1 Stationary limit of the underdamped Fokker-Planck equation

The Fokker-Planck equation for $p(x,p,t)$ reads

$$\dot{p}(x,p,t) = \left(-\frac{p}{m}\partial_x + kx\partial_p + \frac{\xi}{m} + \frac{\xi}{m}p\partial_p + D_p\partial_p^2\right)p(x,p,t)\,. \tag{1}$$

Note that here D_p is a diffusion constant for the momentum p, not for the position x.

1. The stationary solution $p_s(x,p)$ is a product of two Gaussians in x and p. Write the ansatz

$$p_s(x,p) \propto e^{-\lambda_1 x^2} e^{-\lambda_2 p^2}\,. \tag{2}$$

Insert in the above equation and obtain

$$0 = \left(\frac{p}{m}2\lambda_1 x - kx2p\lambda_2 + \frac{\xi}{m} - \frac{\xi}{m}2p^2\lambda_2 + D_p(-2\lambda_2 + 4p^2\lambda_2^2)\right)e^{-\lambda_1 x^2}e^{-\lambda_2 p^2}\,, \tag{3}$$

$$0 = \left(\frac{p}{m}\lambda_1 x - kxp\lambda_2 + \frac{\xi}{2m} - \frac{\xi}{m}p^2\lambda_2 + D_p(-\lambda_2 + 2p^2\lambda_2^2)\right)\,. \tag{4}$$

We notice that the constant term has to vanish independentely of the others: $\frac{\xi}{2m} - D_p\lambda_2 = 0$. From this, we can deduce

$$\lambda_2 = \frac{\xi}{2mD_p}\,. \tag{5}$$

This is consistent with the condition that the terms proportional to p^2 have to vanish too. It follows that λ_1 is given by

$$\lambda_1 = mk\lambda_2 = \frac{k\xi}{2D_p}\,. \tag{6}$$

And thus

$$p_s(x,p) \propto e^{-\frac{k\xi x^2}{2D_p}} e^{-\frac{\xi p^2}{2mD_p}}\,. \tag{7}$$

This is a product of two Gaussians with $\sigma_x^2 = \frac{D_p}{k\xi}$ and $\sigma_p^2 = \frac{mD_p}{\xi}$. The normalization can be found easily:

$$p_s(x,p) = \frac{1}{2\pi\sigma_x\sigma_p}e^{-\frac{x^2}{2\sigma_x}}e^{-\frac{p^2}{2\sigma_p}}\,. \tag{8}$$

2. Comparing the Boltzmann distribution $p_s(x,p) \propto e^{-(T(p)+U(x))/(k_BT)}$, where $T(p) = p^2/(2m)$ is the kinetic energy term, we can identify the following relations

$$D_p = \xi k_B T\,, \tag{9}$$

$$\frac{U(x)}{k_BT} = \frac{k\xi x^2}{2D_p}\,. \tag{10}$$

3. Calculate the first and second moments of the stationary distribution. Explain the physical meaning of your results.

The first momenta correspond to the means μ_x and μ_p and are zero. And the second momenta are therefore the variances σ_x and σ_p.

2 Ideal Gas - Momentum in the microcanonical ensemble

Consider an ideal gas with energy E, volume V and particle number N. Use the fundamental postulate to show that in the microcanonical ensemble the x-component p_1 of the momentum of the first atom is Gaussian-distributed with variance $2mE/(3N)$.

The fundamental postulate states that each microstate corresponding to one macrostate is equally likely in thermal equilibrium. Thus, the probability of finding the x-component p_1 of the momentum of the first atom to be a certain value q is equal to

$$p(q) = \frac{\#\text{ states with } p_1 = q}{\#\text{ states}}. \tag{11}$$

The number of the states is proportional to the phase space volume. The number of all possible states which correspond to the energy E is given by the following phase space integral

$$\begin{aligned}
\#\text{ states} \propto V_{3N}(R) &= \int d^{3N}q \int d^{3N}p\, \delta\left(E - \sum_{i=1}^{3N} \frac{p_i^2}{2m}\right) && (12)\\
&= V^{3N} \int p^{3N-1} dp \int d\Omega_{3N}\, \frac{m}{\sqrt{2mE}}\, \delta\left(p - \sqrt{2mE}\right) && (13)\\
&\approx V^{3N} \cdot \frac{\pi^{\frac{3N}{2}} (2mE)^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2}\right)}, && (14)
\end{aligned}$$

