HW1: Mathematical Modeling (hard copy solution is due on Feb 10, class time)

1. Given a Hamiltonian for N harmonic oscillators

$$H = \sum_{i=1,\dots,3N} \frac{p_i^2}{2m} + \frac{m\omega^2}{2} x_i^2$$

Compute the volume in phase space such that $H < E$. i.e. $\Phi = \int_{H<E} dx \cdot dp$

(a useful formula – a volume of a sphere in D-dimensions with radius of 1 is $\dfrac{\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)}$)

The entropy, S, in the microcanonical ensemble (the set of all states with equal energy) is defined as logarithm of the phase space volume in the layer between E and $E + \Delta E$. Find an expression for the entropy, and for the inverse temperature $\dfrac{1}{T} = \dfrac{dS}{dE}$

2. For a given total energy E_0 compute and compare a time average and a phase space average of x^2 for the harmonic oscillator. The one-dimensional Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2$$

Reminder: the time average is defined as $\left\langle x^2 \right\rangle = \frac{1}{t}\int_0^t x^2(t')\,dt'$, we will be mostly interested in the long time limit. The phase space average is

$$\overline{x}^2 = \frac{\int \delta(E_0 - H)\, x^2 \cdot dx \cdot dp}{\int \delta(E_0 - H) \cdot dx \cdot dp}$$

3. In preparation for future adventures this exercise should prepare you for doing calculations on the Mueller potential. The Mueller potential is a two dimensional energy function which is a sum of exponential functions. I attach five files. One called mueller.eps is a contour plot in two dimensions of the potential energy. The others (matlab files) are mueller.m gauss1.m gauss2.m gauss3.m and gauss4.m and they compute the potential, and the first and second derivatives of it. Your goal is to figure out the code and to generate a contour plot that will be as similar as possible to Mueller.eps