Week 5 Warmups

Week 5 Warmup Problem 1
Demon thermometer G&T 1.8
Due (a) - (d) and (g) but all parts done

° First of all, what is a demon thermometer? It is a little creature with a "sack" that can store energy and trade it with particles of the system. Its energy is called Ed.

° Here is a Monte Carlo algorithm for the demon:

. Choose a particle in the system at random and make a trial change in one of its coordinates. In this case, it changes its Vx, Vy, Vz by a random number.

. Compute ΔE, the change in the energy of the system due to the trial change.

. If $\Delta E \le 0$, the system gives the surplus energy $|\Delta E|$ to the demon, $Ed \rightarrow Ed + |\Delta E|$, and the trial change is accepted.

. If $\Delta E > 0$ and the demon has sufficient energy for this change (remember that Ed is non- negative), then the demon gives the necessary energy to the system, $Ed \rightarrow Ed - \Delta E$, and the trial change is accepted. Otherwise, the trial change is rejected and the microstate is not changed.

. Repeat steps 1–4 many times.

. Compute the averages of the quantities of interest once the system and the demon have reached equilibrium.

° Let's get to the G&T problem ... I'm going to lump parts (a)-(d) together in my solution.

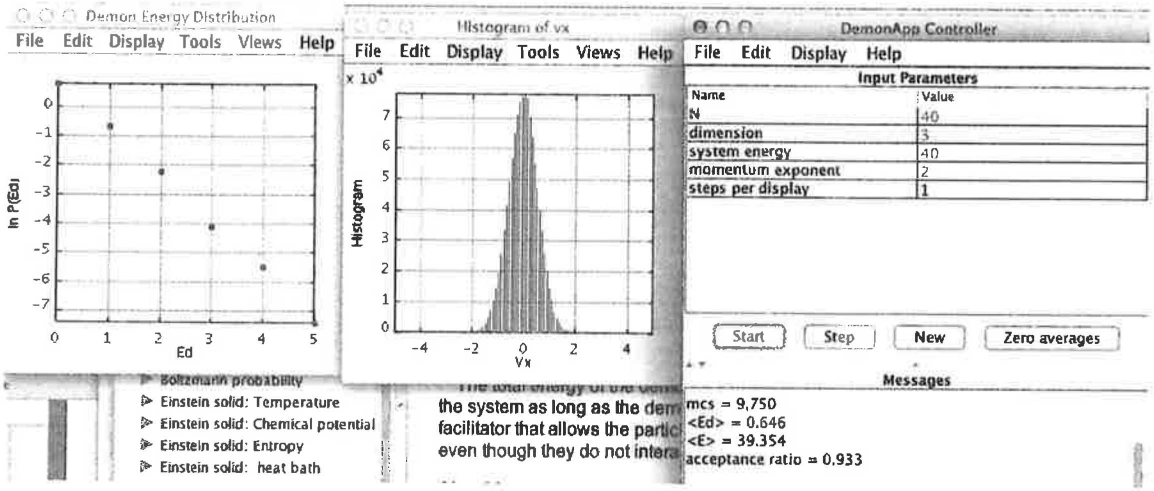
. (a) Run the simulation using the default parameters $N = 40$, $E = 40$, and $d = 3$. Does the mean energy of the demon approach a well-defined value after a sufficient number of energy exchanges with the system? One Monte Carlo step per particle (mcs) is equivalent to N trial changes.

. (b) What is <Ed>, the mean energy of the demon, and <E>, the mean energy of the system? Compare the values of <Ed> and <E>/N.

. (c) Fix $N = 40$ and double the total energy of the system. (Remember that Ed = 0 initially.) Compare the values of <Ed> and <E>/N. How does their ratio change? Consider other values of $N \ge 40$ and E and determine the relation between <Ed> and <E>/N.

. (d) You probably learned in high school physics or chemistry that the mean energy of an ideal gas in three dimensions is equal to (3/2) NkT , where T is the temperature of the gas, N is the number of particles, and k is a constant. Use this relation to determine the temperature of the ideal gas in parts (b) and (c). Our choice of dimensionless variables implies that we have chosen units such that k = 1. Is <Ed> proportional to the temperature of the gas?

Here is what it looks like to run the simulation ...



Here is a table of my results: I tried to run for over 30,000 mcs (Monte Carlo Steps) , zero the averages and then run for about another 30,000. I stayed with N=40 particles in 3 dimensions. I am noting "system energy" which G&T call E as Eo in the table below.

