

Due Apr. 24, Thursday.

**Problem 1** (15 points; Correlation)

- Consider a beam of unpolarized electrons. We sample an electron and measure its spin in the  $z$  direction,  $\sigma_z = \pm 1$  ( $S_z = \sigma_z \hbar/2$ ). Then, we sample another electron to measure its spin in the  $x$  direction,  $\sigma_x = \pm 1$ . Find the correlation between  $\sigma_z$  and  $\sigma_x$ .
- Consider a spin singlet state of two electrons flying in the opposite directions. Alice measures the  $z$ -spin of the right moving electron, ( $\sigma_{z,R} = \pm 1$ ), and then Bob measures the  $z$ -spin of the left moving electron ( $\sigma_{z,L} = \pm 1$ ). Find the correlation between  $\sigma_{z,R}$  and  $\sigma_{z,L}$ .
- Consider, instead, a spin triplet state of two electrons flying in the opposite directions. Find the correlation between  $\sigma_{z,R}$  and  $\sigma_{z,L}$ .

**Problem 2** (20 points; Bayes theorem) Consider a coin toss experiment, in which a single coin is tossed repeatedly ( $N$  times) and the number of its heads are counted ( $n$ ). Let the probability of the head per each toss be  $h$ . You like to investigate whether the coin is a “good” coin ( $h = 1/2$ ) or not. In the Bayesian scheme, one can follow these procedures.

- Assume that anything is possible with equal probability at the beginning. This defines the initial model.
- Gather evidence (do a few coin tosses, for this particular problem) and update the model.
- Repeat.

For this coin toss problem, the initial model can be taken as that in which any value of  $h$  is viewed as equally probable.

- Given this initial model, construct the initial PDF  $p(h)$  ( $0 \leq h \leq 1$ ). This corresponds to the *prior* PDF.
- Let us say that  $n$  heads were found for  $N$  tosses. Given the initial model, show that the probability corresponding to *this specific* outcome,  $p(n)$ , is given by

$$p(n) = \frac{n!(N-n)!}{(N+1)!}.$$

Note that  $p(n)$  is *not* the probability that  $n$  heads will show up in any order, but it is the probability that  $n$  heads will show up in the *exact order* of the actual data. (A better notation of  $p(n)$  would be  $p(\text{evidence})$ .) [Hint: You can use the Beta function,  $B(a,b) = \int_0^1 dh h^{a-1}(1-h)^{b-1} = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$ .]

- (c) Using Bayes theorem, obtain the *posterior* PDF  $p(h|n)$ . [Hint:  $p(h|n)dh \times p(n) = p(n|h) \times p(h)dh$ . The resulting  $p(h|n)$  is the so-called Beta distribution.]
- (d) Show the PDF  $p(h|n)$  has the maximum value at  $h = \frac{n}{N}$ , the mean value  $\frac{n+1}{N+2}$ , and the variance  $\frac{(n+1)(N-n+1)}{(N+2)^2(N+3)}$ .

**Problem 3** (15 points) Consider a container containing an ideal gas. The container is kept at a constant temperature by the environment. Initially, the gas occupies half the container, due to a partitioning wall at the center of the container. However, the partitioning wall has an externally controllable mechanism by which it can open a large opening at its center suddenly (a bit like a camera aperture). As this mechanism is activated, the gas quickly expands to the entire volume of the container, doubling the volume. Now, one can ask—what is the probability that the state of the gas will evolve back to its initial state, in which it occupied only one partition? Since the microscopic laws that govern the dynamics of the gas (electromagnetism and gravity) are time-reversal invariant, such an evolution in time *is clearly a possibility*. The question is *how* possible is it?

