

Homework 1. Due Wednesday, Feb. 13

1. (5pts) Consider a particle in 1D in contact with a heat bath whose states follow the canonical distribution:

$$\mu(x, p) = \frac{1}{Z} e^{-\beta H(x, p)}, \quad \text{where} \quad Z = \int_{\mathbb{R}^2} e^{-\beta H(x, p)} dx dp, \quad (1)$$

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

$$E \left[\frac{p^2}{2} \right] = \frac{1}{Z} \int_{\mathbb{R}^2} \frac{p^2}{2} e^{-\beta(V(x) + p^2/2)} dx dp.$$

- (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

$$\mu(x, p) = \frac{1}{Z} e^{-\beta H(x, p)}, \quad x, p \in \mathbb{R}^{3n}, \quad Z = \int_{\mathbb{R}^{6n}} e^{-\beta H(x, p)} dx dp, \quad (2)$$

$$H(x, p) = V(x) + \frac{1}{2} \sum_{i=1}^{3n} p_i^2.$$

2. (5pts) Suppose you are throwing two dice. Consider the random variables $\eta = \omega_1 + \omega_2$ (the sum of numbers on the top) and $\theta = |\omega_1 - \omega_2|$ (the absolute value of the difference of the numbers on the top).
- Determine whether η and θ are dependent.
 - Calculate $\text{Cov}(\eta, \theta)$.
 - Calculate $E[\eta|\theta]$ and $\text{Var}(\eta|\theta)$.
 - Calculate $E[\theta|\eta]$ and $\text{Var}(\theta|\eta)$.
3. (5pts) Problem 9 from Chorin & Hald, 2nd edition [1], Chapter 2, p. 45. (Matches problem 4, Chapter 2 in the 3rd edition of Chorin & Hald (2013).)
4. (5pts) Problem 10 from Chorin & Hald, 2nd edition [1], Chapter 2, p. 45. (Matches problem 5, Chapter 2 in the 3rd edition of Chorin & Hald (2013).)

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.