V_{\text{drift}}(F) \approx F/\zeta \quad ,$$

as one would expect as the potential has a negligible effect on the diffusion of the particles which can easily jump across the 'low' barriers in their way.

When $W_0 > k_{\text{B}}T$, there will be an interesting interplay between thermal activation (diffusion limited jumps over the barriers) and motion due to the external bias.

For $FL \ll k_{\text{B}}T$, which yields $1 - e^{-\beta FL} \simeq \beta FL + O(F^2)$, we can expand Eq. (IV.38) to linear order in F to obtain the leading order term,

$$V_{\text{drift}}(F) \simeq \underbrace{\frac{1}{\zeta}\left[\frac{(\beta W_0/2)^2}{\sinh^2(\beta W_0/2)}\right]}_{1/\zeta_{\text{eff}}} F \quad . \tag{IV.39}$$

This can be interpreted as a *renormalization* of the drift velocity of a free particle to a smaller value corresponding to a larger effective friction coefficient due to the presence of the barriers which slow down the motion.

However, the most striking feature of Eq. (IV.38) is its asymmetry between positive and negative forces which is most evident in the large force regime, $\beta|F|L \gg 1$. This is due to the underlying asymmetry of the periodic potential.

It is instructive to consider the two cases ($F > 0$, $F < 0$) separately.

(+) For $FL \gg W_0 > k_\mathrm{B}T > 0$, Eq. (IV.38) becomes

$$V^{+}_{\mathrm{drift}}(F) \simeq \frac{\frac{1}{\zeta}\left(F - W_0/L\right)}{1 - \dfrac{\left(1 - e^{-\beta W_0}\right)}{\beta\left(FL - W_0\right)}} \quad . \tag{IV.40}$$

We can further perform an expansion in $1/F$ to obtain the asymptotic behaviour:

$$V^{+}_{\mathrm{drift}}(F) \simeq \frac{F}{\zeta} + \frac{1}{\beta\zeta L}\left[-\beta W_0 + \left(1 - e^{-\beta W_0}\right)\right] + O(1/F) \quad . \tag{IV.41}$$

(−) For $FL \ll -W_0 < -k_\mathrm{B}T < 0$, a similar analysis shows that we have

$$V^{-}_{\mathrm{drift}}(F) \simeq \frac{\frac{1}{\zeta}\left(F - W_0/L\right)}{1 - \dfrac{\left(e^{\beta W_0} - 1\right)}{\beta\left(FL - W_0\right)}} \quad . \tag{IV.42}$$

As above we can further perform an expansion in $1/F$ to obtain the asymptotic behaviour:

$$V^{-}_{\mathrm{drift}}(F) \simeq \frac{F}{\zeta} + \frac{1}{\beta\zeta L}\left[-\beta W_0 + \left(e^{\beta W_0} - 1\right)\right] + O(1/F) \quad . \tag{IV.43}$$

The leading correction to the drift velocity for positive forces is dominated by $-\beta W_0$, while the leading correction for negative forces is dominated by $e^{\beta W_0} - 1$, showing quite different behaviour.

It is particularly illuminating to consider the situation $|F|L \gg W_0 \gg k_\mathrm{B}T > 0$ (the barriers are high compared to $k_\mathrm{B}T$) where the asymptotic behaviour for high $|F|$, of the drift velocity, $V_{\mathrm{drift}}(F)$ will be linear in F (with slope ζ^{-1}) but with vastly different intercepts on the F-axis ($V_{\mathrm{drift}} = 0$) to the left and the right of the origin. For positive forces, the intercept on the F-axis is $\sim W_0/L$, while for negative forces it is $\sim -k_\mathrm{B}Te^{\beta W_0}/L$. The full velocity-force curve is shown in Figure IV.6.

The resulting asymmetric force velocity curve is reminiscent of the current-voltage characteristics of diodes which suggests that Brownian ratchets can be used as *mechanical diodes*.

3. Rectification of Brownian motion

The analogy that we made of Brownian ratchets to diodes suggests immediately that they could be used to rectify motion under oscillatory forcing. The requirement of course is that the underlying periodic potential $W(x)$ is *asymmetric*. If the oscillations in the external force are sufficiently slow (i.e. if the oscillation period is very long compared to the typical escape time for a particle in one of the wells), we can treat the system within a quasi-stationary approximation and analyze the particle behaviour within our steady-state scheme.

Let $F(t)$ be an oscillating function of period T_0 and with zero time-average, i.e. $\frac{1}{\mathsf{T}_0}\int_0^{\mathsf{T}_0} \mathrm{d}t\, F(t) = 0$. Using the analysis of the previous section, we can calculate the instantaneous drift velocity $v_{\mathrm{drift}}(F(t))$ at each value of t. The average drift velocity, $\bar{v}_{\mathrm{drift}}$ is then simply obtained from the time average of the drift velocity over a cycle period, T_0,

$$\bar{V}_{\mathrm{drift}} = \frac{1}{\mathsf{T}_0}\int_0^{\mathsf{T}_0} \mathrm{d}t\, V_{\mathrm{drift}}\left(F(t)\right) \quad . \tag{IV.44}$$

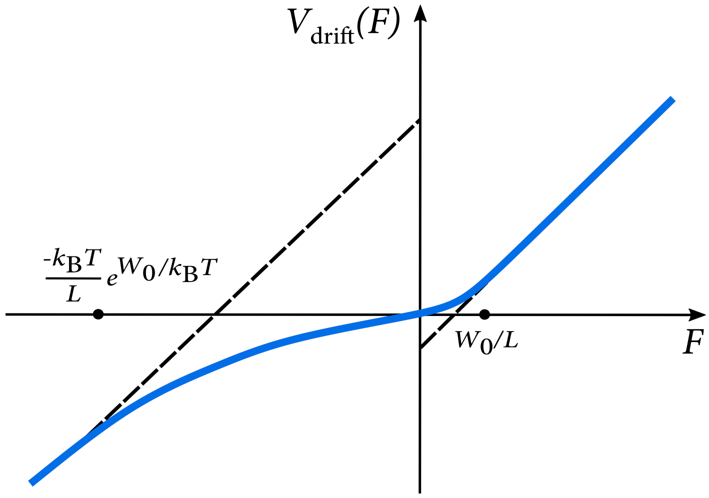

FIG. IV.6 **Nonlinear response.** The drift velocity force curve, $V_{\text{drift}}(F)$, for a particle in a periodic potential of barrier height W_0 and period repeat L.

So even though the time-averaged force is zero there is a non-zero drift velocity due to the asymmetry of the drift velocity as a function of force.

Let us return to the example of the periodic saw-tooth potential, subject to a periodic external force that oscillates between $-F_0$ and F_0 over a period T_0. The oscillating force leads to a rocking of the potential landscape from side to side (and up and down). From the velocity-force curve, we can identify a number of different regimes of behaviour.

For small force amplitudes, such that F_0 is in the linear part of the velocity-force curve, $F_0 L \ll k_B T$, the average drift velocity is zero.

For larger F_0, however, the half period that experiences positive forces gives rise to larger drift speeds (velocity magnitudes) than the half period with negative forces. Taking account of relative signs, Eq. (IV.44), leads to a non-vanishing average velocity. In particular for square wave forcing ($F(t) = F_0$ for $0 \le t < \mathsf{T}_0/2$ and $F(t) = -F_0$ for $\mathsf{T}_0/2 \le t < \mathsf{T}_0$, we can calculate the average velocity as

$$\bar{V}_{\text{drift}} = \frac{1}{2}\left[V_{\text{drift}}\left(F_0\right) + V_{\text{drift}}\left(-F_0\right)\right] \quad , \tag{IV.45}$$

where $V_{\text{drift}}\left(F\right)$ is given by Eq. (IV.38). Equation (IV.45) is sketched in Fig. IV.7.

The average drift velocity increases monotonically with the amplitude of the oscillatory force and saturates at a maximum velocity,

$$V_{\max} = \frac{k_B T}{\zeta L}\left[\sinh\left(\beta W_0\right) - \beta W_0\right] \tag{IV.46}$$

This example demonstrates the remarkable possibility of *fluctuation-driven transport* in which directed motion is extracted from a fluctuating system.

Fluctuations were essential for this to happen (note the dependence of the maximum velocity on $k_B T$) as activated jumps over the barriers need diffusion. At the same time if the fluctuations were too strong then the important features of the potential landscape (i.e. the asymmetry) are not sensed by the particles and no directed motion is achieved (note that $V_{\max}{\to}0$ as $T{\to}\infty$). The ratio of the 'noise' ($k_B T$) to the potential barrier (W_0) should be 'just right' for this mechanism to work.

