Monte Carlo simulation of an Ising spin glass

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1 Part 1

We start by implementing the Exchange Monte Carlo algorith for the Ising spin glass, ehich has a Hamiltonian $H(S) = -\sum_{<i,j>} J_{ij} S_i S_j$, where $S_i = \pm 1$ and J_{ij} are independent random variables with Gaussian distribution with mean zero and variance one. In order to extract these Gaussian numbers, the program $gauss.f$ which uses the Box-Muller algorithm is used. This generates an output file named $gaussian\_numbers.txt$ that is opened in the main program and stored in the $M(i,j)$ variable. Periodic boundary conditions are used.

The code simulates simultaneously with the Metropolis algorithm $2N_T\, replicas H(S^{(a,k)})$, $H(S^{(b,k)})$ of the system, all with the same J_{ij}, with $k = 1, ..., N_T$. The replicas are in different random spin configurations and with temperature T_k linearly spaced in the range $[T_{min}, T_{max}]$.

Every n_{sw} MC steps (1 MCS = N attempted spin flips per replica), $N_T/2$ exchange moves are attempted between $S^{(a,k)}$ and $S^{(a,k+1)}$, and between $S^{(b,k)}$ and $S^{(b,k+1)}$, alternatively for all even k and for all odd k (so that a configuration can travel to all temperatures).

The input variables used are: $L = 20$ (linear size), $T_{min} = 1.0$, $T_{max} = 3.0$, $N_T = L \cdot L = 400$, $n_{sw} = 10$ (number of MCS between attempted exchange moves), $n_{meas} = 10$ (number of MCS between two successive measures), $n_{MCS} = 10000$ (total number of MCS).

The output is: a time series for the overlaps $Q^{(k)} = \sum_{i=1,N} S_i^{a,k} S_i^{b,k}$ and the energy $E^{(k)} = 1/2[H(S^{a,k}) + H(S^{b,k})]$ for each temperature $k = 1, ..., N_T$. The data is saved in an output file named $output\_all\_data$.

2 Part 2

The program is tested on the 2D Ising model by setting $J_{ij} = 1$ (which gives the Ising model). The same input variables described in the last section are used, except for the maximum temperature, which is set to $T_{max} = 500$ in order to compare it with the results of Ferdinand and Fisher, using the program $ferdinand.f$. A second program is created in order to compute the mean energy $\overline{\mathrm{E}}$ with its error for the various temperatures (estimating the error with binning), named $binning\_analysis.f90$. This program takes as input the file $energy\_output$ which has the energy values for the specified temperature range, and generates an output file named $mean\_e\_and\_error$.

In figures 1 and 2, the plots for the mean energy and error for each temperature are shown, the first one being for the model created in this project, and the second one being the results from Ferdinand and Fisher. Both plots are cut at $T_{max} = 300$ in order to visualize better the increasing bbehavior of the curve.

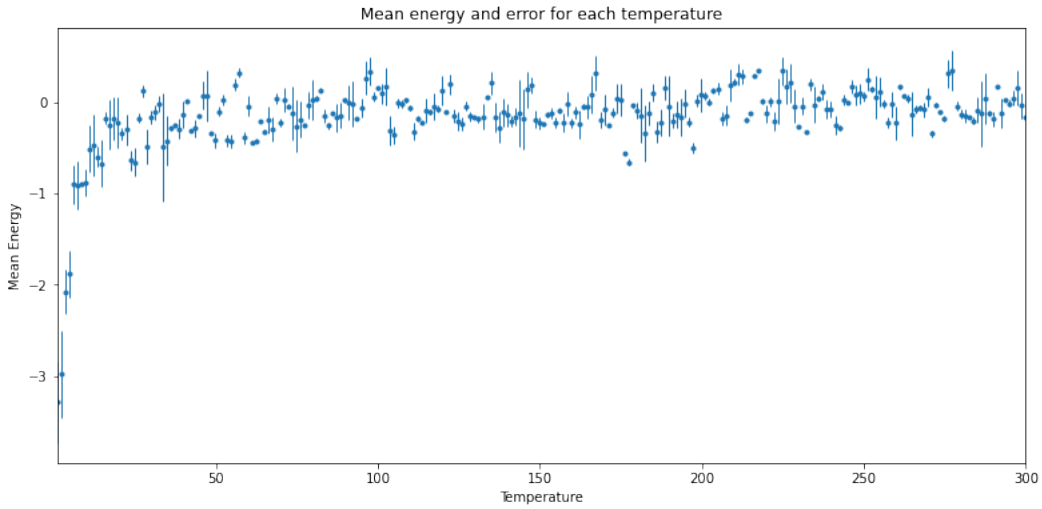

Figure 1: Mean energy and its error for each temperature, plotted with the data obtained using the program created in this project.

