Physics 112L Fall 2023 Lab Four

Exercise 4-1: In Lab 3 you wrote a code in C or python to compute the average energy $\langle E \rangle$, specific heat $C$, entropy $S$, and free energy $F$ for the 1D Ising model for an $N = 10$ site linear chain. Make a copy of that code and modify it to compute also $\langle S_0 \rangle, \langle S_1 \rangle, \cdots, \langle S_9 \rangle$. Can you prove your answer? (It’s a bit tricky!)

Background One:

A very commonly used quantity in statistical mechanics is the ‘correlation function’. Explained in words, the correlation function measures whether the values of different quantities are connected to each other. We encounter this notion all the time outside of physics of course. If I were to define two variables: length of time studying for a class and final course grade, we would find these are not independent. There is no direct connection - some students who work hard do poorly and some students who don’t work hard do well, but on average a student who studies a lot gets a higher grade. On the other hand, there are things that are unrelated. Your course grade in Physics 112L is probably unrelated to the scoring average of LeBron James in the 2023-24 NBA season.

The precise mathematical definition of a correlation function for two quantities $x$ and $y$ is

$$ C(x, y) \equiv \langle xy \rangle - \langle x \rangle \langle y \rangle $$  \hspace{1cm} \text{(1)}

If $C(x, y) = 0$ we say the variables are uncorrelated.

Exercise 4-2: A quantity $x$ can take two values, $x = 2$ with probability $p = 0.3$, and $x = 5$ with probability $p = 0.7$. A second quantity $y$ can take three values, $y = 1$ with probability $p = 0.5$, $y = 3$ with probability $p = 0.4$, and $y = 4$ with probability $p = 0.1$. The probabilities for the different values of $x$ are independent of those of $y$ and vice versa.

What is $\langle x \rangle$?
What is $\langle y \rangle$?
What are the six possible values of the pairs $x, y$?
What is the probability of the each of these pairs?
What does your list of probabilities add up to? What is the value of $xy$ for each these pairs?
What is $\langle xy \rangle$?
What is the correlation function $C(x, y)$?
Explain why your result is reasonable.
Background Two:

In the Ising model, we define the ‘spin-spin correlation function’ for the spin on site \(i = 0\) and the spin on some other site farther down the chain as, to be

\[
C(S_0, S_1) = \langle S_0 S_1 \rangle \\
C(S_0, S_2) = \langle S_0 S_2 \rangle \\
C(S_0, S_3) = \langle S_0 S_3 \rangle \\
\vdots \\
C(S_0, S_9) = \langle S_0 S_9 \rangle
\]  
(2)

A more compact notation is to call \(C(r) = \langle S_0 S_r \rangle\) and refer to \(C(r)\) as the spin-spin correlation function at separation \(r\).

**Exercise 4-3:** Explain why, in Eq. 2, we do not need to subtract anything off as in Eq. 1. You might find your answer to Ex. 4-1 useful.

**Exercise 4-4:** In Lab 3 you wrote a code in C or python to compute the average energy \(\langle E \rangle\), specific heat \(C\), entropy \(S\), and free energy \(F\) for the 1D Ising model for an \(N = 10\) site linear chain. Make a copy of that code and modify it to compute also the ‘spin-spin’ correlation functions \(C(r)\) of Eq. 2. What do you get for \(T = 0.5, T = 1.0, \) and \(T = 1.5\) if you set \(J = 1\)?

**Exercise 4-5:** Make plots of \(\ln C(r)\) versus \(r\) for the three temperatures in Ex. 4.4. What are the shapes of your plots? What does this tell you about how \(C(r)\) depends on \(r\)?

Background Three: For high temperatures, i.e. above the phase transition temperature, correlation functions decay \textit{exponentially} as the degrees of freedom become farther separated. What this tells you is that the different variables lose knowledge of each other very rapidly as their distance apart grows. We write

\[
C(r) = A e^{-r/\xi}
\]  
(3)

where \(\xi\) is called the ‘correlation length’.

**Exercise 4-6:** What is the correlation length \(\xi\) for each of the three temperatures in Ex. 4.5? For each \(T\), compare your values for \(\xi\) with the value of \(-\ln(\tanh J/T)\).

**Exercise 4-7:** Write a code to solve the Ising model on a \(4 \times 4\) lattice. Compute and plot \(\langle E \rangle\) versus \(T\), \(C\) versus \(T\) and \(S\) versus \(T\).