Molecular motors are nanoscale machines which must function, i.e. deliver mechanical work, while being

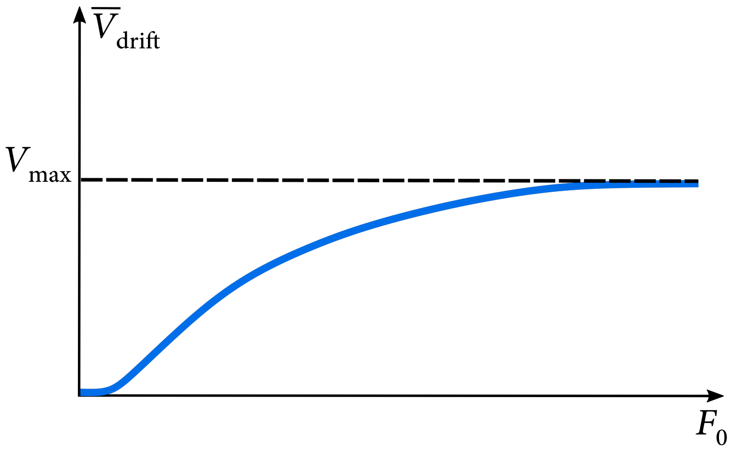

FIG. IV.7 **Fluctuation–driven transport.** The average drift velocity as a function of the force amplitude F_0.

subject to large thermal fluctuations (relative to their sizes). While a detailed understanding of how they operate is still not available, it is thought that their motion can be qualitatively described by such models of rectified fluctuations. It is appealing to think that Nature has exploited this physical mechanism in the making of molecular motors.

4. The flashing ratchet

We close this topic by briefly discussing an alternative scheme to achieve directed motion from nonequilibrium fluctuations, by using fluctuating potentials instead of fluctuating forces. The most convenient way to set up such a problem is by considering a two-state description similar to the telegraph noise in Sec. III.A.1, for the potential landscape and the probability distribution.

Consider a system where it is possible to stochastically switch between two different periodic potentials $W_+(x)$ and $W_-(x)$ at rates $\mu(x)$ and $\lambda(x)$:

$$W_-(x) \underset{\mu}{\overset{\lambda}{\rightleftharpoons}} W_+(x) \quad . \tag{IV.47}$$

The Fokker-Planck equations for the two populations $\mathcal{P}_+(x,t)$ and $\mathcal{P}_-(x,t)$ are written as

$$\begin{aligned} \partial_t \mathcal{P}_+(x,t) &= D\,\partial_x\left[\mathcal{P}_+\partial_x\left(\beta W_+\right) + \partial_x \mathcal{P}_+\right] - \mu \mathcal{P}_+ + \lambda \mathcal{P}_- \quad , \\ \partial_t \mathcal{P}_-(x,t) &= D\,\partial_x\left[\mathcal{P}_-\partial_x\left(\beta W_-\right) + \partial_x \mathcal{P}_-\right] - \lambda \mathcal{P}_- + \mu \mathcal{P}_+ \quad . \end{aligned}$$

Following the case of titling ratchets, these equations can be solved in stationary state, with the relevant boundary conditions, to obtain the probabilities $\mathcal{P}_+(x,t)$ and $\mathcal{P}_-(x,t)$ and the associated fluxes. The governing equation for the total probability $\mathcal{P} = \mathcal{P}_+ + \mathcal{P}_-$, can be written as

$$\partial_t \mathcal{P}(x,t) = D\,\partial_x\left[\mathcal{P}\,\partial_x(\beta U_{\mathrm{eff}}) + \partial_x \mathcal{P}\right] \quad , \tag{IV.48}$$

with the introduction of the *effective potential*, which can be solved from the following expression

$$\partial_x U_{\mathrm{eff}} = \frac{\mathcal{P}_+}{\mathcal{P}}\,\partial_x W_+ + \frac{\mathcal{P}_-}{\mathcal{P}}\,\partial_x W_- \quad . \tag{IV.49}$$

The underlying mechanism behind how flashing ratchets work can be summarized in the following statement. While both $W_+(x)$ and $W_-(x)$ are periodic and without a net bias (tilt), the resulting effective potential $U_{\text{eff}}(x)$ will inherit the periodicity of $W_+(x)$ and $W_-(x)$. However, it can generically also acquire a net bias as if it is under the influence of an effective average force F_{eff}, due to the x-dependence of the $\mathcal{P}_\pm/\mathcal{P}$ ratios. In other words, we can write $U_{\text{eff}}(x) = W_{\text{eff}}(x) - F_{\text{eff}}x$, where $W_{\text{eff}}(x)$ is a resulting effective periodic potential, and F_{eff} is the effective tilting force that can be calculated explicitly as

$$F_{\text{eff}} \equiv -\frac{\Delta U_{\text{eff}}}{L} = -\frac{1}{L}\int_0^L \mathrm{d}x\,\partial_x U_{\text{eff}} = -\frac{1}{L}\int_0^L \mathrm{d}x\left[\frac{\mathcal{P}_+(x)}{\mathcal{P}(x)}\,\partial_x W_+(x) + \frac{\mathcal{P}_-(x)}{\mathcal{P}(x)}\,\partial_x W_-(x)\right] \neq 0 \quad . \tag{IV.50}$$

This is equivalent to having a nonzero value for the net current associated with the total probability $\mathcal{P} = \mathcal{P}_+ + \mathcal{P}_-$, which reads

$$J = -D\partial_x\mathcal{P} - D\left[\mathcal{P}_+\partial_x\left(\beta W_+\right) + \mathcal{P}_-\partial_x\left(\beta W_-\right)\right] \quad . \tag{IV.51}$$

This calculation will show that it is possible to obtain a nonzero current, even in the absence of external forcing. For the special case where we have $W_+(x) = W(x)$ and $W_-(x) = 0$, the system is called *the on-off ratchet*. The choice of sawtooth potential allows for some analytical progress, although the linear algebra associated with the matching of the boundary conditions becomes involved.

We note that when the system satisfies detailed balance, we need to have $\mathcal{P}_+ \sim e^{-\beta W_+}$ and $\mathcal{P}_- \sim e^{-\beta W_-}$ so that the spatial part of the flux vanishes, as well as $\frac{\mu(x)}{\mu(x)+\lambda(x)} = \frac{\mathcal{P}_-}{\mathcal{P}}$ and $\frac{\lambda(x)}{\mu(x)+\lambda(x)} = \frac{\mathcal{P}_+}{\mathcal{P}}$ so that the transition part of the flux vanishes. Therefore, the space dependencies of the transition rates need to be tuned to the changes in the corresponding potentials, i.e. $\mu(x) \sim e^{-\beta W_-}$ and $\lambda(x) \sim e^{-\beta W_+}$. Under such a condition, it is easy to see that the net effective force and the net flux both vanish identically.

V. THE EFFECT OF MULTIPLICATIVE NOISE

For a large class of stochastic systems the noise term appears in a way that depends on the dynamical variable itself. This introduces a subtlety, in terms of an ambiguity that needs to be resolved when in the process of time discretization. We will also encounter this type of ambiguity when constructing a path integral representation for stochastic dynamics in Sec. VI. In this section, we will use a treatment of the discretization procedure and show that the resulting ambiguity, i.e. the well-known Ito versus Stratonovich dilemma, arises from the ambiguity in defining $\Theta(0)$ (the Heaviside step function of the origin). We will continue to present all results with the explicit appearances of $\Theta(0)$, and avoid the commonly used unsatisfactory schemes of either reproducing everything twice or choosing one scheme from the outset over the other.

A. Multiplicative noise: when the underlying physics matters

Before embarking on a formal development of the case of multiplicative noise, it is instructive to examine a specific case that will help us understand how the physical details of the problem will matter when deciding on how to resolve ambiguities. We consider a physically well defined case of a particle with space-dependent friction and space-dependent temperature, and show how a phase-space treatment combined with a moment expansion that allows us to systematically isolate the long time limit of the dynamics gives us very specific recipes of how to deal with the space dependencies that will turn out to be consistent with our physical expectations.

1. Klein-Kramers equation in phase space

Let us consider a particle of mass m that undergoes a stochastic dynamics in the phase-space, described by stochastic trajectory for position $\boldsymbol{r}(t)$ and momentum $\boldsymbol{q}(t)$. We assume a generic (i.e. not necessarily conservative) force-field $\boldsymbol{F}(\boldsymbol{r})$, and space-dependent friction coefficient $\zeta(\boldsymbol{r})$ and temperature profile $T(\boldsymbol{r})$. We shall start from an appropriate generalization of the original Langevin equation, Eq. (I.3), which can be written as

$$m\frac{\mathrm{d}^2\boldsymbol{r}}{\mathrm{d}t^2} = \boldsymbol{F}(\boldsymbol{r}(t)) - \zeta(\boldsymbol{r}(t))\frac{\mathrm{d}\boldsymbol{r}}{\mathrm{d}t} + \boldsymbol{f}(t) \quad , \tag{V.1}$$

where the random force is a Gaussian white noise satisfying the appropriate fluctuation–dissipation theorem $\langle f_i(t)f_j(t')\rangle = 2\zeta(\boldsymbol{r}(t))\,k_{\mathrm{B}}T(\boldsymbol{r}(t))\,\delta_{ij}\delta(t-t')$.