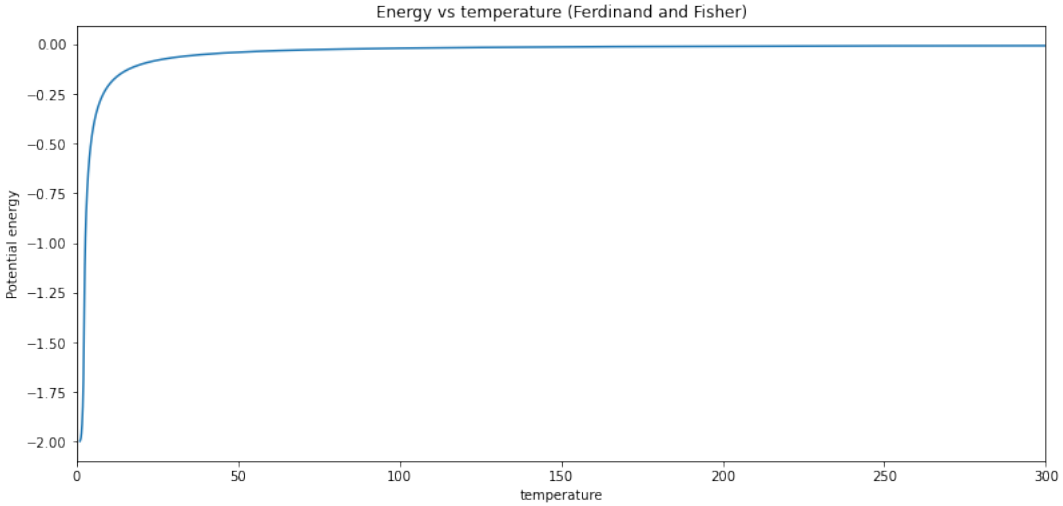

Figure 2: Mean energy and its error for each temperature, plotted with the data of Ferdinand and Fisher.

3 Part 3

A simulation is performed for the 3D spin glass with gaussian Jij with $d = 3$, $L = 4$, $Tmin = 0.2$, $Tmax = 2.0$, for 10^4 MCS, and it is repeated for 10^3 samples (different independent realizations of Jij). The histogram of $P(q)$ of the normalized overlap $q = Q/N$ for each temperature is computed, discarding the first $3 \cdot 10^3$ MCS and averaged over all samples, and two plots are made with the histograms for $T = 0.2$ and $T = 0.5$.

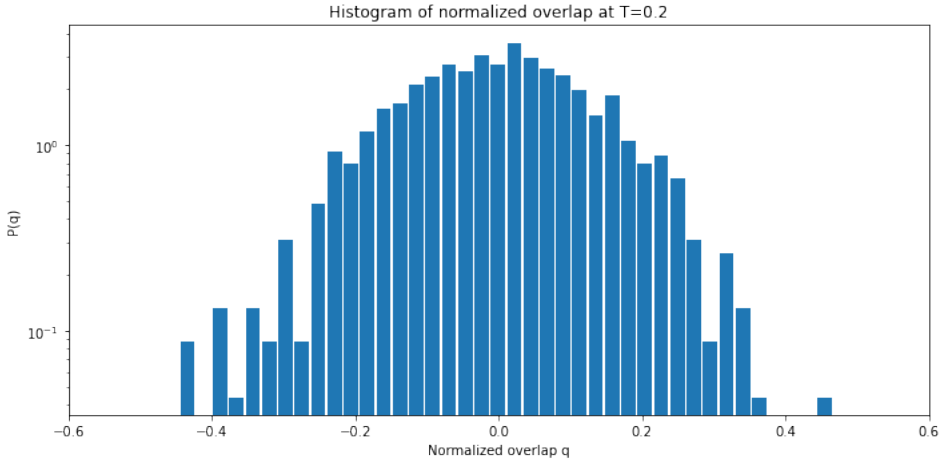

Figure 3: Histogram of the normalized overlap $q = Q/N$ at temperature T = 0.2 for a 3D spin glass.

