1. (10 points) The virial expansion of the pressure of the 3D fluid of hard spheres is
\[ \frac{p}{nk_BT} = 1 + 4\eta + 10\eta^2 + 18.36\eta^3 + 28.23\eta^4 + 39.52\eta^5 + 56.5\eta^6 \ldots \]
Show that this series is well approximated by the Carnahan-Starling equation of state
\[ \frac{p}{nk_BT} = 1 + \eta + \eta^2 - \eta^3 \]
Determine the isothermal compressibility. Determine the Helmholtz free energy for the hard sphere gas by insisting that the result approach the ideal gas in the limit of low density.

2. (20 points) Consider N noninteracting Boltzmann particles in a three dimensional quantum harmonic oscillator. The energy of the system (shifted by \( \frac{3N\hbar\omega}{2} \)) is given by
\[ E = \sum_{j=1}^{N} \hbar\omega(l_{xj} + l_{yj} + l_{zj}) \]
Use that as the energy throughout the problem.

a) First determine analytical expressions for the dimensionless energy per particle and the specific heat
\[ U = \frac{1}{N\hbar\omega}\langle E \rangle \quad \text{and} \quad C = \frac{1}{nk_BT}\langle (E^2) - \langle E \rangle^2 \rangle \quad \text{Use} \quad Z(T) = \frac{1}{N!}(Z_0(T))^{N} = \frac{1}{N!}(Z_0(T))^{3N}. \]

b) Write a Metropolis Monte Carlo program to simulate this system. Develop the code initially with just a few particles. Once you are convinced it is working, try simulating 100 particles. One Monte Carlo step consists of attempting one trial move for all N particles. Choose the particles in order and attempt a trial change of \( l_{xj}, l_{yj}, l_{zj} \) by plus or minus 1 for each quantum number. If the state is illegal (i.e. one or more of the l’s is negative) reject the trial state and move on. If the state is legal and the energy goes down accept the trial state. If the energy goes up, accept the trial state a fraction of the time equal to the Boltzmann factor \( e^{-\beta\Delta E} \) by comparing the Boltzmann factor with a uniformly distributed pseudorandom number. If the trial state is rejected leave the system in the original state. Simulate the system at an evenly spaced set of temperatures \( 0 < \frac{k_BT}{\hbar\omega} \leq 5 \).

You will need to let the system equilibrate at each new temperature before collecting statistics. Keep track of the following quantities:
\[ \langle E \rangle, \quad \langle E^2 \rangle \quad \text{where} \quad \langle f \rangle = \frac{1}{N_{MCS}} \sum_{k=1}^{N_{MCS}} f_k \]. You will need to choose an appropriate value for the number of Monte Carlo Steps \( N_{MCS} \) used to give averages with a reasonably small uncertainty. Plot the dimensionless internal energy per particle and specific heat as functions of \( \frac{k_BT}{\hbar\omega} \) and compare with the exact results. Notice that the crossover from quantum to classical behavior happens at temperatures on the order of the level spacing independent of the number of particles. Note, this is very different from the solution for identical particles with the correct Fermi or Bose statistics that we will do later in the semester.
3. (20 points) The Ising model in zero field is given by

\[ Z_N(T) = \sum_{(s_i = \pm 1)^N} \exp\left( K \sum_{(ij)} s_i s_j \right). \]

Where \( K = \frac{J}{k_B T} \). For \( N \) spins there are \( 2^N \) configurations in the sum.

a) Show the dimensionless internal energy and the dimensionless specific heat determined from derivatives of the free energy can be written as

\[ \frac{U}{NJ} = -\frac{1}{N} \left( \sum_{(ij)} s_i s_j \right) \quad \text{and} \quad \frac{C}{Nk_B} = K^2 \left( \left( \sum_{(ij)} s_i s_j \right)^2 - \left( \sum_{(ij)} s_i s_j \right)^2 \right). \]

Express these quantities terms of ratios of the sums over states.

b) For the two dimensional model (\( N=LxL \)) with periodic boundary conditions, show that the partition function can be expressed as a low-temperature expansion

\[ Z_N(T) = \exp(2NK) \sum_{k=0}^N g_k x^{2k} \]

where \( x = \exp(-2K) \) and the coefficients \( g_k \) are the number of configurations with energy \( 4Jk \) above the ground state. Determine the first few nontrivial coefficients for a large system (\( N>>1 \)). Show that in general \( \sum_{k=0}^N g_k = 2^N \). Show that the energy and heat capacity can be written

\[ \frac{U-U_0}{J} = \frac{4 \sum_{k=0}^N k g_k x^{2k}}{\sum_{k=0}^N g_k x^{2k}} \quad \text{and} \quad \frac{C}{k_B} = 16K^2 \left( \frac{\sum_{k=0}^N k g_k x^{2k}}{\sum_{k=0}^N g_k x^{2k}} - \left( \frac{\sum_{k=0}^N g_k x^{2k}}{\sum_{k=0}^N g_k x^{2k}} \right)^2 \right). \]

c) Determine all \( L^2 + 1 \) coefficients for small systems with \( L=2,3,4 \) (and 5, 6 if you can) by a brute force computer summation. Check that they sum to \( 2^N \).

d) Determine the internal energy and heat capacity numerically for these cases as functions of \( \frac{k_B T}{J} = K^{-1} \) and plot.

4. (10 points) The Mathematica code posted on the web site can be used to calculate the partition function coefficients of the 2-dimensional Ising model for much larger systems than brute-force allows. The code is based on Onsager and Kauffman’s 1949 exact solution. **The code might not work well for the smallest values of \( n \) and \( m \) but is well-checked for larger values.**

a) Test the code against your exact brute-force calculations for \( L=2,3,4 \) (and 5, 6 if you can) to show they give the same coefficients.

b) Use the code to determine the coefficients for much larger systems: \( L=16 \) or larger can be done in a reasonable time. Note that \( L=16 \) includes \( 2^{256} \approx 1.16 \times 10^{77} \) configurations. Determine the internal energy and heat capacity numerically for these cases as functions of \( \frac{k_B T}{J} = K^{-1} \) and plot. Discuss interesting behaviors.

c) Explain why the logarithm of the coefficients as a function of \( k \) represents the entropy as a function of energy. Plot the entropy and discuss the behavior.