In the phase-space picture, we can re-write this second order Langevin equation as a system of two coupled first order Langevin equations

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{q}(t) = \boldsymbol{F}\left(\boldsymbol{r}(t)\right) - \dfrac{1}{m}\cdot\zeta(\boldsymbol{r}(t))\cdot\boldsymbol{q}(t) + \sqrt{2\zeta(\boldsymbol{r}(t))\,k_{\mathrm{B}}T(\boldsymbol{r}(t))}\,\boldsymbol{\xi}(t) \quad , \\[2ex] \dfrac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r}(t) = \dfrac{1}{m}\cdot\boldsymbol{q}(t) \quad , \end{cases} \tag{V.2}$$

where $\xi_i(t)$ is taken to be independent Gaussian white noise of unit strength by construction, i.e. $\langle\xi_i(t)\xi_j(t')\rangle = \delta_{ij}\delta(t-t')$. This form manifestly highlights the multiplicative nature of the noise term. We can now follow the procedure detailed in Sec. II.B as generalized to include both positions and momenta, to derive the corresponding Fokker-Planck equation in the phase-space, for the probability distribution defined as follows

$$\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)=\left\langle \delta^3\left(\boldsymbol{x}-\boldsymbol{r}(t)\right)\delta^3\left(\boldsymbol{p}-\boldsymbol{q}(t)\right)\right\rangle \quad , \tag{V.3}$$

where $\boldsymbol{x}$ and $\boldsymbol{p}$ are to be treated as independent phase-space variables.

We need to calculate the finite-time increments in positions and momenta

$$\begin{aligned}
\Delta q_i(t) &\equiv q_i(t+\Delta t)-q_i(t)=\int_t^{t+\Delta t}\mathrm{d}t_1\left[F_i(\boldsymbol{r}(t_1))-\frac{\zeta(\boldsymbol{r}(t_1))}{m}\,q_i(t_1)+\sqrt{2\zeta(\boldsymbol{r}(t_1))\,k_{\mathrm{B}}T(\boldsymbol{r}(t_1))}\,\xi_i(t_1)\right] \quad ,\\
\Delta r_i(t) &\equiv r_i(t+\Delta t)-r_i(t)=\frac{1}{m}\int_t^{t+\Delta t}\mathrm{d}t_1 q_i(t_1) \quad ,
\end{aligned} \tag{V.4}$$

and use them to make estimates of their first and second moments up to first order in Δt. We find

$$\langle \Delta q_i\rangle = F_i(\boldsymbol{x})\,\Delta t-\frac{1}{m}\,\zeta(\boldsymbol{x})\,p_i\,\Delta t+O(\Delta t^{3/2}) \quad , \tag{V.5}$$

$$\langle \Delta r_i\rangle = \frac{1}{m}\,p_i\,\Delta t+O(\Delta t^{3/2}) \quad , \tag{V.6}$$

$$\langle \Delta q_i \Delta q_j\rangle = 2\,\zeta(\boldsymbol{x})\,k_{\mathrm{B}}T(\boldsymbol{x})\,\delta_{ij}\,\Delta t+O(\Delta t^{3/2}) \quad , \tag{V.7}$$

$$\langle \Delta r_i \Delta r_j\rangle = O(\Delta t^{3/2}) \quad , \tag{V.8}$$

which are to be used in the appropriate generalization of the calculations performed in Sec. II.B using the probability distribution defined in Eq. (V.3) to yield the following generalized Fokker-Planck equation in phase-space

$$\partial_t\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)=-\frac{1}{m}\boldsymbol{\nabla}_{\boldsymbol{x}}\cdot\Big[\boldsymbol{p}\,\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)\Big]-\boldsymbol{\nabla}_{\boldsymbol{p}}\cdot\left[\Big(\boldsymbol{F}(\boldsymbol{x})-\frac{1}{m}\,\zeta(\boldsymbol{x})\,\boldsymbol{p}\Big)\,\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)\right]+\boldsymbol{\nabla}_{\boldsymbol{p}}^2\Big[\zeta(\boldsymbol{x})\,k_{\mathrm{B}}T(\boldsymbol{x})\,\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)\Big] \quad , \tag{V.9}$$

which is often called the Klein-Kramers equation in the literature.

The next task is to take the long time limit of this equation, and in the process, project the equation onto only the position subspace. This calculation is not as simple as the procedure we carried out in the case of the Langevin equations and requires the introduction of a new tool, which we will develop in the following sub-section.

2. Moment expansion and the long time limit

How can we extract the Fokker-Planck equation for $\mathcal{P}(\boldsymbol{x},t)$ from the corresponding equation for $\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)$? Since the original equation has much more information than needed for the governing equation of $\mathcal{P}(\boldsymbol{x},t)$, we can simply project Eq. (V.9) onto the relevant sector in phase-space. Since by definition $\mathcal{P}(\boldsymbol{x},t)=\int \mathrm{d}^3\boldsymbol{p}\,\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)$, this amounts to integrating Eq. (V.9) over $\boldsymbol{p}$. This yields

$$\partial_t\mathcal{P}(\boldsymbol{x},t)=-\boldsymbol{\nabla}\cdot\left[\frac{1}{m}\int \mathrm{d}^3\boldsymbol{p}\,\boldsymbol{p}\,\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)\right] \quad , \tag{V.10}$$

which is, however, not closed as it involves the first moment of the distribution with respect to momentum. Attempting to calculate the same equation for the first moment, will result in an equation that involves the second moment, etc, leading to a *hierarchy* of coupled equations that need to be solved together.

Let us introduce the notation $\rho(\boldsymbol{x},t)=\mathcal{P}(\boldsymbol{x},t)=\int \mathrm{d}^3\boldsymbol{p}\,\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)$, $\langle\boldsymbol{p}\rangle\,\rho=\int \mathrm{d}^3\boldsymbol{p}\,\boldsymbol{p}\,\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)$, and so on, to define more explicitly various moments of the momentum $\boldsymbol{p}$ (and avoid the confusion between $\mathcal{P}(\boldsymbol{x},t)$

and $\mathcal{P}(\boldsymbol{x},\boldsymbol{p},t)$ when the arguments are not shown). Then, the hierarchy of coupled equations derived for various moments of the distribution from Eq. (V.9) will read as follows

$$\begin{aligned} \partial_t \rho &= -\boldsymbol{\nabla}\cdot\left(\frac{1}{m}\langle \boldsymbol{p}\rangle \rho\right) \quad , && \text{(V.11)} \\ \partial_t\big[\rho\langle p_i\rangle\big] &= -\partial_j\left(\frac{1}{m}\langle p_i p_j\rangle \rho\right) + F_i\rho - \frac{1}{m}\zeta(\boldsymbol{x})\langle p_i\rangle\rho \quad , && \text{(V.12)} \\ \partial_t\left[\frac{1}{2}\rho\langle \boldsymbol{p}^2\rangle\right] &= -\partial_i\left(\frac{1}{2m}\langle \boldsymbol{p}^2 p_i\rangle\rho\right) + \boldsymbol{F}\cdot\langle\boldsymbol{p}\rangle\rho - \frac{1}{m}\zeta(\boldsymbol{x})\langle\boldsymbol{p}^2\rangle\rho + 3\zeta(\boldsymbol{x})k_{\rm B}T(\boldsymbol{x})\rho \quad , && \text{(V.13)} \end{aligned}$$

and so on. Since we are interested in the behaviour of the system in the long time limit when $t \gg m/\zeta$, we need to isolate the relevant parts of the hierarchy of governing equations. This can be simply achieved due to the way the equations are structured, as we can see from a rewriting of Eq. (V.12) below

$$\left(\partial_t + \frac{\zeta}{m}\right)\big[\rho\langle\boldsymbol{p}\rangle\big] = -\boldsymbol{\nabla}\cdot\left(\frac{1}{m}\langle\boldsymbol{p}\rangle\langle\boldsymbol{p}\rangle\rho\right) - \boldsymbol{\nabla}\left(\frac{1}{3m}\langle\boldsymbol{p}^2\rangle_c\rho\right) + \boldsymbol{F}\rho \quad ,$$

in which we have incorporated an assumption of isotropy of space for the fluctuations of momentum by using $\langle p_i p_j\rangle = \langle p_i\rangle\langle p_j\rangle + \frac{1}{3}\langle\boldsymbol{p}^2\rangle_c\delta_{ij}$. In the limit of $t \gg m/\zeta$, this yields

$$\langle\boldsymbol{p}\rangle\rho = \frac{m}{\zeta}\left[-\boldsymbol{\nabla}\left(\frac{1}{3m}\langle\boldsymbol{p}^2\rangle_c\rho\right) + \boldsymbol{F}\rho\right] + O\left((m/\zeta)^2\right) \quad . \tag{V.14}$$