where we used the properties of the delta function

$$\delta(f(x)) = \sum_{x_0 : f(x_0)=0} \frac{\delta(x - x_0)}{|f'(x_0)|} \tag{15}$$

and the fact that for large N, the volume of a $3N$-dimensional hypersphere with radius $R = \sqrt{2mE}$ is almost completely on its surface. For a better explaination, see `https://homepage.univie.ac.at/franz.vesely/sp_english/sp/node15.html`.
By constraining $p_1 = q$, we go from a $3N$-dimensional hypersurface to a $(3N-1)$-dimensional hypersurface. So we have

$$p(q) = \frac{V_{3N-1}(R')}{V_{3N}(R)} \propto \frac{R'^{3N-1}}{R^{3N}}. \tag{16}$$

From $E = \frac{q^2}{2m} + \sum_{i=2}^{3N} \frac{p_i^2}{2m}$, we see that $R' = \sqrt{2mE - q^2}$ and thus

$$\begin{aligned}
p(q) &\propto \frac{1}{\sqrt{2mE - q^2}} \left(1 - \frac{q^2}{2mE}\right)^{\frac{3N}{2}} && (17)\\
&\approx \frac{1}{\sqrt{2mE}} \left(\exp\left(-\frac{q^2}{2mE}\right)\right)^{\frac{3N}{2}} && (18)\\
&\propto e^{-\frac{3Nq^2}{4mE}}. && (19)
\end{aligned}$$

We used the approximation that the momentum of the single particle is much smaller than the total energy $q^2 \ll 2mE$. This is a Boltzmann distribution with variance $\sigma^2 = \frac{2mE}{3N}$.

Note: This is just a sketch. A lot of details are skipped but you get the idea how to do it.

3 Computer exercise - Monte Carlo integration

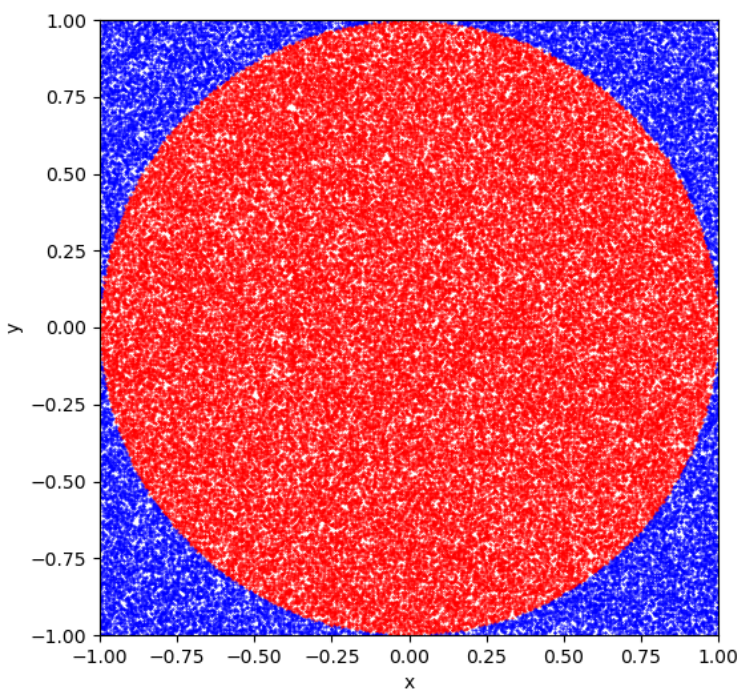
The algorithm can be implemented using the following python code snippet:

```python
import numpy as np

A = 0

N = 100000
for _ in range(N):
    x = np.random.uniform(-1, 1)
    y = np.random.uniform(-1, 1)
    if x**2 + y**2 <= 1:
        A += 1

z = 4 * A / N
print(z)
```

With this, a value for π can be estimated, running the above code returns 3.14312. The ratio of A to N is directly proportional to another ratio, namely that of a the area of a unit circle to the area of a square with side length 2. One could thus in principle calculate π by e.g. throwing darts onto a square surface with a circle drawn on it. This is because the number of "hits" can be assumed to be proportional to the hit probability, which again is directly proportional to the respective area. This method can only work if the distribution of random numbers is uniform and N is large enough.
Converges like $\sim 1/\sqrt{N}$ (law of large numbers).

Visualization: