Particle – potential energy

$$U(h) = mgh$$

Particle is coupled to a heat bath with temperature T.

① Hamiltonian?

$$H(h,v) = \frac{1}{2} m v^2 + mgh$$

② Classical approx to the part func Q?

$$Q_{NVT} = \frac{1}{N!\,(2\pi\hbar)^{3N}} \int d\vec{r}^N d\vec{p}^N e^{-\beta H(r^N, p^N)}$$

$$\beta = 1/k_B T$$

$$N = 1 \implies Q_{NVT} = \frac{1}{(2\pi\hbar)^3} \int dr\, dp\, e^{-\beta \frac{1}{2} m\vec{v}^2} e^{-\beta mgh} =$$

$$Q = \frac{1}{(2\pi\hbar)^3} \int_0^\infty dh\, e^{-\beta mgh} \int_{-\infty}^{\infty} dp\, e^{-\beta \frac{p^2}{2m}} =$$

$$= \frac{1}{(2\pi\hbar)^3} \frac{-1}{\beta mg} \underbrace{\left[e^{-\beta mgh}\right]_{h=0}^{\infty}}_{1} \left(\frac{2\pi m}{\beta}\right)^{3/2} =$$

$h \to \infty \ldots e^{-h} \to 0$

$h = 0 \ldots e^{-h} = 1$

$$= \frac{1}{(2\pi\hbar)^3} \frac{-1}{\beta mg} \left(\frac{2\pi m}{\beta}\right)^{3/2}$$

③ Internal energy E?

Helmholtz free energy: $F = -k_B T \ln Q$

$$F = -k_B T \ln\left(\frac{1}{(2\pi\hbar)^3}\frac{-1}{\beta m g}\left(\frac{2\pi m}{\beta}\right)^{3/2}\right) = -k_B T \ln\left(\frac{-m^{1/2}}{(2\pi)^{3/2}\hbar^3 g\,\beta^{5/2}}\right)$$

$$\frac{\partial(\beta F)}{\partial\beta} = F + \beta\frac{\partial F}{\partial\beta} = F + \beta\underbrace{\left(-\frac{1}{k_B\beta^2}\right)}_{=-T}\underbrace{\frac{\partial F}{\partial T}}_{=-S} = F + TS = E$$ ..energy

$$E = \frac{\partial}{\partial\beta}\left(-\ln\left(\frac{-m^{1/2}}{(2\pi)^{3/2}\hbar^3 g\,\beta^{5/2}}\right)\right) = -k_B T\,\frac{(2\pi)^{3/2}\hbar^3 g\,\beta^{5/2}}{m^{1/2}}\cdot T^{-3/2}\cdot\left(\frac{-3}{2}\right)$$

④ Observable $A(h)$ exp. value $\langle A\rangle$?

$$Z = \frac{-1}{\beta m g}$$

$$\langle A(h)\rangle = -mg\beta\int_0^\infty dr\, A(h)\, e^{-\beta m g h}$$

2 Monte-carlo simulation

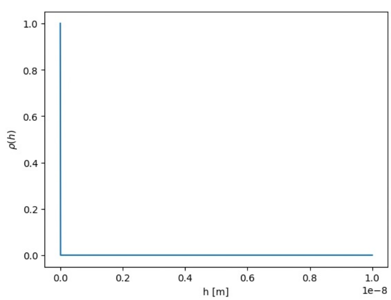
$A(h) = h$

$$\underbrace{\langle A(h)\rangle}_{\langle g(h)\rangle} = -mg\beta\int_0^\infty dh\, \underbrace{h}_{g(h)}\, \underbrace{e^{-\beta m g h}}_{f(h)}$$

Because we are interested in $\langle A(h)\rangle$ and according to the formula the $g(h)$ should be found in the integral

Implementation

I am not sure how I should implement ‘the ξi are a samples from ϱ’. The code gives me the following plot for rho.



From this plot I would suggest that the partile is in the hight zero.

Used code:

```
# expected height of a particle in homogeneous gravitational field calculated by Monte Carlo method

# %% import modules
import numpy as np
import matplotlib.pyplot as plt
from scipy.constants import Boltzmann as kB
from scipy.constants import g

# %% define constants
m = 4.66e-26 # mass of the particle [kg]
T = 300.0 # temperature [K]
beta = 1/(kB*T) # inverse temperature [1/K]

def f(h):
    return np.exp(-beta*g*h)

# %% Monte Carlo method

N = 1 # number of particles
h = np.linspace(0, stop=1e-8, num=1000) # height of the particle [m]

# %% calculate the expected height of the particle

def rho(h):
    return np.exp(-beta*g*h)

# plot the probability density function
plt.plot(h, rho(h))
plt.xlabel('h [m]')
plt.ylabel(r'$\rho (h)$')
plt.show()

# %%

exp_g = 1/N * np.sum(rho(h))
print(f"expected height is {exp_g}")
# %%
```