Putting this result back in Eq. (V.11) gives the following

$$\partial_t\rho = -\boldsymbol{\nabla}\cdot\left\{\frac{1}{\zeta}\left[-\boldsymbol{\nabla}\left(\frac{\langle\boldsymbol{p}^2\rangle_c}{3m}\rho\right) + \boldsymbol{F}\rho\right]\right\} + O\left(m/\zeta\right) \quad , \tag{V.15}$$

which is still not a closed equation as it involves $\langle\boldsymbol{p}^2\rangle_c$. To close the hierarchy, we can use the following approximation $\langle\boldsymbol{p}^2 p_i\rangle \simeq \langle\boldsymbol{p}^2\rangle\langle p_i\rangle = \left(\langle\boldsymbol{p}\rangle\cdot\langle\boldsymbol{p}\rangle + \langle\boldsymbol{p}^2\rangle_c\right)\langle p_i\rangle$ in Eq. (V.13), which can now be written as

$$\left(\frac{1}{2}\partial_t + \frac{\zeta}{m}\right)\big[\rho\langle\boldsymbol{p}^2\rangle\big] = -\partial_i\left[\frac{1}{2m}\left(\langle\boldsymbol{p}\rangle\cdot\langle\boldsymbol{p}\rangle + \langle\boldsymbol{p}^2\rangle_c\right)\langle p_i\rangle\rho\right] + \boldsymbol{F}\cdot\langle\boldsymbol{p}\rangle\rho + 3\,\zeta\,k_{\rm B}T\,\rho \quad .$$

Ignoring the time derivative (long time limit), the above equation yields

$$\frac{1}{m}\langle\boldsymbol{p}^2\rangle_c = 3\,k_{\rm B}T(\boldsymbol{x}) + O\left(m/\zeta\right) \quad . \tag{V.16}$$

This is the appropriate nonequilibrium generalization of equipartition theorem, which amounts to its local implementation. Inserting Eq. (V.16) back in Eq. (V.15) gives the following closed equation for the concentration field

$$\partial_t\rho(\boldsymbol{x},t) = -\boldsymbol{\nabla}\cdot\left\{\frac{1}{\zeta(\boldsymbol{x})}\left[-\boldsymbol{\nabla}\Big(k_{\rm B}T(\boldsymbol{x})\,\rho\Big) + \boldsymbol{F}\rho\right]\right\} \quad . \tag{V.17}$$

This result has a number of remarkable features, which we discuss below.

The first thing to note is how the dependence on the friction coefficient is separated from the dependence on temperature. The structure of Eq. (V.17) guarantees that when the temperature profile is uniform and the force is conservative (i.e. $\boldsymbol{F} = -\boldsymbol{\nabla}U$), a stationary-state corresponding to thermodynamic equilibrium can be achieved irrespective of how the friction coefficient might depend on space. This is, for example, relevant to studies of colloidal particles near solid boundaries; while the presence of a wall will affect how long it takes for the colloid to relax to its equilibrium (due to the change in friction coefficient), the nature of the equilibrium state is not affected by the hydrodynamic effects due to the wall.

When the temperature profile is nonuniform, Eq. (V.17) gives rise to a nonuniform distribution of particles in the stationary state. In particular, for the case of $\boldsymbol{F} = 0$ we find $\rho(\boldsymbol{x}) \propto 1/T(\boldsymbol{x})$, which means that the particles will preferentially evacuate the hotter regions and accumulate in the colder regions; a phenomenon that is called positive *thermophoresis* in the context of linear response theory. When $\boldsymbol{F} \neq 0$, Eq. (V.17) can give rise to a richer variety of behaviour, including negative thermophoresis or accumulation of the particles in the hotter region.

B. Stochastic dynamics with position-dependent noise

After our consideration of a specific class of nonequilibrium systems using a phase-space description, let us go back to the position-space description of the stochastic dynamics and consider the situation where the strength of the noise experienced by a Brownian particle depends on the position of the particle. The stochastic dynamics in such cases could be described by a general Langevin equation of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{r}(t) = \boldsymbol{v}\left(\boldsymbol{r}(t)\right) + \sqrt{2D(\boldsymbol{r}(t))}\,\boldsymbol{\xi}(t) \quad , \tag{V.18}$$

where, as above, $\xi_i(t)$ is a Gaussian white noise of unit strength, i.e. $\langle \xi_i(t)\xi_j(t')\rangle = \delta_{ij}\delta(t-t')$. We now follow the procedure detailed in Sec. II.B to derive the corresponding Fokker-Planck equation for the probability distribution $\mathcal{P}(\boldsymbol{x},t) = \left\langle \delta^3\left(\boldsymbol{x} - \boldsymbol{r}(t)\right)\right\rangle$.

We start by integrating Eq. (V.18) over a finite, but small, time interval Δt to obtain

$$\begin{aligned}
\Delta r_i(t) \;&\equiv\; r_i(t+\Delta t) - r_i(t) = \int_t^{t+\Delta t} \mathrm{d}t_1 v_i(\boldsymbol{r}(t_1)) + \int_t^{t+\Delta t} \mathrm{d}t_1 \sqrt{2D(\boldsymbol{r}(t_1))}\,\xi_i(t_1) \quad , \\
&\simeq\; \Delta t\, v_i(\boldsymbol{r}(t)) + \int_t^{t+\Delta t} \mathrm{d}t_1 \left[\sqrt{2D(\boldsymbol{r}(t))} + \frac{\partial_j D(\boldsymbol{r}(t))}{\sqrt{2D(\boldsymbol{r}(t))}}\left(r_j(t_1) - r_j(t)\right)\right]\xi_i(t_1) \quad , \\
&=\; \Delta t\, v_i(\boldsymbol{r}(t)) + \sqrt{2D(\boldsymbol{r}(t))}\int_t^{t+\Delta t} \mathrm{d}t_1 \xi_i(t_1) + \partial_j D(\boldsymbol{r}(t)) \int_t^{t+\Delta t} \mathrm{d}t_1 \int_t^{t_1} \mathrm{d}t_2\, \xi_i(t_1)\xi_j(t_2) \\
&+\; O(\Delta t^{3/2}) \quad .
\end{aligned} \tag{V.19}$$

Averaging over noise now yields

$$\begin{aligned}
\langle \Delta r_i \rangle \;&=\; \Delta t\, v_i(\boldsymbol{x}) + \Delta t\, \Theta(0)\partial_i D(\boldsymbol{x}) \quad , &(\mathrm{V.20})\\
\langle \Delta r_i \Delta r_j \rangle \;&=\; 2D(\boldsymbol{x})\Delta t\, \delta_{ij} \quad , &(\mathrm{V.21})
\end{aligned}$$

to the lowest order in Δt. Following the procedure detailed in Sec. II.B, we can now write

$$\begin{aligned}
\mathcal{P}(\boldsymbol{x}, t+\Delta t) - \mathcal{P}(\boldsymbol{x},t) \;&=\; \left\langle \delta^3\left(\boldsymbol{x} - \boldsymbol{r}(t+\Delta t)\right)\right\rangle - \left\langle \delta^3\left(\boldsymbol{x} - \boldsymbol{r}(t)\right)\right\rangle \\
&=\; -\partial_i \left\langle \Delta r_i\, \delta^3\left(\boldsymbol{x} - \boldsymbol{r}(t)\right)\right\rangle + \frac{1}{2}\,\partial_i\partial_j \left\langle \Delta r_i \Delta r_j\, \delta^3\left(\boldsymbol{x} - \boldsymbol{r}(t)\right)\right\rangle \\
\Delta t\, \partial_t \mathcal{P}(\boldsymbol{x},t) \;&=\; -\partial_i\left[\langle \Delta r_i\rangle \mathcal{P}(\boldsymbol{x},t)\right] + \frac{1}{2}\,\partial_i\partial_j\left[\langle \Delta r_i \Delta r_j\rangle \mathcal{P}(\boldsymbol{x},t)\right] \quad .
\end{aligned} \tag{V.22}$$

