Computational Physics - Project 4

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As a first benchmark test for our program, we calculated the expectation values $< E >$, $< |M| >$, $< C_V >$ and $< \chi >$ of a 2×2-lattice for different temperatures. Those results could be easily compared to the analytical values from the part **??**. In fig. 1 – 8, you can see our results for these expectation values compared with the analytical solutions as functions of T. We took 10000 Monte Carlo cycles for each temperature to achieve good results. You can see that the results fit very well to the analytical solutions which means that our program passed this benchmark test and works fine.

In the following table, we compared the analytical results for the different expectation values for a temperature $T = 1.0$. It shows that all numerical results have a precision of at least two, in most cases of even three leading digits.

In the next step, we took a closer look at the effect of thermalization. This term describes the process of the system

Table 1: Analytical and numerical value of different expectaion values for $T = 1.0$ in a 2×2-lattice

	Analytical value	Numerical results
$< E >$	-7.983928	-7.984080
$< \|M\| >$	3.994642	3.994760
$< c_v >$	0.128329	0.127107
$< \chi >$	0.016043	0.015494

slowly reaching the most likely state for a given temperature. When we start with a random setup, it is very unlikely that the system is already in this state at the beginning, but it will need some time (or, in our case, some Monte Carlo cycles) to reach it.

To get more insight in the process of thermalization, we observed the development of $< E >$ and $< |M| >$ of a 20×20-lattice for temperatures of $T = 1.0$ and $T = 2.4$, for both starting with a random setup and a lattice with all spins pointing in one direction. You can see that development in the figures **??** – **??**, where these expectation values are plotted as function of the number of Monte Carlo cycles. We also plotted how many ‚moves'(flipping of spins) got accepted as a function of the number of cycles in fig. **??** – **??** It is obvious that this value is proportional to the number of cycles and that, the higher the temperature is, the faster the number of accepted moves increases.

All these plots show that we need a bit more than 1000 cycles in order to reach a stable state. This duration seems not to depend on the temperature, but obviously on the initial set-up: If this is close to a setup corresponding to the given temperature, it will not take long time to reach a stable state.

For later calculation, we set up a function called *thermalization* for our program. This function performs the Metropolis algorithm without collecting data, instead it evaluates the energy after every 10 cycles. When the change between two measurements is less than 1%, the program starts collecting data. This takes in account the process described above and ensures that we reached a stable state before the actual calculations start.

In the next step, we took a closer look at the probability of the single values of E to appear. We observed a 2×2-lattice at a temperature of $T = 1.0$ respectively $T = 2.4$ again and did two histograms of how often an energy value occurred. Obviously, that distribution is expanded for a higher temperature. This correspondents with the fact that the variation of the energy for these temperatures is higher, which means that more values are accessed. Both histograms can be found in fig **??** – **??**.

