

Statistical Physics IV: Non-equilibrium statistical physics
ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL)

Solutions to Exercise No.1

1.1 Solution: Langevin equation

(a) Straightforward computation gives,

$$m \frac{d}{dt} \langle xv \rangle = m \left(\frac{dx}{dt} v + x \frac{dv}{dt} \right) = mv^2 + x(-\alpha v + F_L). \quad (1)$$

(b) When doing the stochastic average, with respect to all possible realization of the random force, the only thing that can happen is that one of the two averages does not exist. For nice and smooth functions, it should always be possible to interchange the order of the derivative and the average.

(c) Taking the ensemble average of Eq. 1,

$$m \frac{d}{dt} \langle xv \rangle = \langle mv^2 \rangle - \alpha \langle xv \rangle.$$

If we consider the long-time limit, when the system goes toward a stationary solution, we can identify this to thermal equilibrium. The equipartition theorem then states that $\langle mv^2 \rangle = k_B T$.

(d) We have

$$\frac{d \langle x^2 \rangle}{dt} = 2 \langle xv \rangle.$$

From the previously derived equation, $\langle xv \rangle$ converges to $k_B T / \alpha$ for long times. We then have $\langle x^2(t) \rangle = 2Dt$ for long times, with the diffusion constant $D = \frac{k_B T}{\alpha}$.

(e) For a particle of charge q , in a homogeneous stationary electric field E , and being impressed upon by a Langevin force, the equation of motion reads,

$$m \frac{dv}{dt} + \alpha v = qE + F_L.$$

Integrating this:

$$\begin{aligned} v(t) &= v(0)e^{-\alpha t/m} + \frac{1}{m} \int_0^t (qE + F_L(t')) e^{-\alpha(t-t')/m} dt' \\ &= v(0)e^{-\alpha t/m} + \frac{qE}{\alpha} (1 - e^{-\alpha t/m}) + \frac{1}{m} \int_0^t F_L(t') e^{-\alpha(t-t')/m} dt'. \end{aligned}$$

Taking the limit $t \rightarrow \infty$, and ensemble averages:

$$\lim_{t \rightarrow \infty} \langle v(t) \rangle = \frac{qE}{\alpha} \quad \Rightarrow \quad \mu = \frac{q}{\alpha}.$$

Finally using the expression for the diffusion constant from above,

$$\mu/D = q/k_B T.$$

1.2 Solution: Smoluchowski equation

The discrete probability $p(n\Delta, (k+1)\tau)$ can be related to $p((n-1)\Delta, k\tau)$ and $p((n+1)\Delta, k\tau)$:

$$\begin{aligned} p(n\Delta, (k+1)\tau) &= r(n\Delta)p((n-1)\Delta, k\tau) + l(n\Delta)p((n+1)\Delta, k\tau) \\ &= \left[\frac{1}{2} + \Delta\alpha(n-1)\Delta\right] \times p((n-1)\Delta, k\tau) + \left[\frac{1}{2} - \Delta\alpha(n+1)\Delta\right] \times p((n+1)\Delta, k\tau) \end{aligned} \quad (2)$$

By subtracting $p(n\Delta, k\tau)$ on each side of the equality, one obtains:

$$\begin{aligned} p(n\Delta, (k+1)\tau) - p(n\Delta, k\tau) &= \frac{1}{2}[p((n+1)\Delta, k\tau) - 2p(n\Delta, k\tau) + p((n-1)\Delta, k\tau)] \\ &\quad - \Delta[\alpha(n+1)\Delta \times p((n+1)\Delta, k\tau) - \alpha(n-1)\Delta \times p((n-1)\Delta, k\tau)] \end{aligned} \quad (3)$$

By dividing by τ on each side, one obtains:

$$\begin{aligned} \frac{p(n\Delta, (k+1)\tau) - p(n\Delta, k\tau)}{\tau} &= \frac{\Delta^2}{2\tau} \left[\frac{p((n+1)\Delta, k\tau) - 2p(n\Delta, k\tau) + p((n-1)\Delta, k\tau)}{\Delta^2} \right] \\ &\quad - \frac{2\Delta^2}{\tau} \left[\frac{\alpha(n+1)\Delta \times p((n+1)\Delta, k\tau) - \alpha(n-1)\Delta \times p((n-1)\Delta, k\tau)}{2\Delta} \right] \end{aligned} \quad (4)$$

Notice that:

$$\begin{aligned} \frac{p((n+1)\Delta, k\tau) - 2p(n\Delta, k\tau) + p((n-1)\Delta, k\tau)}{\Delta^2} &= \frac{1}{\Delta} \left[\frac{p((n+1)\Delta, k\tau) - p(n\Delta, k\tau)}{\Delta} \right. \\ &\quad \left. - \frac{p(n\Delta, k\tau) - p((n-1)\Delta, k\tau)}{\Delta} \right] \end{aligned} \quad (5)$$

Taking the limit $\Delta \rightarrow 0$ and $\tau \rightarrow 0$, one gets the differential equation for continuous probability distribution $P(x, t)$:

$$\frac{\partial P(x, t)}{\partial t} = D \frac{\partial^2}{\partial x^2} P(x, t) - 4D \frac{\partial}{\partial x} [\alpha(x) P(x, t)] \quad (6)$$

where we set $\frac{\Delta^2}{2\tau} = D$.

Dimensional analysis incites us to write $4D\alpha(x) = \frac{F(x)}{m\gamma}$, where $F(x)$ is the force acting on the particle. Thus,

$$\frac{\partial P(x, t)}{\partial t} = D \frac{\partial^2}{\partial x^2} P(x, t) - \frac{1}{m\gamma} \frac{\partial}{\partial x} [F(x) P(x, t)] \quad (7)$$