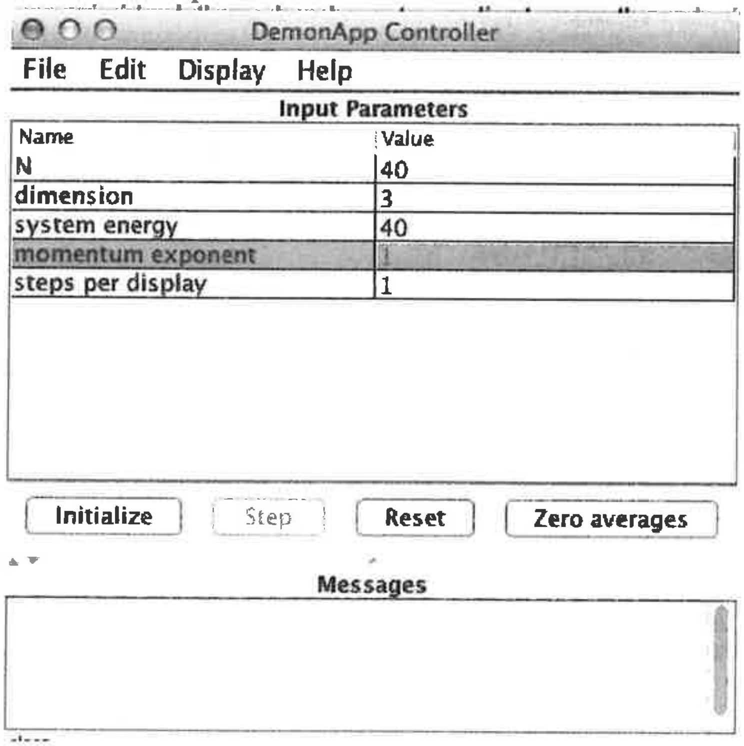
Eo	<Ed>	<E>	<E>/N	T = (2/3) <E>/N	<Ed>/(<E>/N)
40	0.655	39.345	0.98	0.653	0.668
80	1.308	78.692	1.967	1.31	0.665
120	1.959	118.041	2.951	1.96	0.664

So what's the take-home? We note that as we double and then triple the energy, Eo, given to the system, the typical demon thermometer's energy, <Ed>, also doubles and triples. If we look at the last column, the ratio of the typical demon to typical gas particle energy, it is suspiciously like 0.666 = 2/3, independent of Eo. Finally, if we use the high school definition of temperature, it is exactly equal to the demon energy. (I'd settle for proportionality and be happy.) Good demon!

(e) Here is what G&T want:

(e) Suppose that the energy momentum relation of the particles is not $\varepsilon = p^2/2m$, but is $\varepsilon = cp$, where c is a constant (which we take to be 1). Consider various values of N and E as you did in part (c). Is the dependence of Ed on E/N the same as you found in part (d)? We will find (see Problem 4.30) that Ed is still proportional to the temperature.

For relativistic particle, E ~ p . So here we changed "momentum exponent" in the program from $E \sim p^2$ to $E \sim p$ to turn classical into relativistic particles.



And below are data for E_d and <E>/N with E_o = 40, 80, 120 as before

mcs = 19,750
<Ed> = 0.327
<E> = 39.673
acceptance ratio = 0.928

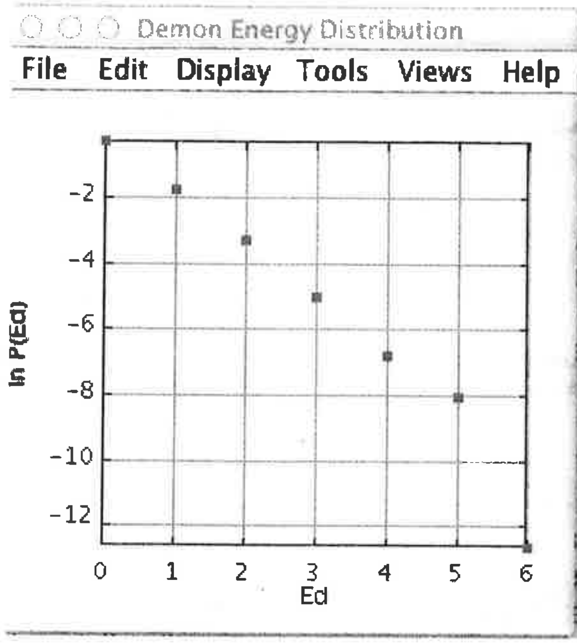
mcs = 23,500
<Ed> = 0.673
<E> = 79.327
acceptance ratio = 0.964

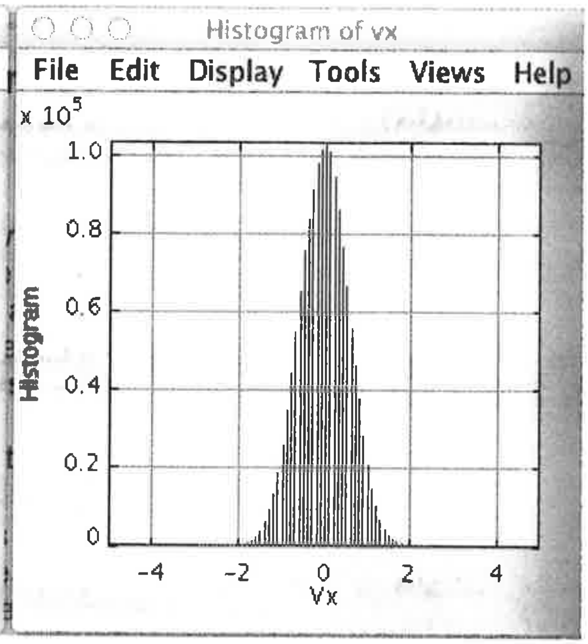
mcs = 26,250
<Ed> = 0.983
<E> = 119.017
acceptance ratio = 0.977

We conclude that again, Ed is proportional to <E>. <E>/N would be .99, 1.98, 2.97 or about 1, 2, and 3 for E_o = 40, 80, 120.
In each of these relativistic cases, E_d is about 1/3 <E>/N. In classical case, E_d is about 2/3 <E/N>. Interesting!

