

PH-M31 Assignment Question 3

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1. Question 3 - Add the routine that computes the energy and the magnetisation to the MPI code. Describe your modifications.

The current MPI program takes measurements in parallel and then afterwards does an MPI_Reduce of the local energy and magnetisation values into total values for the global lattice, then we must perform statistical analysis on the results for the global lattice, we can perform this analysis serially as there is no real benefit to parallelizing this section of code because we are working on a relatively small amount of data points and jackknife bins.

Define a function perform the statistical analysis on the energy and magnetisation observables which we will pass to the function. The function will perform averaging, binning and jackknifing. Jackknifing is required to remove bias from the system.

The function begins by taking the simple average of the observable by summing over all measurements of the observable and then dividing by the number of measurements. Then we divide the data into bins, where the number of data points inside each bin is given by (number of measurements/number of bins). We then take partial averages on the bins by dividing each bin by the number of data points in the bin.

Then we form the jackknife bins using the standard formula of $jackbin[i] = (1/(N-1)) * \text{Sum}(\text{bin}[j])$, where $i \neq j$.

Then we perform analysis on the jackknife bins to compute the error in the observable, where the $(\text{Error})^2 = (\text{Standard Deviation})^2$.

Using $(\text{Standard Deviation}) = ((N-1)/N) * \text{Sum}((jackbin[i] - \text{Average})^2)$. We then take the square root to compute the error in the observable value.

Then print values to the console/output file.