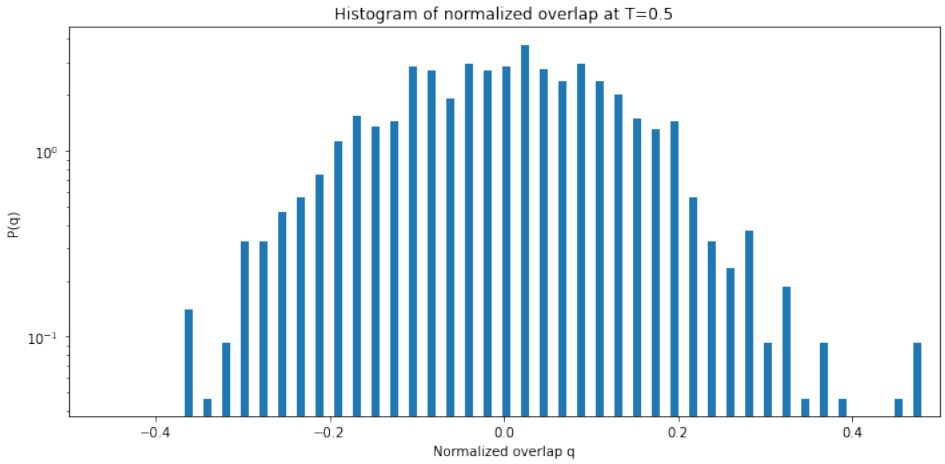

Figure 4: Histogram of the normalized overlap $q = Q/N$ at temperature T = 0.5 for a 3D spin glass.

If we compare these plots with Fig.2 and Fig.3 of Katzgraber et al., we can see that P(q) follows a different distribution; instead of having the peak at large q and the tail down to q=0, the histograms show the opposite behavior. There could be several reasons why the results don't match with those of Katzgraber et al. One could be because of insufficient equilibration, which means that the simulation has not been run long enough for the system to equilibrate, therefore the results may not be accurate. However this is not very probable, since the simulation has been done for $10^4\,MCS$ which should be enough to simulate an accurate representation of the system. The error might also be becasue of an incorrect calculation of the overlap, causing the results to differ from those of the article.

4 Part 4

A simulation is performed for the spin glass with gaussian Jij with $d = 3$, $L = 8$, $Tmin = 0.2$, $Tmax = 2.0$, for 10^6 MCS. The estimates of $\langle q^2 \rangle$ (where $q = Q/N$ is the normalized overlap) and $\langle E \rangle/N$ and their statistical errors (using binning) are computed, for the data in different intervals of time: $[10^4{:}3 \cdot 10^4]$ MCS, $[3 \cdot 10^4{:}10^5]$ MCS, $[10^5{:}3 \cdot 10^5]$ MCS, and $[3 \cdot 10^5{:}10^6]$ MCS. An output file named *mean_values.txt* is generated, having 9 columns: the first one being the temperature values, the second and third columns the mean values for q and E in the first time interval, and the same thing for columns 4 and 5 (second time interval), 6 and 7 (third time interval) and 8 and 9 (last time interval). Two different plots are made, one for $\langle q^2 \rangle$ (figure a 5) and another for $\langle E \rangle/N$ (figure 6).

It can be seen how both the normalized overlaps and the energies converge to equilibrium for the lowest temperatures. $\langle q^2 \rangle$ converges at around 0.9 for T = 0.2, while the curve for $\langle E \rangle/N$ shows a more lineal behaviour, but it starts to converge at 0.001 for T = 0.2.

