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: $F = -k_B T \ln Q$

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

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

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

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

$A(h) = h$

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

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