Upon insertion of Eqs. (V.20) and (V.21), we find the Fokker-Planck equation

$$\partial_t \mathcal{P}(\boldsymbol{x},t) = -\boldsymbol{\nabla}\cdot\left[\Big(\boldsymbol{v}(\boldsymbol{x}) + \Theta(0)\boldsymbol{\nabla} D\Big)\,\mathcal{P}(\boldsymbol{x},t)\right] + \boldsymbol{\nabla}^2\left[D(\boldsymbol{x})\mathcal{P}(\boldsymbol{x},t)\right] \quad , \tag{V.23}$$

when we take the limit $\Delta t \to 0$. Due to the space dependence of the diffusion coefficient, a new contribution to the drift term proportional $\boldsymbol{\nabla} D$ arises in the Fokker-Planck equation, with the ill-defined prefactor $\Theta(0)$. The most common choices for this prefactor are $\Theta(0) = 0$, which corresponds to the Ito formulation, and $\Theta = 1/2$, which corresponds to the Stratonovich formulation. Another noteworthy feature of Eq. (V.23) is the way the space-dependent diffusion coefficient is placed in with respect to the two $\boldsymbol{\nabla}$ operators. It is, for example, appealing to define a flux $\boldsymbol{J}(\boldsymbol{x}) = \boldsymbol{v}_{\rm drift}(\boldsymbol{x})\mathcal{P} - D(\boldsymbol{x})\boldsymbol{\nabla}\mathcal{P}$ and write the Fokker-Planck equation as a continuity equation $\partial_t \mathcal{P} + \boldsymbol{\nabla} \cdot \boldsymbol{J} = 0$. In this representation, the drift term will have a different form:

$$\partial_t \mathcal{P}(\boldsymbol{x}, t) = -\boldsymbol{\nabla} \cdot \Big[\Big(\boldsymbol{v}(\boldsymbol{x}) + [\Theta(0) - 1]\,\boldsymbol{\nabla} D\Big)\,\mathcal{P}(\boldsymbol{x}, t)\Big] + \boldsymbol{\nabla} \cdot \big[D(\boldsymbol{x})\boldsymbol{\nabla}\mathcal{P}(\boldsymbol{x}, t)\big] \quad . \tag{V.24}$$

The choice of the drift term needs particular attention when the dynamics is described by a potential and an equilibrium reference for the system can be identified. In this case, the intrinsic drift velocity has the form of $\boldsymbol{v}(\boldsymbol{x}) = -\mu(\boldsymbol{x})\boldsymbol{\nabla} U(\boldsymbol{x}) = -D(\boldsymbol{x})\beta\boldsymbol{\nabla} U(\boldsymbol{x})$, if we generalize the fluctuation-dissipation theorem to include space-dependent mobilities. Putting this in Eq. (V.24) gives

$$\partial_t \mathcal{P}(\boldsymbol{x}, t) = -\boldsymbol{\nabla} \cdot \Big[\Big(-D(\boldsymbol{x})\beta\boldsymbol{\nabla} U(\boldsymbol{x}) + [\Theta(0) - 1]\,\boldsymbol{\nabla} D\Big)\,\mathcal{P}(\boldsymbol{x}, t)\Big] + \boldsymbol{\nabla} \cdot \big[D(\boldsymbol{x})\boldsymbol{\nabla}\mathcal{P}(\boldsymbol{x}, t)\big] \quad . \tag{V.25}$$

However, since thermal equilibrium should manifestly result from the equation irrespective of the form of $D(\boldsymbol{x})$, we expect the correct Fokker-Planck equation to be as follows

$$\partial_t \mathcal{P}(\boldsymbol{x}, t) = \boldsymbol{\nabla} \cdot \Big[D(\boldsymbol{x})\Big(\beta\boldsymbol{\nabla} U(\boldsymbol{x})\,\mathcal{P}(\boldsymbol{x}, t) + \boldsymbol{\nabla}\mathcal{P}(\boldsymbol{x}, t)\Big)\Big] \quad , \tag{V.26}$$

suggesting that our coarse-graining (or generalization of the fluctuation-dissipation theorem) should be such that the drift term has an additional contribution of the from

$$\boldsymbol{v}(\boldsymbol{x}) = -D(\boldsymbol{x})\beta\boldsymbol{\nabla} U(\boldsymbol{x}) \quad \longrightarrow \quad \boldsymbol{v}(\boldsymbol{x}) = -D(\boldsymbol{x})\beta\boldsymbol{\nabla} U(\boldsymbol{x}) + [1 - \Theta(0)]\,\boldsymbol{\nabla} D \quad , \tag{V.27}$$

to cancel the existing $\boldsymbol{\nabla} D$ drift term in Eq. (V.36) to ensure thermal equilibration. This additional term, which needs to be added by hand, is called the *spurious drift* in the literature. An alternative to adding this term is to interpret the freedom afforded by the presence of $\Theta(0)$ differently; the (so-called anti-Ito) choice of $\Theta(0) = 1$ will not necessitate the addition of a spurious drift term. In arbitrary nonequilibrium cases where equilibration is not a constraint, the appropriate choice of the drift term will need to be made using guidance from the information that is available about the specific system; it is not possible to make generic comments about the validity of either of the interpretations. We have seen an example of how such description guides us to the physically correct rendition of the nonequilibrium formulation in Sec. V.A.1.

1. Anisotropic diffusion

The above scheme can be generalized to the case where the space-dependent diffusion coefficient is anisotropic, i.e. it is a tensor $D_{ij}(\boldsymbol{r})$. The corresponding Langevin equation will need to be generalized as follows

$$\frac{\mathrm{d}}{\mathrm{d}t} r_i(t) = v_i\left(\boldsymbol{r}(t)\right) + \sqrt{2}\,\sigma_{ij}(\boldsymbol{r}(t))\,\xi_j(t) \quad , \tag{V.28}$$

where $\xi_i(t)$ is a Gaussian white noise of unit strength as above, and σ_{ij} is the "square-root" of the noise strength that is set by the anisotropic diffusion tensor

$$D_{ij}(\boldsymbol{r}) = \sigma_{im}(\boldsymbol{r})\sigma_{jm}(\boldsymbol{r}) \quad , \tag{V.29}$$

as will be shown explicitly below. Integrating Eq. (V.28) over the time interval Δt and following the steps used to calculate Eq. (V.19), we find

$$\begin{aligned}\Delta r_i(t) \;&\equiv\; r_i(t+\Delta t) - r_i(t) = \Delta t\, v_i(\boldsymbol{r}(t)) + \sqrt{2}\,\sigma_{ij}(\boldsymbol{r}(t)) \int_t^{t+\Delta t} \mathrm{d}t_1\, \xi_j(t_1) \\ &+\; 2\,\partial_k \sigma_{ij}(\boldsymbol{r}(t))\,\sigma_{kl}(\boldsymbol{r}(t)) \int_t^{t+\Delta t} \mathrm{d}t_1 \int_t^{t_1} \mathrm{d}t_2\, \xi_j(t_1)\xi_l(t_2) + O(\Delta t^{3/2}) \quad . \end{aligned} \tag{V.30}$$

Averaging over noise gives

$$\langle \Delta r_i(t) \rangle \;=\; \Delta t\, v_i(\boldsymbol{x}) + 2\Delta t\,\Theta(0)\,\sigma_{kj}(\boldsymbol{x})\,\partial_k \sigma_{ij}(\boldsymbol{x}) \quad , \tag{V.31}$$

$$\langle \Delta r_i(t) \Delta r_j(t) \rangle \;=\; 2 D_{ij}(\boldsymbol{x}) \Delta t \quad , \tag{V.32}$$

to the lowest order in Δt, where Eq. (V.29) has been used in Eq. (V.32). Finally, we find the Fokker-Planck equation as follows

$$\partial_t \mathcal{P}(\boldsymbol{x},t) = -\partial_i \left[\Big(v_i(\boldsymbol{x}) + 2\Theta(0)\,\sigma_{kj}\partial_k\sigma_{ij} \Big)\, \mathcal{P}(\boldsymbol{x},t) \right] + \partial_i\partial_j \left[D_{ij}(\boldsymbol{x}) \mathcal{P}(\boldsymbol{x},t) \right] \quad . \tag{V.33}$$

Rewriting the Fokker-Planck equation such that the structure of a diffusive flux is manifest yields

$$\partial_t \mathcal{P}(\boldsymbol{x},t) = -\partial_i \left[\Big(v_i(\boldsymbol{x}) + 2\Theta(0)\,\sigma_{kj}\partial_k\sigma_{ij} - \partial_j D_{ij} \Big)\, \mathcal{P}(\boldsymbol{x},t) \right] + \partial_i \left[D_{ij}(\boldsymbol{x}) \partial_j \mathcal{P}(\boldsymbol{x},t) \right] \quad . \tag{V.34}$$

Note that the two additional drift terms are not identical in form, as expanding the divergence of the diffusivity tensor shows:

$$\partial_k D_{ik} = \partial_k \left[\sigma_{ij}\sigma_{kj} \right] = \sigma_{kj}\partial_k\sigma_{ij} + \sigma_{ij}\partial_k\sigma_{kj} \quad . \tag{V.35}$$

When the dynamics is described by a potential, the intrinsic drift velocity will have the form of $v_i(\boldsymbol{x}) = -\mu_{ij}(\boldsymbol{x})\partial_j U(\boldsymbol{x})$, which includes an anisotropic mobility tensor μ_{ij}. This can be written as $v_i(\boldsymbol{x}) = -D_{ij}(\boldsymbol{x})\beta\partial_j U(\boldsymbol{x})$, if we generalize the fluctuation-dissipation theorem accordingly. In this case, the requirement of thermal equilibration gives us the Fokker-Planck equation

$$\partial_t \mathcal{P}(\boldsymbol{x},t) = \partial_i \left[D_{ij}(\boldsymbol{x}) \Big(\beta\partial_j U(\boldsymbol{x})\, \mathcal{P}(\boldsymbol{x},t) + \partial_j \mathcal{P}(\boldsymbol{x},t) \Big) \right] \quad . \tag{V.36}$$

which can be rendered by making the following transformation

$$v_i(\boldsymbol{x}) = -D_{ij}(\boldsymbol{x})\beta\partial_j U(\boldsymbol{x}) \quad \longrightarrow \quad v_i(\boldsymbol{x}) = -D_{ij}(\boldsymbol{x})\beta\partial_j U(\boldsymbol{x}) - 2\Theta(0)\,\sigma_{kj}\partial_k\sigma_{ij} + \partial_j D_{ij} \quad , \tag{V.37}$$

i.e. adding spurious drift terms to the microscopic Langevin equation.

