NOTE: As this assignment is quite short, the report and directory itself are not split up exactly into exercises like previous assignments.

1 Directory Structure

All the functions already written are saved in the main directory. Any extra scripts written to plot or parse data are also saved in this directory. Any data files are stored in the subdirectory 'files' and all plots are stored in the subdirectory 'plots'.

2 Variational Wave Function

The main metropolis program was compiled and run using the README file provided. It was edited slightly to stored files in the data directory but all changes made were superficial. Once ran once, we had all the data needed for the rest of the analysis.

The end goal of this exercise is to calculate the fraction of particles in the Bose-Einstein condensate. However, in order to do this we must first find a good approximation of the wave function. This is done by taking a trial function which is very similar to what we would expect and varying a parameter to find a better approximation. The parameter we are interested in is called a_1 and the trial function in terms of this parameter is given by

$$f(r) = exp\left(-\left(\frac{a_1}{r}\right)^5\right)$$

Here we want to find the value of a_1 that minimises the expected energy in order to find the best approximate wave function. This method is called the variational method and it works because we are looking for the ground state wave function so we want the energy to be minimised.

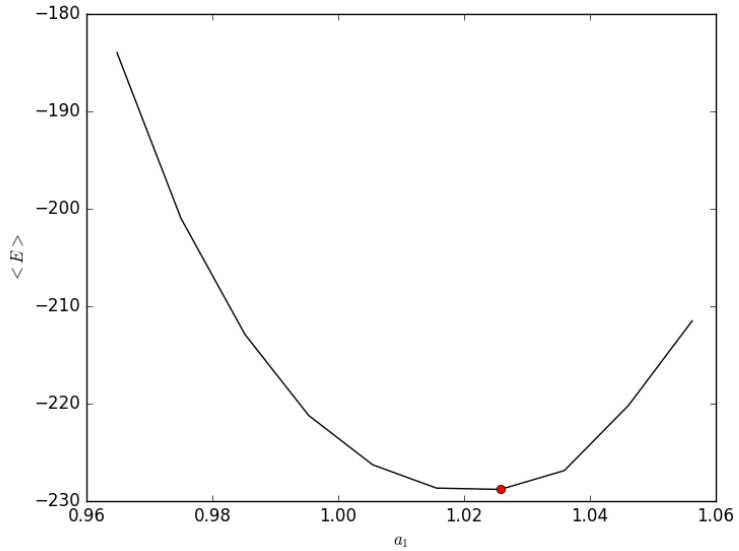

Figure 1: Expected energy vs a_1

When the simulation was run, data for the expected energy vs a_1 was saved in the file 'energy_vs_a1'. Using this file the script a1_plot.py plots a graph of the expected energy vs a_1 (see *Figure 1*) and finds the value of a_1 that minimises this energy. The value of a_1 found to minimise the expected energy is

$$a_1 = 1.026$$

in the units used in this simulation. Converting to Angstroms by multiplying by 2.56 we have

$$a_1 = 2.627\mathring{A}$$

This agrees extremely well with the value found by McMillan in 1964, $a_1 \approx 2.6\mathring{A}$. Therefore we can continue the rest of the analysis with confidence in the value chosen for a_1.

3 Pair Distribution Function

Now that we have a good approximate ground state wave function we want to plot both the pair distribution function and the single-particle density matrix for a_1 found previously.

The python script 'pair_dist.py' plots both of these curves and using the large distance behaviour of the single-particle density matrix, the fraction of the Bose-Einstein condensate was found. The two plots are shown below

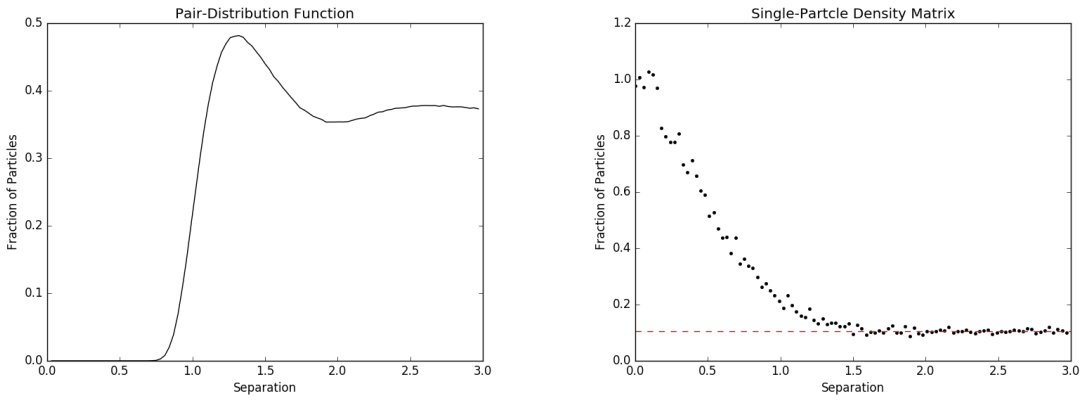

Figure 2: Plots of both the pair-distribution function and the single-particle density matrix

The most important plot relating to Bose-Einstein condensation is the single-particle density matrix. This is an important quantity because when it's normalised with respected to the density (which is the function plotted above) it was shown by the physicists Penrose and Onsager that for large separations, this normalised quantity approaches the fraction of particles in the zero-momentum state. Bose-Einstein condensation occurs when a large fraction of atoms exist in this state and so looking at the graph on the right above, we can see that because this curve doesn't approach zero, rather it approaches some finite value, Bose-Einstein condensation is occurring. We can quantify the fraction of atoms in this state by finding out what value the curve approaches in the large separation limit. This was done by taking the last 20% of the data points i.e. where it has settled, and taking an average. Doing this the fraction of atoms in the Bose-Einstein condensate was found to be

$$f_{BE} = 0.106 = 10.6\%$$

This agrees very well with McMillan's result of 11% which is quite close to the theoretical value of 8% calculated by Penrose and Onsager.