(f) and (g) These parts want us to read a histogram which bins the energy Ed, and reports on how often a certain Ed is found. (So for example, the average <Ed> is the average of the histogram, but the histogram has more info ... it is proportional to the probability distribution p(Ed).

There is a histogram-labelled plot, but this is Vx. I believe that these parts of the problem are referring to the plot on the left, which is labelled p(Ed), the probability density that the demon has energy Ed.



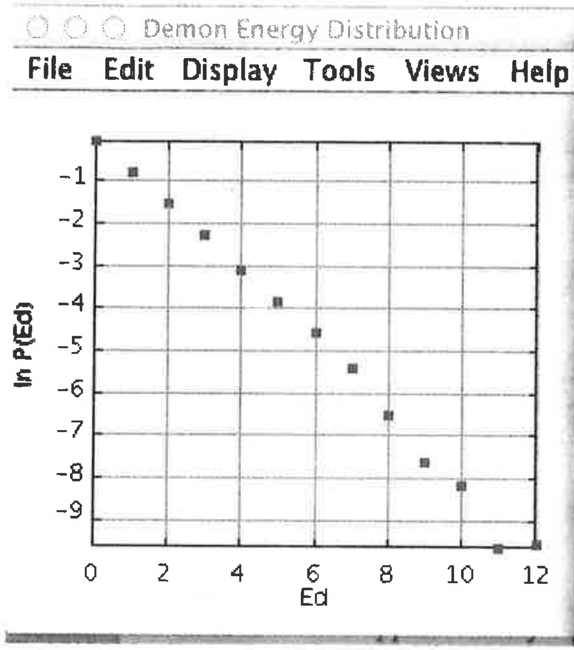


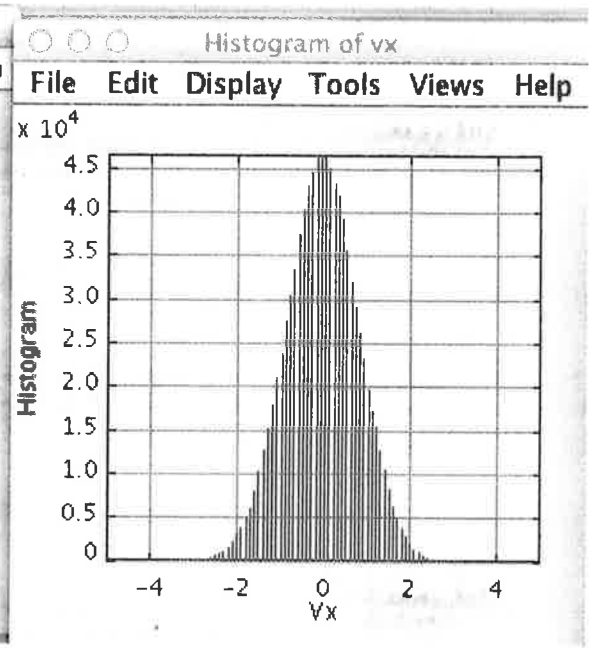
It looks like the likeliest energy for the demon is a low one, and it becomes progressively less likely to have a higher energy. In fact, since the log plot is a straight line, it seems as if this is an exponential form as the problem suggests for part (g).

- (g) Verify the exponential form of $p(Ed) = Ae-\beta Ed$, where A and β are parameters. How does the value of $1/\beta$ compare to the value of Ed? We will find that the exponential form of p(Ed) is universal, that is, independent of the system with which the demon exchanges energy, and that $1/\beta$ is proportional to the temperature of the system.

- The slope appears to be -8/5 for the case above, where <E>/N was about 1, <Ed>was about 2/3 (and thus T is about 2/3). If this slope is considered $-\beta$, then $1/\beta$ is around 5/8. Is 5/8 approximately equal to 2/3? Sure! 0.625 vs. 0.666. Close!

- We can try another Ed too, and will get similarly good results. See below:





Here, <Ed> was about 1.3, because Eo was set to 80. The slope is about -5.5/7 = 0.786 = - β so 1/ β = 1.27 which is marvelously close to 1.3 the demon typical energy ... and also the temperature :-)

(h) Finally, what makes this demon an ideal thermometer? Well besides the cool factor of having your very own demon to tell you the temperature, it is

> accurate: always telling you T by virtue of its expected energy <Ed>

> tiny, so that it doesn't take a lot of energy out of the system. If I put Eo in, less than 1% is typically in the posession of the demon. (Hence demonic posession, but on a very manageable size scale ;-)