Homework 1. Due Thursday, Feb. 11

1. (**5pts**) Consider a particle in 1D in contact with a heat bath whose states follow the canonical distribution:
$$\mu(x,p) = \frac{1}{Z}e^{-\beta H(x,p)}, \quad \text{where} \quad Z = \int_{\mathbb{R}^2} e^{-\beta H(x,p)}dxdp, \tag{1}$$
where $H(x,p) = V(x) + \frac{p^2}{2}$ is its energy and $\beta = (k_B T)^{-1}$ (k_B is Boltzmann's constant).

   (a) Show that the mean kinetic energy equals to $k_B T/2$, i.e., calculate the expected value of
$$E\left[\frac{p^2}{2}\right] = \frac{1}{Z}\int_{\mathbb{R}^2}\frac{p^2}{2}e^{-\beta(V(x)+p^2/2)}dxdp.$$

   Solution

$$\begin{aligned}
Z &= \int_{R^2} dxdp \exp(-\beta(V(x)) \exp(-\beta p^2/2) \\
&= \left[\int_{-\infty}^{\infty} dx \exp(-\beta(V(x))\right]\left[\int_{-\infty}^{\infty} dp \exp(-\beta p^2/2)\right] = Z_x Z_p \\
t &= p\sqrt{\beta/2}, \quad dp = dt\sqrt{2/\beta}, \quad \int_{-\infty}^{\infty}\exp(-t^2)dt = \sqrt{\pi} \\
Z_p &= \int_{-\infty}^{\infty} dt\sqrt{2/\beta}\exp(-t^2) = \sqrt{2\pi/\beta} \\
E[p^2/2] &= Z_x^{-1}Z_p^{-1}\left[\int_{-\infty}^{\infty} dx \exp(-\beta(V(x))\right]\left[\int_{-\infty}^{\infty}\frac{p^2}{2}dp\exp(-\beta p^2/2)\right] \\
&= \sqrt{\beta/2\pi}\int_{-\infty}^{\infty}\frac{p^2}{2}dp\exp(-\beta p^2/2), \\
&\int_{-\infty}^{\infty} t^2\exp(-t^2)dt = \sqrt{\pi}/2
\end{aligned}$$

   (b) Use your result to show that for a system consisting of n particles of unit mass each of which is moving in 3D, the mean kinetic energy is $(3/2)nk_B T$. The canonical distribution of this system is given by
$$\mu(x,p) = \frac{1}{Z}e^{-\beta H(x,p)}, \quad x,p \in \mathbb{R}^{3n}, \quad Z = \int_{\mathbb{R}^{6n}} e^{-\beta H(x,p)}dxdp, \tag{2}$$
$$H(x,p) = V(x) + \frac{1}{2}\sum_{i=1}^{3n} p_i^2.$$

2. (**5pts**) Let η be the number that comes up when you throw a die[1] . Evaluate
$$E[\eta|(\eta-3)^2].$$

   Hint: You may want to represent your answer as a table of values of $E[\eta|(\eta-3)^2]$ for different values of $(\eta-3)^2$.

[1]Problem 11 from Chorin & Hald, 2nd edition [1], Chapter 2, p. 45.

References

[1] A. Chorin and O. Hald, Stochastic Tools in Mathematics and Science, 2nd edition, Springer 2009. You can download a pdf file with the whole book from the UMD library.