3 Comparison and discussion of results

4 source code

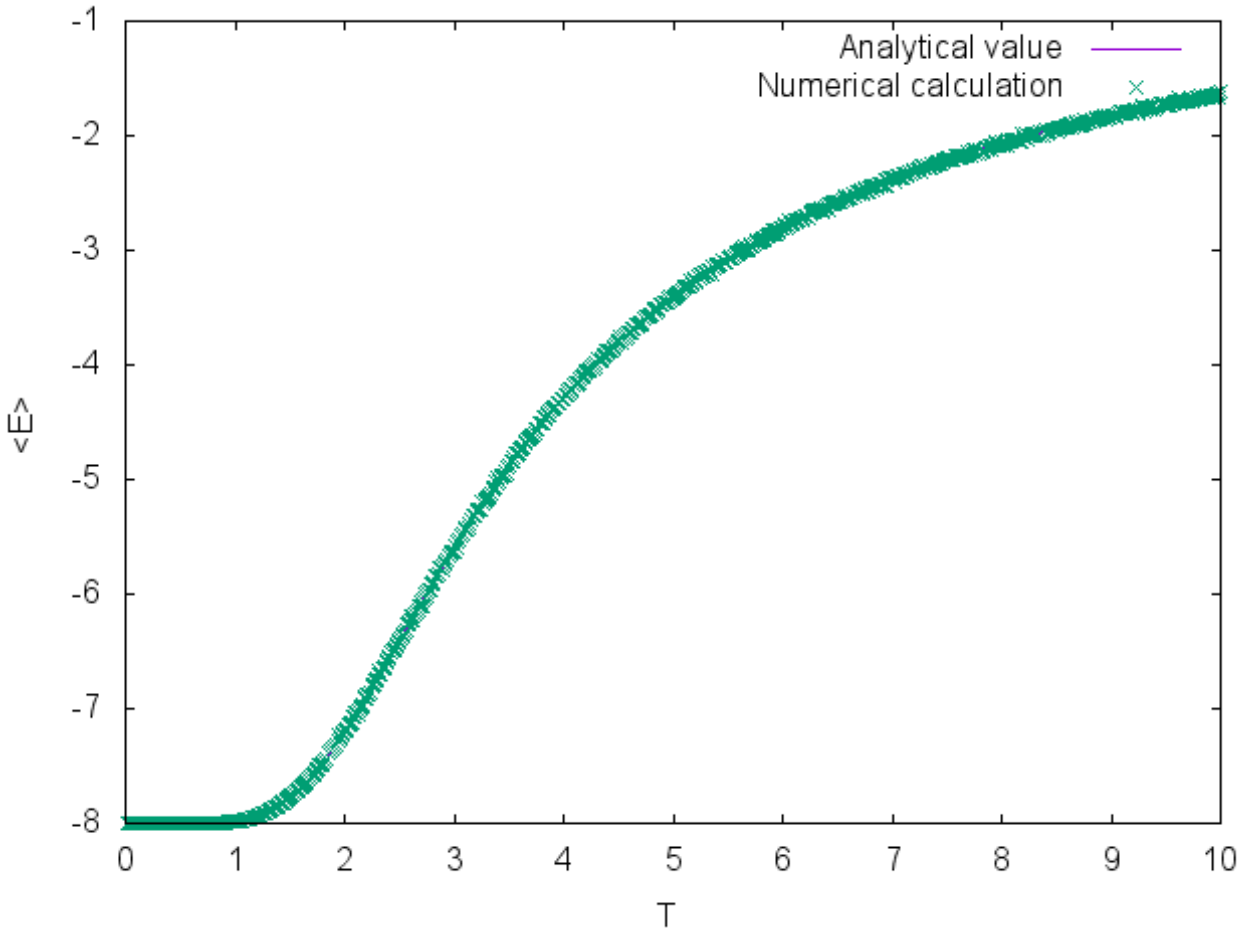

Figure 1: $< E >$ in a 2×2-lattice for different temperatures

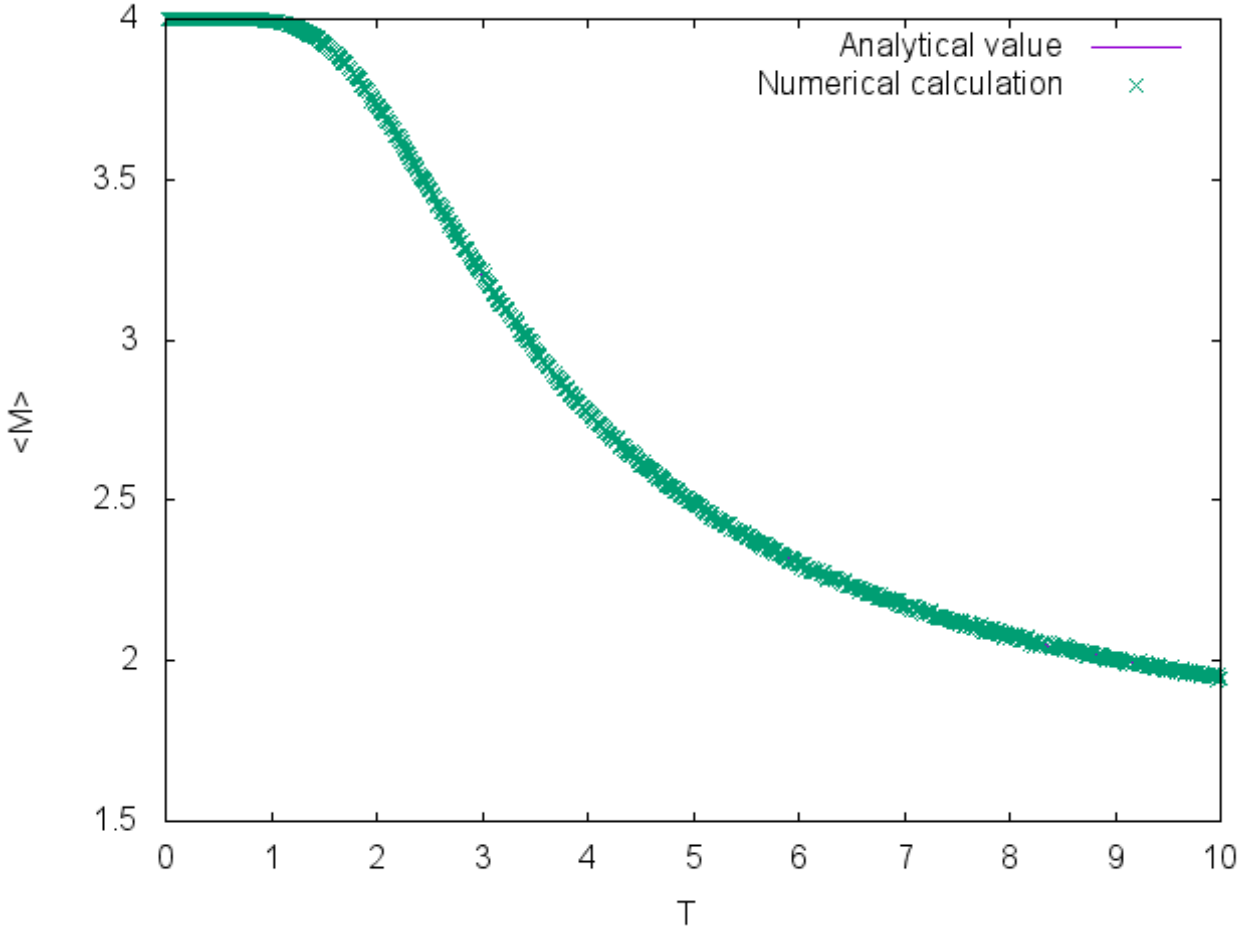