2. Coordinate transformation

Using the equations for the stochastic dynamics in a given coordinate system, how can we construct the corresponding equations in a different coordinate system? While it is naturally possible to use standard methods to transform partial differential equations to other coordinate systems, our derivation of the Fokker-Planck equation lends itself to a relatively straightforward way to this end.

Let us start with the Fokker-Planck equation [Eq. (V.33)]

$$\partial_t \mathcal{P} = -\partial_i \left[w_i\, \mathcal{P} \right] + \partial_i\partial_j \left[D_{ij} \mathcal{P} \right] \quad . \tag{V.38}$$

where the effective drift term is defined as

$$w_i = v_i + 2\,\Theta(0)\,\sigma_{km}\,\partial_k\sigma_{im} \quad . \tag{V.39}$$

We now consider a coordinate transformation $x_i \mapsto x'_i$, and define the corresponding Jacobian matrix $K_{ij} = \partial x'_i/\partial x_j$. We define $\mathcal{P}'(\boldsymbol{x}', t) = \left\langle \delta^3\left(\boldsymbol{x}' - \boldsymbol{r}'(t)\right)\right\rangle$ and note that normalization of the probability distribution implies $\mathcal{P}' = J\mathcal{P}$, where $J = |\det(\partial x_i/\partial x'_j)|$ is the Jacobian of the transformation.

Following the same procedure as in Eq. (V.22) in the primed coordinate, we find

$$\Delta t\,\partial_t\mathcal{P}' = -\partial'_i\left[\langle\Delta r'_i(t)\rangle\,\mathcal{P}'\right] + \frac{1}{2}\,\partial'_i\partial'_j\left[\left\langle\Delta r'_i(t)\Delta r'_j(t)\right\rangle\mathcal{P}'\right] \quad . \tag{V.40}$$

On the other hand, the coordinate transformation

$$\mathrm{d}r'_i = K_{ij}(\boldsymbol{r})\,\mathrm{d}r_j \quad , \tag{V.41}$$

can be used to find an expression for finite position increments in the primed coordinate system as

$$\begin{aligned}
\Delta r'_i &= \int_t^{t+\Delta t} \mathrm{d}r_j\,K_{ij}\left(\boldsymbol{r}\right) = \int_t^{t+\Delta t} \mathrm{d}t_1\,K_{ij}\left(\boldsymbol{r}(t_1)\right)\frac{\mathrm{d}r_j(t_1)}{\mathrm{d}t_1} \quad , \\
&= \int_t^{t+\Delta t} \mathrm{d}t_1\left[K_{ij}\left(\boldsymbol{r}(t)\right) + \partial_k K_{ij}\left(\boldsymbol{r}(t)\right)\Big(r_k(t_1) - r_k(t)\Big)\right]\frac{\mathrm{d}r_j(t_1)}{\mathrm{d}t_1} \quad , \\
&= K_{ij}\left(\boldsymbol{r}(t)\right)\Delta r_j + \partial_k K_{ij}\left(\boldsymbol{r}(t)\right)\int_t^{t+\Delta t}\mathrm{d}t_1\int_t^{t_1}\mathrm{d}t_2\,\frac{\mathrm{d}r_k(t_2)}{\mathrm{d}t_2}\,\frac{\mathrm{d}r_j(t_1)}{\mathrm{d}t_1} \quad , \\
&= K_{ij}\left(\boldsymbol{r}(t)\right)\Delta r_j + 2\,\partial_k K_{ij}\left(\boldsymbol{r}(t)\right)\sigma_{kl}\left(\boldsymbol{r}(t)\right)\sigma_{jm}\left(\boldsymbol{r}(t)\right)\int_t^{t+\Delta t}\mathrm{d}t_1\int_t^{t_1}\mathrm{d}t_2\,\xi_l(t_2)\xi_m(t_1)
\end{aligned} \tag{V.42}$$

where only terms of order Δt are kept in the expression. Averaging over noise yields

$$\begin{aligned}
\langle\Delta r'_i\rangle &= K_{ij}w_j\Delta t + 2\,\Theta(0)\,\partial_k K_{ij}D_{jk}\Delta t \quad , & \text{(V.43)}\\
\left\langle\Delta r'_i\Delta r'_j\right\rangle &= 2K_{im}K_{jn}D_{mn}\Delta t \quad . & \text{(V.44)}
\end{aligned}$$

Note the similarity of our calculations above and the procedure we followed in Sec. V.B.1, and hence the occurrence of $\Theta(0)$. Combining Eqs. (V.43) and (V.44) with Eqs. (V.31) and (V.32) gives

$$\begin{aligned}
\langle\Delta r'_i\rangle &= K_{ij}\left\langle\Delta r_j\right\rangle + \Theta(0)\,\partial_k K_{ij}\left\langle\Delta r_j\Delta r_k\right\rangle \quad , & \text{(V.45)}\\
\left\langle\Delta r'_i\Delta r'_j\right\rangle &= K_{im}K_{jn}\left\langle\Delta r_m\Delta r_n\right\rangle \quad , & \text{(V.46)}
\end{aligned}$$

which are equivalent to the following connection between the finite stochastic position increments

$$\Delta r'_i = K_{ij}\left(\boldsymbol{x} + \Theta(0)\boldsymbol{\Delta r}\right)\Delta r_j = K_{ij}\Delta r_j + \Theta(0)\,\partial_k K_{ij}\Delta r_j\Delta r_k \quad . \tag{V.47}$$

Inserting Eqs. (V.43) and (V.44) back in Eq. (V.40) gives

$$\partial_t\mathcal{P}' = -\partial'_i\left[w'_i\,\mathcal{P}'\right] + \partial'_i\partial'_j\left[D'_{ij}\mathcal{P}'\right] \quad , \tag{V.48}$$

where the primed coefficients are related to the unprimed coefficient using the following transformation rules:

$$\begin{aligned}
w'_i &= K_{ij}w_j + 2\,\Theta(0)\,\partial_k K_{ij}D_{jk} \quad , & \text{(V.49)}\\
D'_{ij} &= K_{im}K_{jn}D_{mn} \quad . & \text{(V.50)}
\end{aligned}$$

Note that the above results are consistent with a transformation rule

$$\sigma'_{ij} = K_{im}\sigma_{mj} \quad , \tag{V.51}$$

for the square-root of the diffusivity tensor. This can be understood by regarding the noise term in Eq. (V.28) as belonging to a different vector space from that of the position space, hence considering σ_{im} as a rank-1 tensor with regards to coordinate transformations. The next section will shed some more light on this.

C. Stochastic dynamics on Riemannian manifolds

There are many important examples in nature where stochastic dynamics is confined to a particular space with nontrivial geometry. Two most prominent examples are diffusion of lipids and proteins on the 2-dimensional cell membranes and diffusion of proteins in charge of transcription along the 1-dimensional DNA. The peculiar transformation properties of the stochastic dynamics under a change of coordinate system as studied in Sec. V.B.2 suggests that constructing a geometrically consistent structure to the equations of stochastic dynamics might prove a subtle task.

