4 Exercises lectures 8 and 9 (due 26 Feb)

4.1 Langevin dynamics for thermostatting

Find the Fokker-Planck equation somewhere in the literature (even Wikipedia will do). For a particle subjected to langevin dynamics, the probability density is governed by the FP equation.

a) Write down the langevin equation for a point particle in a potential well in one dimension.

b) From the langevin equation, argue why the 2×2 diffusion tensor in the FP equation for this particle has only one nonzero element. Argue that this element does not depend on the position or velocity.

c) Show that for a one-dimensional particle in a potential well, langevin dynamics produce a probability density equal to the canonical probability distribution. Langevin dynamics thus produce a suitable thermostat.

4.2 Drawing a variable from a non-uniform distribution

Random number generators usually produce homogeneously distributed random numbers. Often this is not really the distribution you want. Suppose you have at your disposal a random number generator which produces random numbers x distributed uniformly between 0 and 1.

a) Using a method similar to the one described in the lecture for Gaussian random numbers, devise a way to obtain a random number y distributed between 0 and ∞ according to the density

$$\rho(y) = \frac{1}{l} \exp\left(-\frac{y}{l}\right) \quad , \tag{7}$$

where l is some positive constant. Prove that your scheme gives the correct distribution. For the Monte-Carlo simulation of the random Lorentz gas, which we have used as an example in the lecture, you would need this distribution for the free-flight times (see exercise 1.1).

b) The other distribution in the Lorentz-gas exercise was

$$\rho(\phi) = \frac{1}{2} \cos\phi, \text{with} - \frac{\pi}{2} < \phi < \frac{\pi}{2} \ . \tag{8}$$

There are other ways to get nonuniform distributions, for instance by first drawing from a uniform distribution, and then rejecting the outcome with some probability that depends on the value of the random number. Find such a way to draw from the distribution in Eq. (8).