Figure 2: $< |M| >$ in a 2×2-lattice for different temperatures

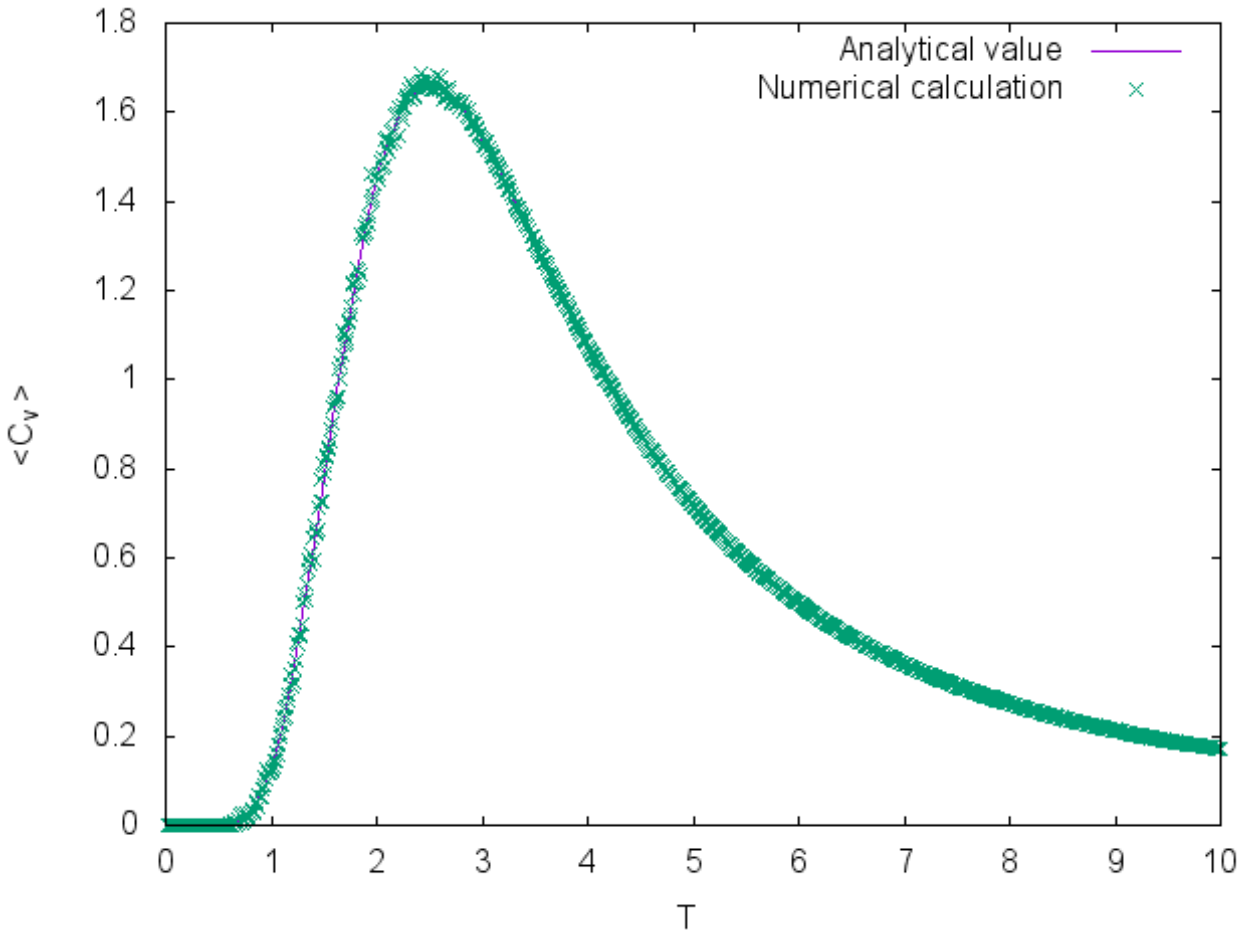

Figure 3: $< c_v >$ in a 2×2-lattice for different temperatures

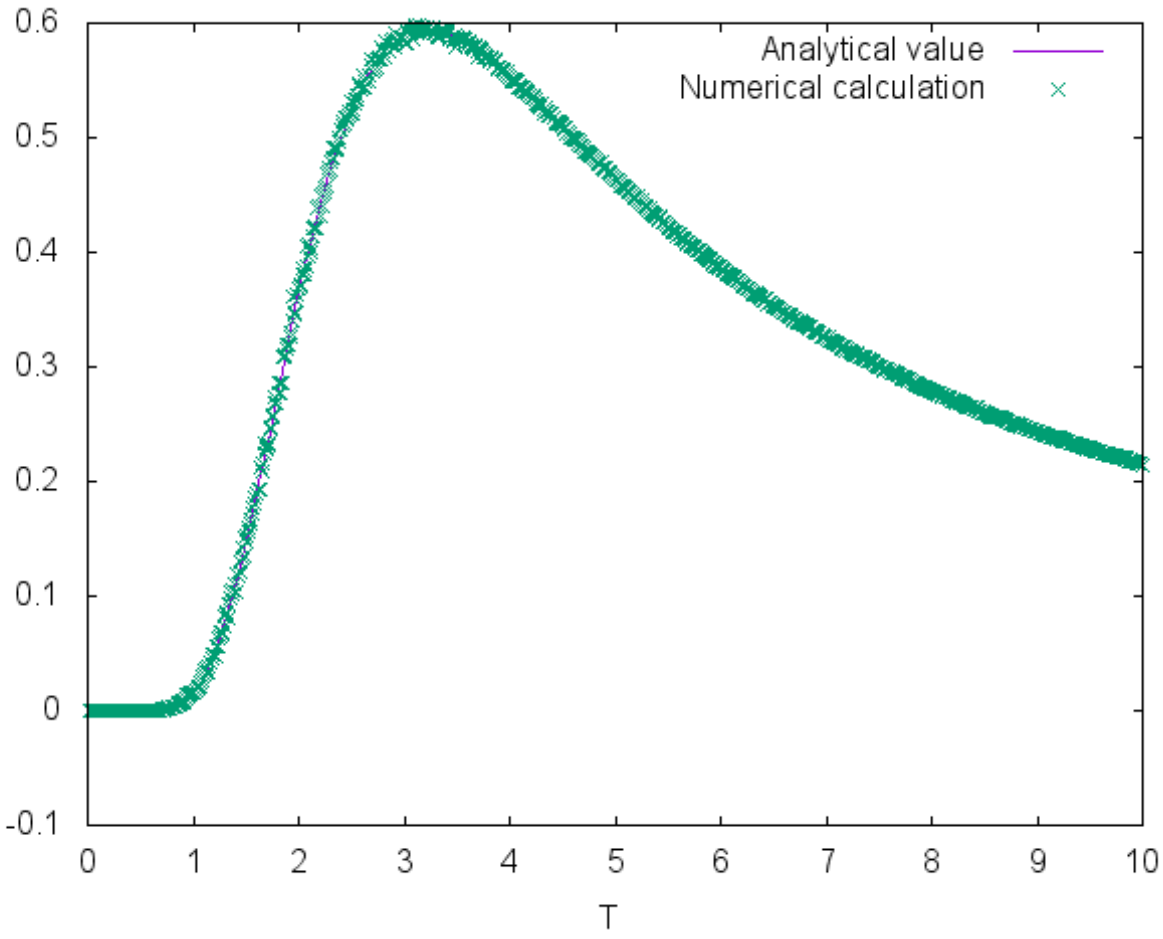

