Discussion 4

Name and section: ______________________________

1. Consider a four level system of N particles with energies $E_1 = 0$, $E_2 = 5$, $E_3 = 12$, and $E_4 = 20$. The probabilities are normalized: $\sum_{i=1}^{4} p_i = 1$.

   (a) Subject to the constraint that the probabilities are normalized, maximize the energy. What are the probabilities $p_i \quad \forall \quad i \in [1, 4]$ for this system with maximized energy?

$$
\begin{aligned}
p_1 = p_2 = p_3 &= 0 \\
p_4 &= 1
\end{aligned}
$$

   (b) Now, subject to to the same constraint, maximize the entropy. Again, give the probabilities for this state with maximum entropy.

$$p_1 = p_2 = p_3 = p_4 = \frac{1}{4}$$

   (c) What is the expected energy of the system with maximized entropy?

$$
\begin{aligned}
U_{\text{tot}} &= N\left(\sum_{i=1}^{4} p_i E_i\right) \\
&= \frac{1}{4} N\,(0 + 5 + 12 + 20) \\
&= \frac{37}{4} N
\end{aligned}
$$

   (d) What are the changes in energy ΔU and entropy ΔS in going from the system with maximum entropy to the system with maximum energy?

$$
\begin{aligned}
\Delta U &= U_{\max U} - U_{\max S} \\
&= 20N - \frac{37}{4} N \\
&= \frac{43}{4} N \\
\frac{\Delta S}{k_B} &= S_{\max U} - S_{\max S} \\
&= -1 \ln 1 + 4 \frac{1}{4} \ln \frac{1}{4} \\
&= -\ln 4
\end{aligned}
$$

2. Consider the function $f(x) = x^2 - 2x - 1$ for the following problems. We are trying to find the zeros of this function $f(x^*) = 0$.

   (a) Using Newton's iterative method for finding solutions of a function and using as your first guess $x_0 = 0$, do two iterations to find an estimate of a solution to this function. This will use the formula derived in class:

   $$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{1}$$

   where $f'(x)$ is the first derivative of the function f evaluated at the point x.

   $$\begin{aligned} f'(x) &= 2x - 2 \\ x_0 &= 0 \\ x_1 &= 0 - \frac{-1}{-2} \\ x_2 &= -\frac{1}{2} - \frac{1/4}{-3} \\ &= -\frac{5}{12} \end{aligned}$$

   (b) Using some other guess of a solution for x_0, do two iterations from that new starting point. Do the two starting points approach the same value?

   Depending on where you choose to start, it can approach the same answer or a different answer, and it may be difficult to tell exactly after only two iterations.

   (c) If you continued both parts above until convergence $n \to \infty$, would they converge to the same solution?

   Again, it depends on exactly what starting point you choose, it could or it may not.

   (d) This system is easily analytically solvable using several different possible methods. What are the exact solutions to this function?

   $$\begin{aligned} x^* &= \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \\ &= \frac{2 \pm 2\sqrt{2}}{2} \\ &= 1 \pm \sqrt{2} \\ &\approx (-0.414, 2.414) \end{aligned}$$

   (e) How do your estimates of the solutions using Newton's method compare to the true answer? Were the iterations approaching the correct solutions or were they diverging?

   The estimation in (a) gave us $x^2 \approx -0.417$ which is pretty close after only two iterations.

   For a quadratic function, Newton's method is guaranteed to converge exactly after infinite iterations, but from one starting point it will only give you one of the solutions.