- (a) A simple way to estimate this probability is to calculate at a given time, the probability of a single molecule to be in half the volume, and then exponentiate the number  $N$  times, assuming all molecules are independent, and  $N$  is the number of molecules. Estimate the probability this way, using  $N = 200$ , a smallish number that is still much larger than 1, and  $N = 10^{23}$ , for a typical macroscopic amount.
- (b) Note that a small probability does not necessarily mean that the event will not happen. A more realistic question is in what time scale would the event occur once? To estimate *the lower bound* of this time scale, we must know the “relaxation time scale”—the time scale in which the system readjusts locally. The relaxation time for a gas system in a typical ambient condition is well-known: it is about 0.1 ns. Estimate the lower bound of the time scale, in unit of years, in which the “spontaneous volume contraction” will occur for  $N = 200$  and  $N = 10^{23}$ .
- (c) According to recent studies (Phys. Rev. E, vol. 60, 2721 (1999) and subsequent papers citing it), the following identity holds.

$$\frac{P_F(\Delta S)}{P_R(-\Delta S)} = e^{\frac{\Delta S}{k_B}}$$

where  $P_F(\Delta S)$  is the probability for a forward process involving  $\Delta S$ , and  $P_R(-\Delta S)$  is the probability for its time-reversed process. If we take the forward process as the expansion process after the partitioning wall opened, then clearly  $P_F$  must be close to, or practically equal to, 1. Assuming ideal

gas, for which the entropy function is well-known (Eq. 6.13), calculate  $P_R(-\Delta S)$ , and compare your answer with the answer for part (a).

**Problem 4** (30 points) *Poincaré period*. This problem will show you how to estimate the Poincaré period.

- (a) Consider two oscillatory functions  $\psi_1 = \exp(-i\omega_1 t)$  and  $\psi_2 = \exp(-i\omega_2 t)$ . We assume that  $\omega_1 \neq \omega_2$  and furthermore that they are incommensurate with each other. We can interpret  $\psi_1$  and  $\psi_2$  as representing two points on a unit radius circle. As written, at  $t = 0$ , the two points coincide. After some time the two points will be at a finite angular distance away from each other, since  $\omega_1 \neq \omega_2$ . The question one can ask is: how long would it take for the two points to come back to the zero angle position within a small tolerance  $\Delta\theta$ ? [Note that  $\Delta\theta$  here can be identified with  $\epsilon/\sqrt{2}$  in Eq. 5.22.] Now, the first point has the period of  $T_1 = 2\pi/\omega_1$  and it spends time  $t_1 = T_1\Delta\theta/(2\pi)$  in the “sweet zone” ( $\Delta\theta$ ) per revolution. For the second point,  $T_2 = 2\pi/\omega_2$  and  $t_2 = T_2\Delta\theta/(2\pi)$ . We define *coincidence* as the state in which both of these points are in the sweet zone. How frequently this coincidence occurs is characterized by the recurrence period. In order to figure out the recurrence period, it is helpful to consider the following function  $t_{12}(\theta_1)$ . Without loss of generality, assume  $T_1 > T_2$ . Consider the moment when point 2 is just entering the sweet zone. Point 1 can be anywhere on the circle at this moment. Let its position be  $\theta_1$  ( $-\pi < \theta_1 \leq \pi$ ). As a function of  $\theta_1$ , we can calculate how long, if at all, the two points will be in the sweet zone together before point 2 leaves the sweet zone after time  $t_2$  has passed. This *duration of coincidence* as a function of  $\theta_1$  is defined as  $t_{12}(\theta_1)$ . Obtain this function.
- (b) (This part is optional, since it is not absolutely necessary. However, you must read this part, and understand the final result. See the next part for a quicker way of proving the final result.) With the function  $t_{12}(\theta_1)$  thus obtained, one can calculate the *average coincidence lifetime*  $\tau_C$  as

$$\tau_C = \frac{\text{the average of } t_{12}}{\text{the probability of the coincidence}}$$

Note that the probability of the coincidence is proportional to the extent of  $\theta_1$  in which  $t_{12}(\theta_1)$  is non-zero.  $\tau_C$  represents the average duration of the coincidence given the condition that a coincidence happened. Show that

$$\frac{1}{\tau_C} = \frac{1}{t_1} + \frac{1}{t_2}$$

- (c) Explain the last result by considering the following. Suppose that a coincidence is observed at time  $t$ . Consider the probability that this coincidence

will be broken within the next infinitesimal time interval  $dt$ . By definition, this probability is  $dt/\tau_C$ . It can also be expressed in terms of  $t_1$ ,  $t_2$ , and  $dt$ . Show clearly that this consideration leads exactly to the above result (“Matthiessen’s rule”).