Figure 4: $< \chi >$ in a 2×2-lattice for different temperatures

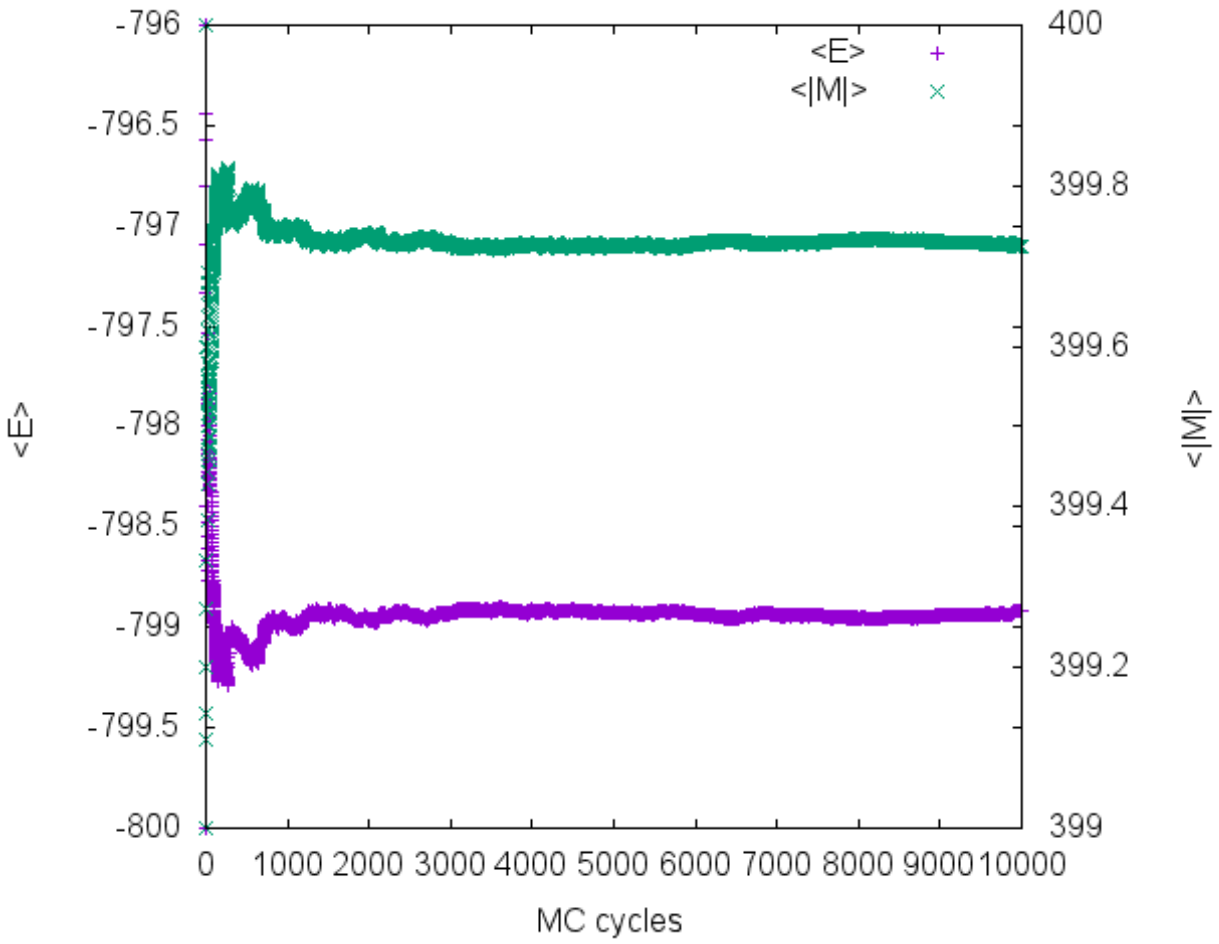

Figure 5: $< E >$ and $< |M| >$ in a 20×20-lattice as a function of the number of Monte Carlo cycles, starting with ordered spins at $T = 1.0$