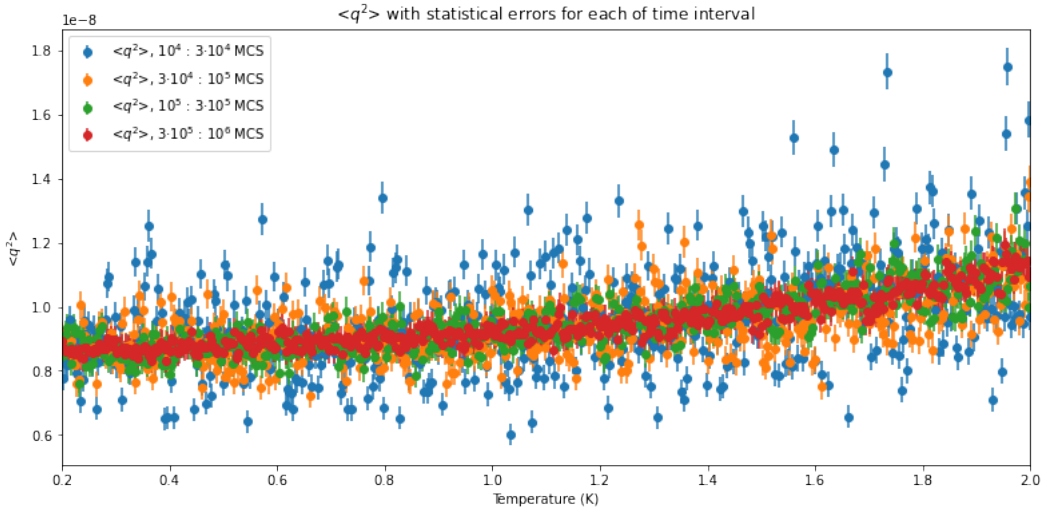

Figure 5: $\langle q^2 \rangle$ values and their statistical errors for each temperature and time interval.

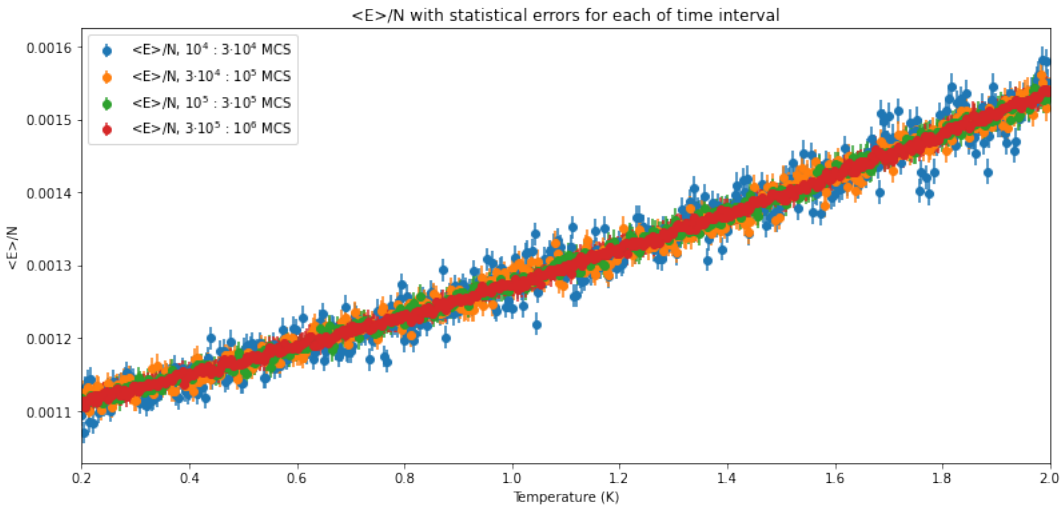

Figure 6: $\langle E \rangle / N$ values and their statistical errors for each temperature and time interval.

5 Part 5

Using only the data in the last time interval, $\langle q^2 \rangle$ and $\langle E \rangle$ are plotted as a function of temperature. The squared mean of the overlaps is shown in figure 7 and the mean values of the energies for each temperature in figure 8.