- (d) Now generalize to the case when there are  $M$  oscillators with mutually incommensurate periods. By using the same argument, prove that

$$\frac{1}{\tau_C} = \sum_{i=1}^M \frac{1}{t_i}$$

where  $t_i \equiv T_i \Delta\theta / (2\pi)$  and  $T_i$  is the period of the  $i$ -th oscillator.

- (e) In the limit of running the system to the infinity of time, we can express the probability of coincidence in two ways. The first way is simple:  $(\frac{\Delta\theta}{2\pi})^M$ . The second way is  $\tau_C / T_{pc}$ , where  $T_{pc}$  is the recurrence period, or the Poincaré cycle. By equating these two quantities, and using the results above, show that

$$T_{pc} = \frac{2\pi}{\omega_{ave}} \frac{1}{M} \exp \left[ (M-1) \log \frac{2\pi}{\Delta\theta} \right]$$

where  $\omega_{ave}$  is the average frequency of the  $M$  oscillators.

- (f) As an example of a classical mechanical system, consider normal modes of linearly coupled oscillators as applicable to the molecular vibrations in a one dimensional solid. The typical frequency is the Debye frequency so that  $2\pi/\omega_{ave} \sim 10^{-12}$  sec. If there are 101 atoms in a linear chain, then  $M = 100$  (excluding one translational mode that has zero frequency). Evaluate and discuss the value of  $T_{pc}$ .
- (g) As a quantum mechanical example, we may consider an electron gas. When this system goes out of equilibrium (due to an external field or a temperature gradient), it relaxes to a local equilibrium by collision processes. This time scale is what we discussed in class as  $\tau_X$ . By a conservative estimate,  $\tau_X \sim 1$  ns, while it is typically *much* shorter than 1 ns. Note that  $\tau_X$  gives a lower bound for the energy width  $\Delta E$  through the Heisenberg uncertainty relation. To estimate the corresponding lower bound of the number of frequency modes, one must divide  $\Delta E$  by the energy increment of the system. This is roughly<sup>1</sup>  $\hbar^2 4\pi^2 / (2mL^2)$  where  $L$  is the sample size or the mean free path  $v_F \tau_X$ , whichever is larger. So, for  $\tau_X \sim 1$  ns, we have  $L \sim v_F \tau_X \sim 1$  mm at least, if  $\hbar v_F \sim 5$  eV Å. Estimate  $M$  based on these parameters and the corresponding  $T_{pc}$ . Discuss the relationship between the irreversibility

---

<sup>1</sup>This estimate is based on the independent particle picture. In an interacting system, this estimate will tend to become smaller, e.g., due to the formation of “heavy fermions.”

time scale (note:  $\tau_X$  is the time scale in which the local equilibrium is established) and  $T_{pc}$ , if any. [Hint:  $\hbar c = 1973 \text{ eV \AA}$ , and  $mc^2 = 0.511 \text{ MeV}$  would be useful.]

**Problem 5** (15 points) The *entropy function* of a PDF is defined as

$$s = - \sum_j p_j \log p_j \quad j = 1, 2, \dots, N$$

where the random variable is assumed to be discrete, and the extension to a continuous variable is obvious (while such an extension is not without an issue—see LN 5). Note that  $p_j \geq 0$ , by definition. If  $p_j = 0$ , then it contributes to 0 to the sum, since  $0^+ \log 0^+ = 0$ .

- (a) Show that  $k_B \cdot s$  becomes the “Boltzmann entropy”  $S = k_B \log N$ , if  $p_j$  is uniformly distributed over  $N$  possible outcomes.
- (b) Prove that for any non-uniform distribution,  $s$  is smaller than the one in the previous part. [Hint: Here, the Lagrange multiplier method is the way to go. As there is a constraint,  $\sum_j p_j = 1$ , on the  $N$  variables  $\{p_j\}$ , one examines the extrema of the function,  $f(\{p_j\}) = - \sum_j p_j \log p_j - \alpha(1 - \sum_j p_j)$ . Get  $N+1$  coupled equations to solve,  $N$  by differentiating  $f$  and 1 from the constraint equation itself, and solve them for  $N+1$  unknowns ( $\{p_j\}$  and  $\alpha$ ).]