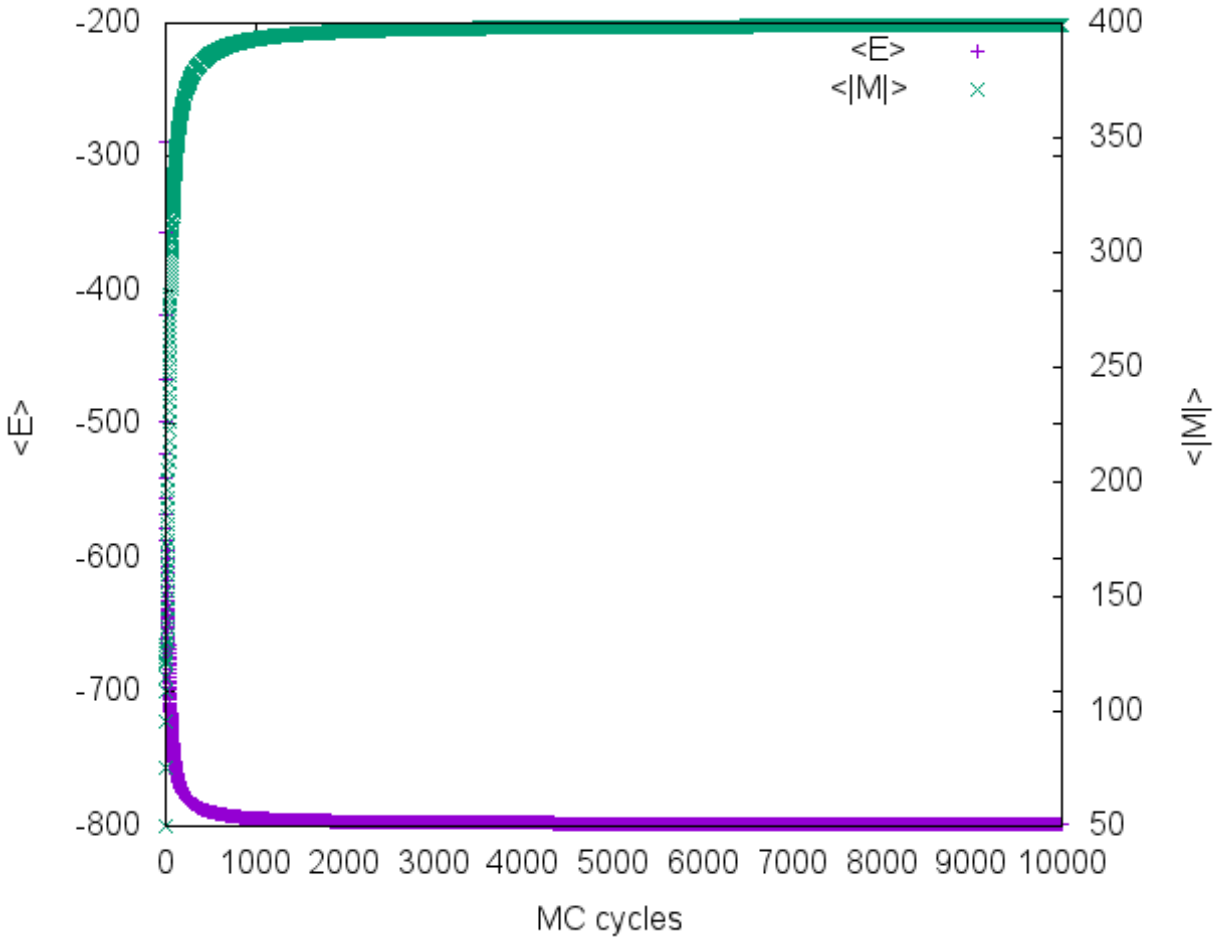

Figure 6: $< E >$ and $< |M| >$ in a 20×20-lattice as a function of the number of Monte Carlo cycles, starting with random spins at $T = 1.0$

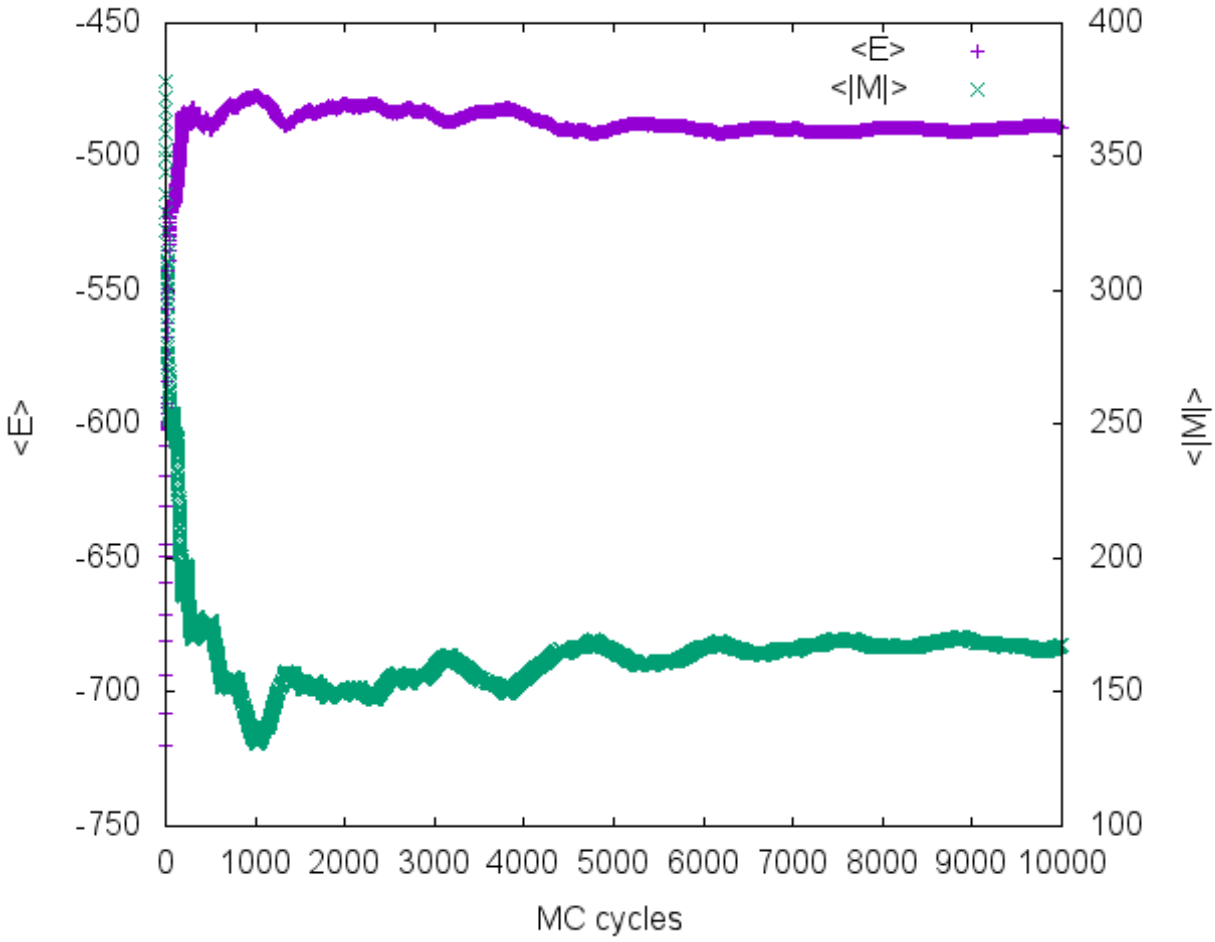

Figure 7: $< E >$ and $< |M| >$ in a 20×20-lattice as a function of the number of Monte Carlo cycles, starting with ordered spins at $T = 2.4$