We take an intuitive approach and build this geometric construction using embedding of arbitrary spaces in a $d-$dimensional Euclidean space. We start by writing the Langevin equation in *contravariant* coordinates

$$\frac{\mathrm{d}}{\mathrm{d}t} r^i(t) = v^i\left(\boldsymbol{r}(t)\right) + \sqrt{2D}\, e^i_a(\boldsymbol{r}(t))\, \xi_a(t) \quad , \tag{V.52}$$

where the noise terms are taken to be along the tangent vectors of the manifold, which are indexed by a. $\xi_a(t)$ is a Gaussian white noise of unit strength, i.e. $\langle \xi_a(t)\xi_b(t')\rangle = \delta_{ab}\delta(t-t')$. Note that nontrivial geometry will make the noise multiplicative. The drift term v^i could in general have components both inside and outside of the tangent space. For simplicity, we consider a scalar and space-independent diffusion coefficient D and focus on the role of geometry, but the generalization to include these additional features is straightforward. The set of the tangent vectors or the *vielbein* gives us the contravariant metric tensor

$$g^{ij}(\boldsymbol{x}) = e^i_a(\boldsymbol{x}) e^j_a(\boldsymbol{x}) \quad , \tag{V.53}$$

from which we can also define the complementary covariant metric tensor g_{ij}. We have

$$g^{ij} g_{jk} = \delta^i_k \quad , \tag{V.54}$$

and we can define

$$g = \det(g_{ij}) = 1/\det(g^{ij}) \quad , \tag{V.55}$$

which will give us the measure $\mathrm{d}V = \mathrm{d}^d\boldsymbol{x}\sqrt{g}$ that is invariant under arbitrary coordinate transformations. To see this, let us consider a coordinate transformation $x^i \mapsto x'^i$, which gives the Jacobian matrix $K^i_j = \partial x'^i/\partial x^j$, and its inverse $K^{-1i}_j = \partial x^i/\partial x'^j$. Covariance of the metric tensor gives

$$g_{ij} = K^k_i\, K^l_j\, g'_{kl} \qquad \Rightarrow \qquad g' = J^2\, g \qquad \Rightarrow \qquad \mathrm{d}^d\boldsymbol{x}\sqrt{g} = \mathrm{d}^d\boldsymbol{x}'\, J\sqrt{g} = \mathrm{d}^d\boldsymbol{x}'\sqrt{g'} \quad , \tag{V.56}$$

where $J = |\det(\partial x^i/\partial x'^j)|$ is the Jacobian of the transformation.

The invariant probability distribution will be defined as

$$\mathcal{P}_g(\boldsymbol{x},t) = \frac{1}{\sqrt{g}} \left\langle \delta^d \left(\boldsymbol{x} - \boldsymbol{r}(t)\right)\right\rangle \quad , \tag{V.57}$$

which is manifestly normalized using the invariant measure, i.e. $\int \mathrm{d}^d\boldsymbol{x}\sqrt{g}\,\mathcal{P}_g = 1$.

To construct the Fokker-Planck equation, we can follow our standard procedure [see e.g. Eq. (V.22)] that yields

$$\Delta t\, \partial_t \left\langle \delta^d \left(\boldsymbol{x} - \boldsymbol{r}(t)\right)\right\rangle = -\partial_i \left[\left\langle \Delta r^i \right\rangle \left\langle \delta^d \left(\boldsymbol{x} - \boldsymbol{r}(t)\right)\right\rangle\right] + \frac{1}{2}\,\partial_i\partial_j \left[\left\langle \Delta r^i \Delta r^j \right\rangle \left\langle \delta^d \left(\boldsymbol{x} - \boldsymbol{r}(t)\right)\right\rangle\right] \quad , \tag{V.58}$$

and replace $\left\langle \delta^3 \left(\boldsymbol{r} - \boldsymbol{r}(t)\right)\right\rangle$ by the invariant probability distribution defined in Eq. (V.57). The finite displacement can be calculated by integrating Eq. (V.52), which yields

$$\begin{aligned} \Delta r^i(t) \;\equiv\; & r^i(t+\Delta t) - r^i(t) = \Delta t\, v^i(\boldsymbol{r}(t)) + \sqrt{2D}\, e^i_a(\boldsymbol{r}(t)) \int_t^{t+\Delta t} \mathrm{d}t_1\, \xi_a(t_1) \\ &+\; 2D\, e^k_b(\boldsymbol{r}(t))\, \partial_k e^i_a(\boldsymbol{r}(t)) \int_t^{t+\Delta t} \mathrm{d}t_1 \int_t^{t_1} \mathrm{d}t_2\, \xi_a(t_1)\xi_b(t_2) + O(\Delta t^{3/2}) \quad . \end{aligned} \tag{V.59}$$

The next step is averaging over noise, which gives

$$\left\langle \Delta r^i \right\rangle \;=\; \Delta t\, v^i + 2D\Delta t\, \Theta(0)\, e^k_a\, \partial_k e^i_a \quad , \tag{V.60}$$

$$\left\langle \Delta r^i \Delta r^j \right\rangle \;=\; 2D\, g^{ij}\, \Delta t \quad , \tag{V.61}$$

to the lowest order in Δt, where Eq. (V.53) has been used to introduce the metric tensor. Putting these together, and restricting ourselves to the case where the geometry is not time-dependent, we find the Fokker-Planck equation as follows

$$\partial_t \mathcal{P}_g(\boldsymbol{x},t) = -\frac{1}{\sqrt{g}}\,\partial_i \left[\left(v^i(\boldsymbol{x}) + 2D\,\Theta(0)\, e^k_a\, \partial_k e^i_a\right)\sqrt{g}\,\mathcal{P}_g(\boldsymbol{x},t)\right] + \frac{D}{\sqrt{g}}\,\partial_i\partial_j \left[g^{ij}\sqrt{g}\,\mathcal{P}_g(\boldsymbol{x},t)\right] \quad . \tag{V.62}$$

We now need to examine whether Eq. (V.62) is reparametrization invariant. To this end, we first rewrite the second derivative term such that the structure of a diffusive flux is manifest, and absorb the resulting terms into the drift term. This yields

$$\partial_t \mathcal{P}_g = -\frac{1}{\sqrt{g}}\,\partial_i \left[\sqrt{g}\, W^i\, \mathcal{P}_g\right] + \frac{D}{\sqrt{g}}\,\partial_i \left[\sqrt{g}\, g^{ij} \partial_j \mathcal{P}_g\right] \quad , \tag{V.63}$$

where

$$W^i = v^i + 2D\,\Theta(0)\, e^k_a\, \partial_k e^i_a - \frac{D}{\sqrt{g}}\,\partial_j \left(\sqrt{g}\, g^{ij}\right) \quad . \tag{V.64}$$

On the right hand side of Eq. (V.63), the first term has the form of a covariant divergence, i.e.

$$\nabla_i V^i = \frac{1}{\sqrt{g}}\,\partial_i \left(\sqrt{g}\, V^i\right) \quad , \tag{V.65}$$

and the second term has the covariant form of the Laplace-Beltrami operator on manifolds

$$\Delta_g \equiv \frac{1}{\sqrt{g}}\partial_i \left[\sqrt{g}\, g^{ij} \partial_j\right] \quad . \tag{V.66}$$

Since $\mathcal{P}_g$ is a scalar, to make Eq. (V.63) fully covariant we need to show that W^i is a contravariant vector under arbitrary coordinate transformation.

To probe this, let us look at the transformation explicitly*

$$\begin{aligned}
K^i_j\, W^j &= K^i_j\, v^j + 2D\,\Theta(0)\, K^i_j\, e^k_a\, \partial_k e^j_a - \frac{D}{\sqrt{g}}\, K^i_j\, \partial_k \left(\sqrt{g}\, g^{jk}\right) \quad , \\
&= K^i_j\, v^j + 2D\,\Theta(0)\, e^k_a\, \partial_k \left(K^i_j\, e^j_a\right) - 2D\,\Theta(0)\, e^k_a\, e^j_a\, \partial_k K^i_j - \overbrace{\frac{D}{\sqrt{g}}\, \partial_k \left(K^i_j\, \sqrt{g}\, g^{jk}\right)}^{\bullet} + D\, g^{jk}\, \partial_k K^i_j \quad , \\
&= v'^i + 2D\,\Theta(0)\, e'^l_a\, \partial'_l e'^i_a - \overbrace{\frac{D}{\sqrt{g'}}\, \partial'_l \left(\sqrt{g'}\, g'^{il}\right)}^{\bullet} + D\left[1 - 2\Theta(0)\right]\, g^{jk}\, \partial_k K^i_j \quad , \\
&= W'^i + D\left[1 - 2\Theta(0)\right]\, g^{jk}\, \partial_k K^i_j \quad .
\end{aligned} \tag{V.67}$$

Remarkably, Eq. (V.67) tells us that the reparametrization invariance necessitates the choice of $\Theta(0) = 1/2$! Therefore, our covariant Fokker-Planck equation will be given by Eq. (V.63) with the following choice for the drift term

$$W^i = v^i + D\, e^k_a\, \partial_k e^i_a - \frac{D}{\sqrt{g}}\, \partial_k \left(\sqrt{g}\, g^{ik}\right) \quad , \tag{V.68}$$

which can be re-written [using Eqs. (V.53) and (V.65)] in the following manifestly covariant form

$$W^i = v^i - D\, e^i_a\, \nabla_k e^k_a \quad . \tag{V.69}$$

D. Hydrodynamic interaction

A particular phenomenon in which multiplicative noise plays a prominent role is the many-body stochastic dynamics of particles (colloids, polymers, proteins, etc) with hydrodynamic interactions. For an earlier discussion of many-body stochastic dynamics, see Sec. II.B.2. Hydrodynamic interactions are generalizations of the locally defined Stokes law of viscous friction, in the sense that the force experienced by any particle will affect the velocity of any other particle by generating a long-range viscous hydrodynamic flow.