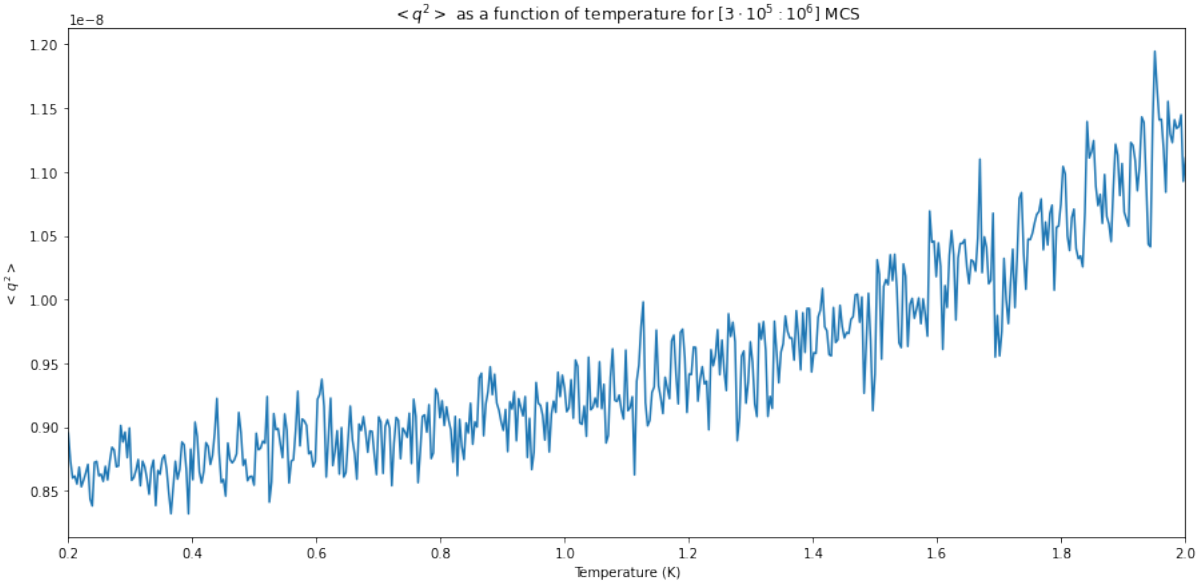

Figure 7: $\langle q^2 \rangle$ values as a function of temperature for the last time interval (from $3 \cdot 10^5$ to 10^6 Monte Carlo steps).

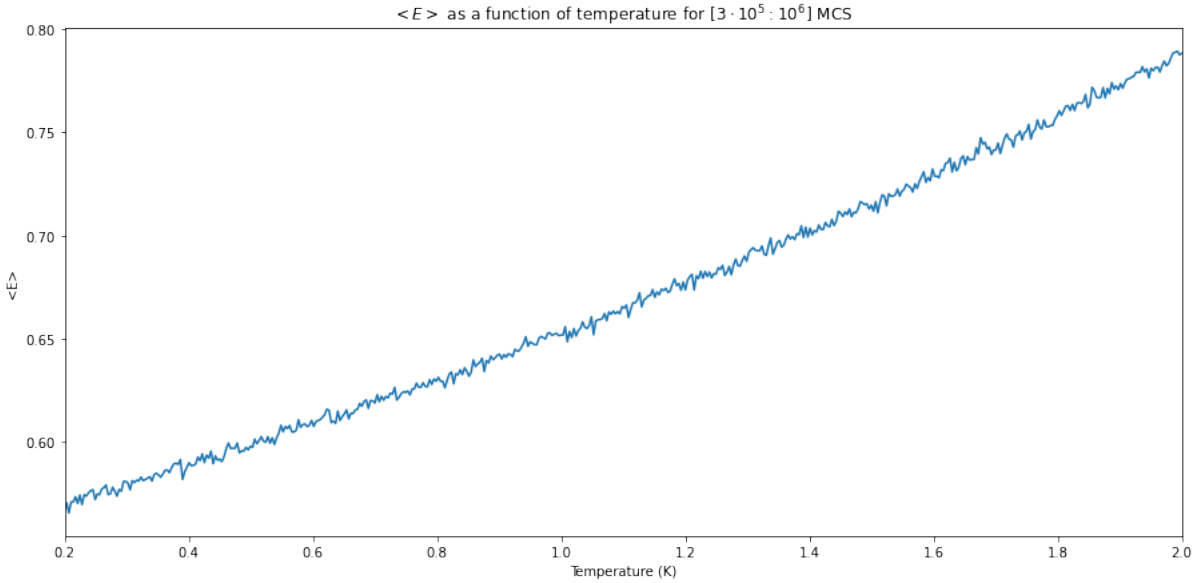

Figure 8: $\langle E \rangle$ values as a function of temperature for the last time interval (from $3 \cdot 10^5$ to 10^6 Monte Carlo steps).

It can be seen how $\langle q^2 \rangle$ grows exponentially with temperature, starting from $\langle q^2 \rangle = 0.85$ at $T = 0.2$, and it reaches $\langle q^2 \rangle = 1.15$ at $T = 2.0$. The mean energy values, on the other hand have a more linear growth, starting from $\langle E \rangle = 0.56$ at $T = 0.2$, and reaching $\langle E \rangle = 0.79$ at $T = 2.0$.