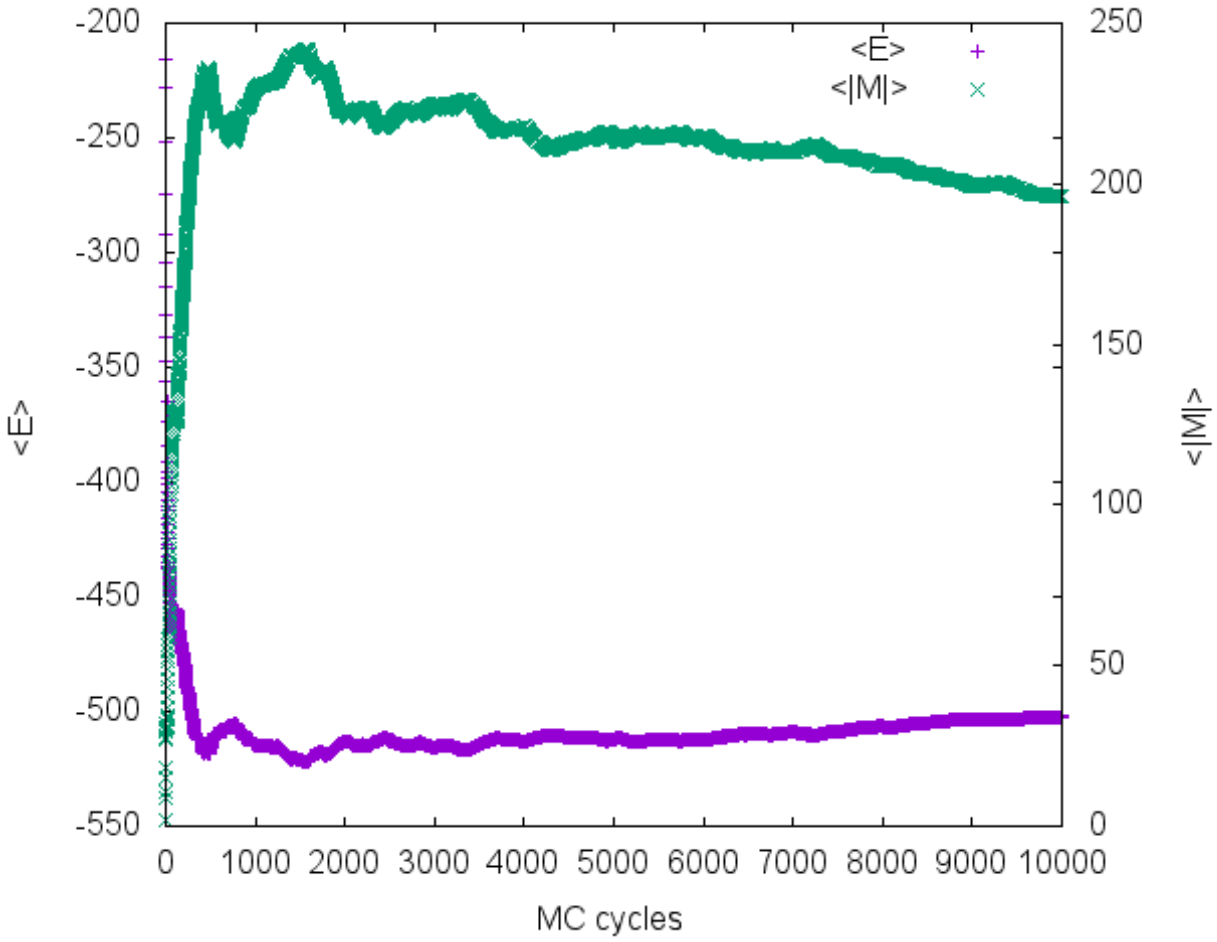

Figure 8: $< E >$ and $< |M| >$ in a 20×20-lattice as a function of the number of Monte Carlo cycles, starting with random spins at $T = 2.4$