Consider a system with N particles, with the position of the αth particle described as $\boldsymbol{R}^\alpha(t)$, where $\alpha \in \{1, \ldots, N\}$. The Langevin equation the αth particle is written as

$$\frac{\mathrm{d}}{\mathrm{d}t} R^\alpha_i(t) = M^{\alpha\beta}_{ij} F^\beta_j + \sqrt{2k_{\mathrm{B}}T}\, \Sigma^{\alpha\beta}_{ij}\, \xi^\beta_j(t) \quad , \tag{V.70}$$

where summation convention is implied both for component indices and particle indices. In Eq. (V.70), $\xi^\alpha_i(t)$ represents Gaussian white noise of unit strength with the following correlator $\left\langle \xi^\alpha_i(t) \xi^\beta_j(t') \right\rangle = \delta^{\alpha\beta}\delta_{ij}\delta(t-t')$, and $\Sigma^{\alpha\beta}_{ij}$ is the "square-root" of the mobility tensor

$$M^{\alpha\beta}_{ij} = \Sigma^{\alpha\nu}_{im}\Sigma^{\beta\nu}_{jm} \quad , \tag{V.71}$$

as will be shown below. Note that the force $\boldsymbol{F}^\beta$ could be externally imposed or the outcome of two-body

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* The transformation between the two terms highlighted by • requires the use of the identity $\partial_k f = \frac{1}{J}\partial'_l \left(K^l_k J f\right)$, or equivalently $\frac{1}{J}\partial'_l \left(K^l_k J\right) = 0$. To prove this, in the latter form, we can rewrite it as $-\partial_k \ln J = \partial'_l K^l_k = K_l^{-1m}\partial_m K^l_k = K_l^{-1m}\partial_k K^l_m$, which is now in a form that can be obtained by applying ∂_k to both sides of the identity $\mathrm{tr}\ln K = \ln\det K$.

interactions between particles, as discussed in Sec. II.B.2. In the far field limit, the mobility tensor is defined as follows

$$M_{ij}^{\alpha\beta}(\boldsymbol{R}^\alpha, \boldsymbol{R}^\beta) = \begin{cases} \dfrac{\delta_{ij}}{6\pi\eta a} & , \quad \alpha = \beta \\ \\ \mathcal{G}_{ij}(\boldsymbol{R}^\alpha - \boldsymbol{R}^\beta) & , \quad \alpha \neq \beta \end{cases} \tag{V.72}$$

where the Oseen tensor

$$\mathcal{G}_{ij}(\boldsymbol{r}) = \frac{1}{8\pi\eta r}\left[\delta_{ij} + \frac{r_i r_j}{r^2}\right] \quad , \tag{V.73}$$

is the Green's function (in free space) for Stokes equation of hydrodynamics, describing the velocity profile of viscous and incompressible fluid flow generated by a point force (at the origin). Note that $\partial_i \mathcal{G}_{ij} = 0$ due to the incompressibility constraint.

We now follow the procedure and integrate Eq. (V.70) over the time interval Δt, which yields

$$\begin{aligned} \Delta R_i^\alpha \;&\equiv\; R_i^\alpha(t+\Delta t) - R_i^\alpha(t) = \Delta t\, M_{ij}^{\alpha\beta} F_j^\beta + \sqrt{2k_\mathrm{B}T}\,\Sigma_{ij}^{\alpha\beta}\int_t^{t+\Delta t} \mathrm{d}t_1 \xi_j^\beta(t_1) \\ &+\; 2k_\mathrm{B}T\,\partial_k^\gamma \Sigma_{ij}^{\alpha\beta}\,\Sigma_{kl}^{\gamma\delta}\int_t^{t+\Delta t}\mathrm{d}t_1\int_t^{t_1}\mathrm{d}t_2\,\xi_j^\beta(t_1)\xi_l^\delta(t_2) + O(\Delta t^{3/2}) \quad . \end{aligned} \tag{V.74}$$

The next step is noise averaging, which gives

$$\langle \Delta R_i^\alpha \rangle \;=\; \Delta t\, M_{ij}^{\alpha\beta} F_j^\beta + 2k_\mathrm{B}T\Delta t\,\Theta(0)\,\Sigma_{kj}^{\gamma\beta}\,\partial_k^\gamma \Sigma_{ij}^{\alpha\beta} \quad , \tag{V.75}$$

$$\left\langle \Delta R_i^\alpha \Delta R_j^\beta \right\rangle \;=\; 2k_\mathrm{B}T M_{ij}^{\alpha\beta}\Delta t \quad , \tag{V.76}$$

to the lowest order in Δt, where Eq. (V.71) has been used in Eq. (V.76).

We can now define the N-particle distribution function as

$$\mathcal{P}(\boldsymbol{X}^1, \ldots, \boldsymbol{X}^N, t) \equiv \mathcal{P}(\{\boldsymbol{X}^\alpha\}, t) = \left\langle \prod_{\alpha=1}^N \delta^3(\boldsymbol{X}^\alpha - \boldsymbol{R}^\alpha(t)) \right\rangle \quad , \tag{V.77}$$

and generalize the procedure used in Sec. II.B to write

$$\begin{aligned} \mathcal{P}(\{\boldsymbol{X}^\alpha\}, t+\Delta t) - \mathcal{P}(\{\boldsymbol{X}^\alpha\}, t) &= \left\langle \prod_{\alpha=1}^N \delta^3(\boldsymbol{X}^\alpha - \boldsymbol{R}^\alpha(t+\Delta t)) \right\rangle - \left\langle \prod_{\alpha=1}^N \delta^3(\boldsymbol{X}^\alpha - \boldsymbol{R}^\alpha(t)) \right\rangle \\ \Delta t\,\partial_t \mathcal{P} = -\partial_i^\alpha\left[\langle \Delta R_i^\alpha \rangle \mathcal{P}\right] + \frac{1}{2}\partial_i^\alpha \partial_j^\beta &\left[\left\langle \Delta R_i^\alpha \Delta R_j^\beta \right\rangle \mathcal{P}\right] \quad . \end{aligned} \tag{V.78}$$

Putting in Eqs. (V.75) and (V.76), we find the N-particle Fokker-Planck equation

$$\partial_t \mathcal{P} = -\partial_i^\alpha\left[\left(M_{ij}^{\alpha\beta}F_j^\beta + 2\,\Theta(0)\,k_\mathrm{B}T\,\Sigma_{kj}^{\gamma\beta}\,\partial_k^\gamma \Sigma_{ij}^{\alpha\beta}\right)\mathcal{P}\right] + k_\mathrm{B}T\partial_i^\alpha\partial_j^\beta\left[M_{ij}^{\alpha\beta}\mathcal{P}\right] \quad , \tag{V.79}$$

in the limit $\Delta t \to 0$, or alternatively

$$\partial_t \mathcal{P} = -\partial_i^\alpha\left[\left(M_{ij}^{\alpha\beta}F_j^\beta + 2\,\Theta(0)\,k_\mathrm{B}T\,\Sigma_{kj}^{\gamma\beta}\,\partial_k^\gamma \Sigma_{ij}^{\alpha\beta} - k_\mathrm{B}T\partial_j^\beta M_{ij}^{\alpha\beta}\right)\mathcal{P}\right] + k_\mathrm{B}T\partial_i^\alpha\left[M_{ij}^{\alpha\beta}\partial_j^\beta\mathcal{P}\right] \quad , \tag{V.80}$$

which is the form where the diffusive flux is manifest. Note that $\partial_j^\beta M_{ij}^{\alpha\beta} = 0$ due to the incompressibility constraint and the fact that the friction coefficient is independent of position; see Eq. (V.72). However, the friction coefficient can become position dependent in the vicinity of boundaries.

Since we expect thermal equilibration from the Fokker-Planck equation, we will need to modify it as

$$\partial_t \mathcal{P}(\{\boldsymbol{X}^\alpha\}, t) = \partial_i^\alpha \left[M_{ij}^{\alpha\beta} \Big(- F_j^\beta \, \mathcal{P}(\{\boldsymbol{X}^\alpha\}, t) + k_{\mathrm{B}} T \partial_j^\beta \mathcal{P}(\{\boldsymbol{X}^\alpha\}, t) \Big) \right] \quad , \tag{V.81}$$

by incorporating the following transformation

$$M_{ij}^{\alpha\beta} F_j^\beta \quad \longrightarrow \quad M_{ij}^{\alpha\beta} F_j^\beta - 2\,\Theta(0)\, k_{\mathrm{B}} T\, \Sigma_{kj}^{\gamma\beta}\, \partial_k^\gamma \Sigma_{ij}^{\alpha\beta} + k_{\mathrm{B}} T \partial_j^\beta M_{ij}^{\alpha\beta} \quad , \tag{V.82}$$

in the microscopic Langevin equation [Eq. (V.70)].