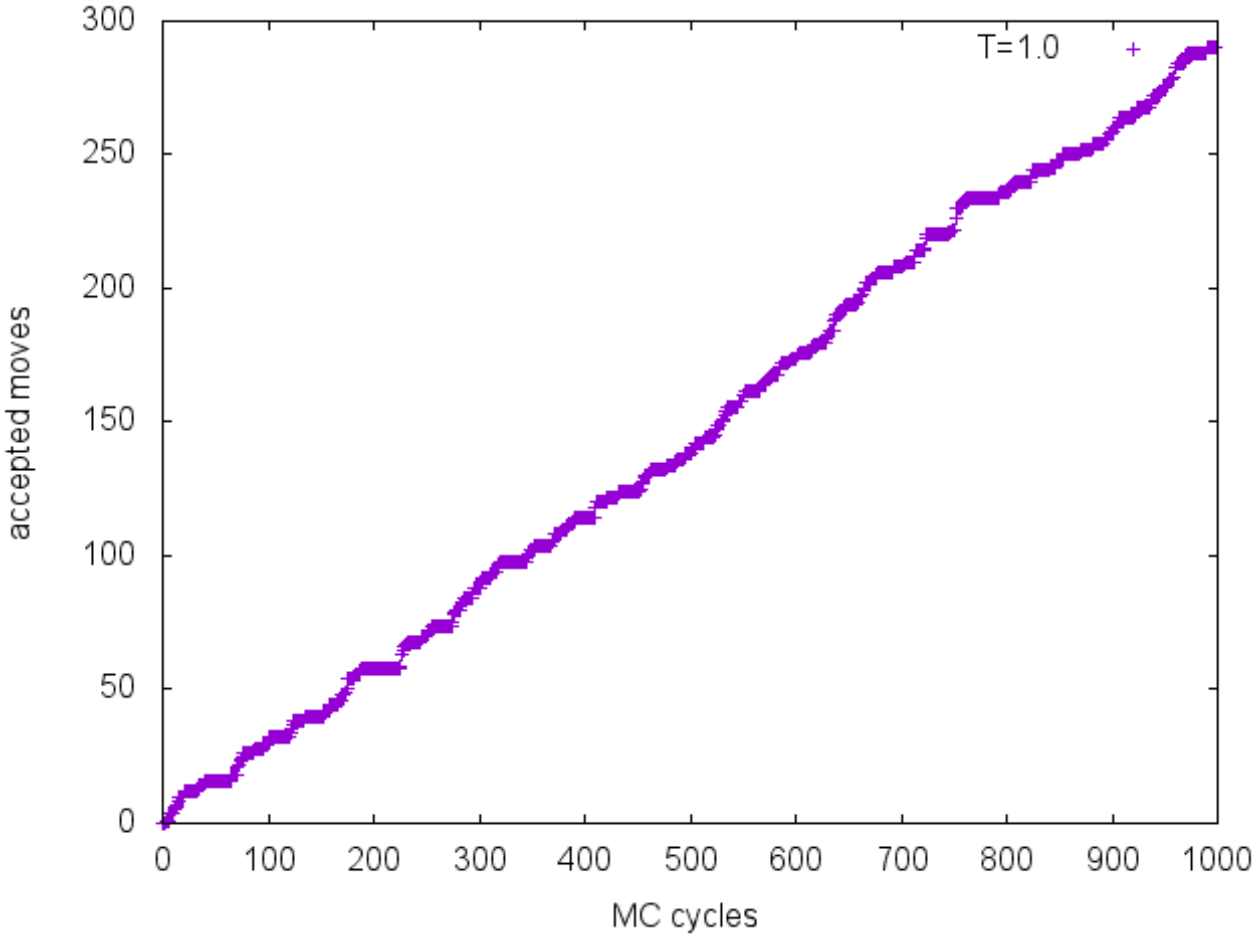

Figure 9: The number of accepted spin flips as function of the number of cycles at $T = 1.0$

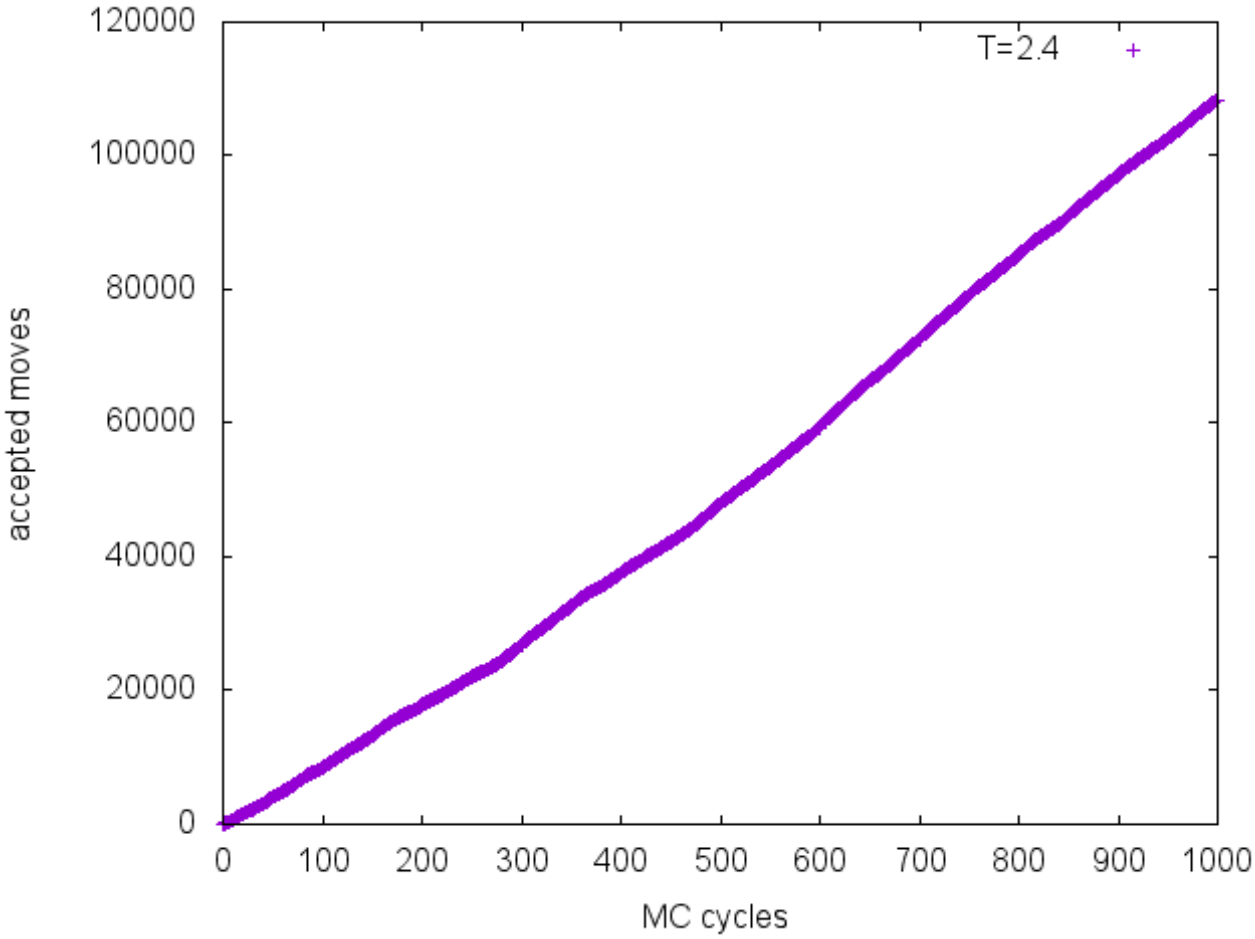

Figure 10: The number of accepted spin flips as function of the number of cycles at $T = 2.4$

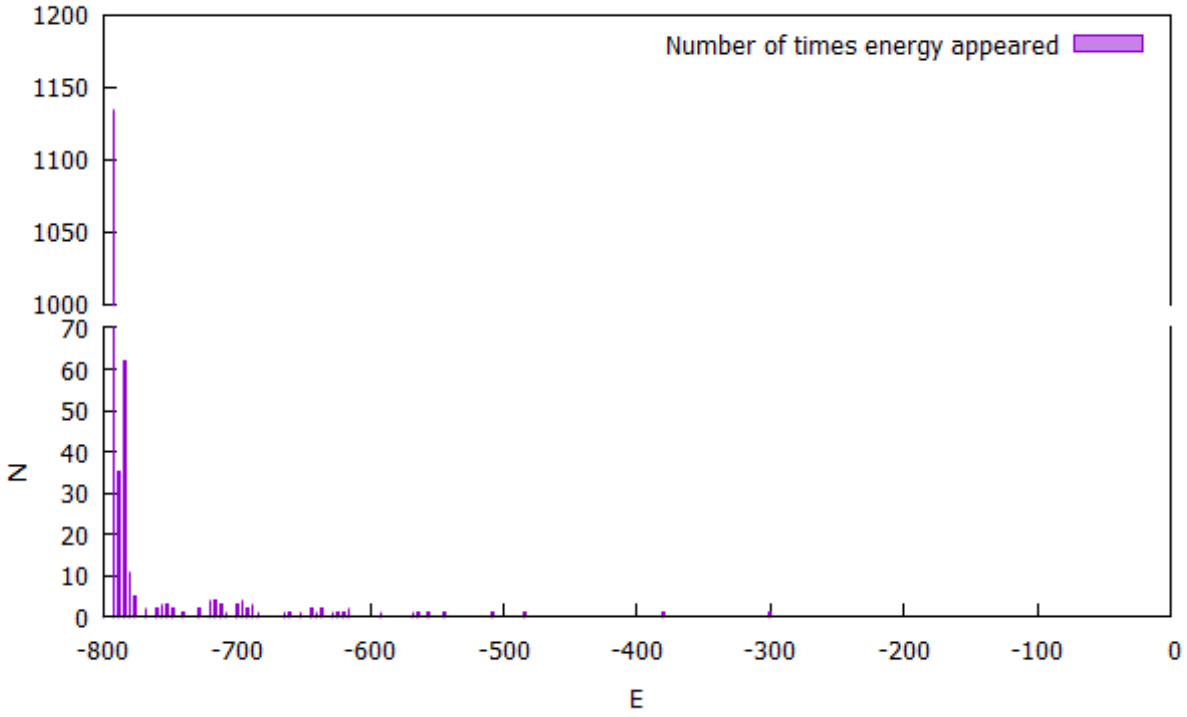

Figure 11: Frequency of occurrence for different energies at $T = 1.0$

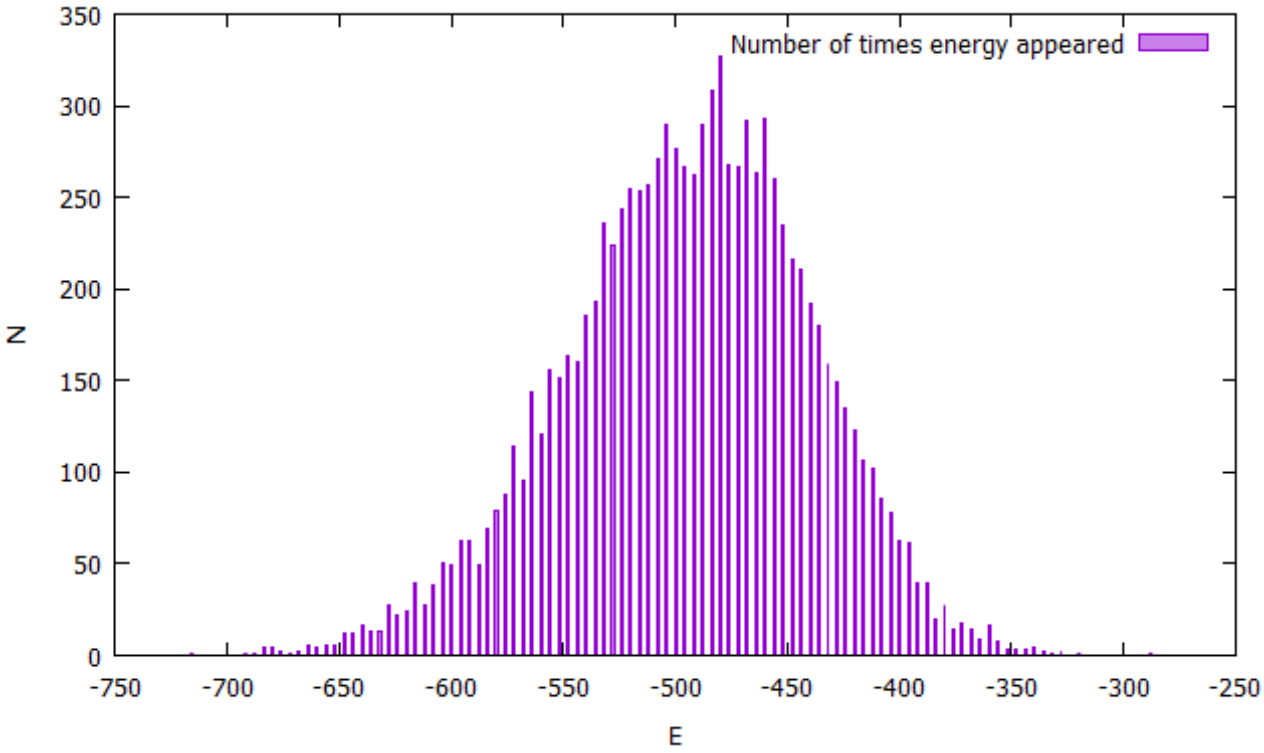

Figure 12: Frequency of occurrence for different energies at $T = 2.4$