Uppsala Universitet

Computational Physics
1FA573

Final Projects

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Part A - Scattering by central potential

Introduction

The first half of this report simulates and studies the scattering of particles via a central potential. The particle enters the potential from a large distance and retains its energy after leaving the potential. We want to look at the angle Θ between the original path and its path after the scattering.

Project 1

The potential in the first project was given to be a square potential, that is, $V(r) = U_0$ when $r < r_{max}$ and 0 for $r > r_{max}$. The equation to be solved is:

$$\Theta = 2b\Big[\int_b^{r_{max}} \frac{dr}{r^2}\Big(1 - \frac{b^2}{r^2}\Big)^{-1/2} - \int_{r_{min}}^{r_{max}} \frac{dr}{r^2}\Big(1 - \frac{b^2}{r^2} - \frac{V}{E}\Big)^{-1/2}\Big], \tag{1}$$

where b is the impact parameter and E is the kinetic energy of the particle. r_{min} is defined as the distance when particle is closest to the source of the potential. It is found by solving the equation when the root in the second integral is set to zero. r_{max} is the distance when the potential no longer has any effect on the particle. The solution depends on the relation between the kinetic energy and the potential. If $E < V$, the particle does not have enough energy to enter the potential and therefore, $r_{min} = r_{max}$ and the second integral vanishes. The solution reads:

$$\Theta = \pi - 2\arcsin\Big(\frac{b}{r_{max}}\Big). \tag{2}$$

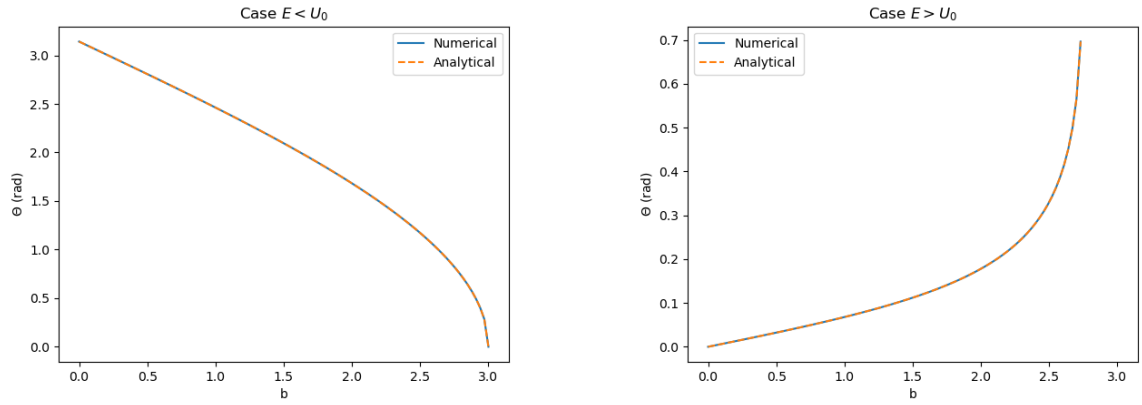
If $E > V$, both integrals are non-zero and the solution reads:

$$\Theta = -2\arcsin\Big(\frac{b}{r_{max}}\Big) - 2\arcsin\left(\frac{b}{r_{max}\sqrt{1 - \frac{U_0}{E}}}\right). \tag{3}$$

Equation 1 can also be solved using quadrature. In order to do that, one must use clever substitutions in order to get rid of the singularities. For the first integral, we use $p = \sqrt{r - b}$. Similarly, for the second integral we take $p = \sqrt{r - r_{min}}$. With a little algebra, equation 1 becomes:

$$\Theta = \int_0^{\sqrt{r_{max}-b}} \frac{4bp \cdot dp}{p^2 + b}\Big(1 - \frac{b^2}{p^2 + b}\Big)^{-1/2} - \int_0^{\sqrt{r_{max}-r_{min}}} \frac{4bp \cdot dr}{p^2 + r_{min}}\Big(1 - \frac{b^2}{p^2 + r_{min}} - \frac{V}{E}\Big)^{-1/2}. \tag{4}$$

In this project, we vary b from 0 to r_{max}. However, this poses the problem by dividing by zero when $p = b = 0$ in the first integral. To counter this, we replace the integrals by their limit, which is π.
Now, we are ready to compute the integrals analytically and numerically.



(a) The first phase.

(b) The second case. $E = 6$ and $U_0 = 1$

Figure 1: Solutions for the two cases. $r_{max} = 3$.

When the sign of the potential is flipped, the first case clearly is not affected, since it does not depend on it. For the other case, the results can be seen in figure 2.

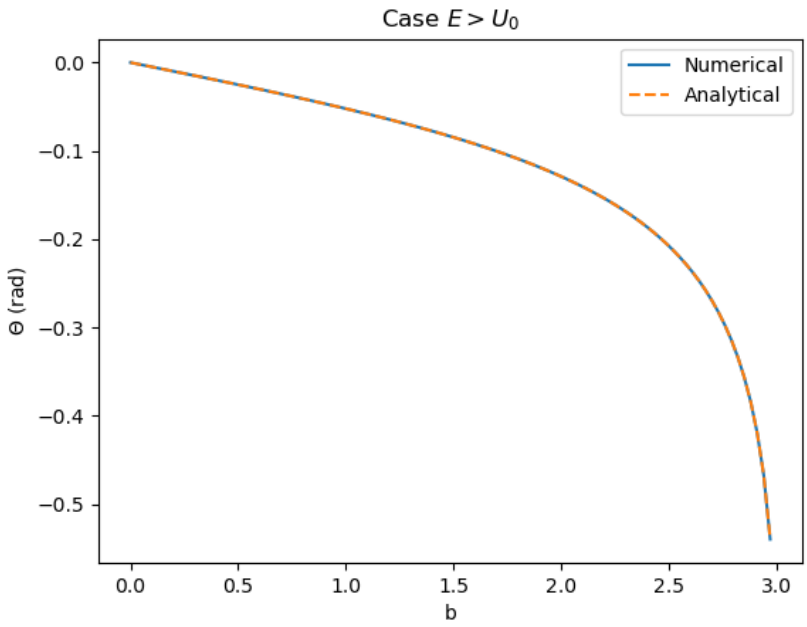


Figure 2: Solution for $U_0/E = -1/6$.

Project 2

Now, let us use the solution from project 1 to look at a little more complex case. The potential in this problem is a Lennard-Jones potential, which models der Waals interactions. It is defined as:

$$V(r) = 4V_0\Big((\frac{a}{r})^{12} - (\frac{a}{r})^6\Big). \tag{5}$$

The assignment stated that the value of E should vary from $0.1V_0$ to $100V_0$. r_{max} was again set to 3. The instructions also said that a could be taken as $r_{max}/3$, meaning $a = 1$. V_0 was also conveniently set to 1. Now, equation 4 was solved again using quadrature,

but this time with equation 5 as potential. The results from the simulation with some different b values can be seen in figure 3.

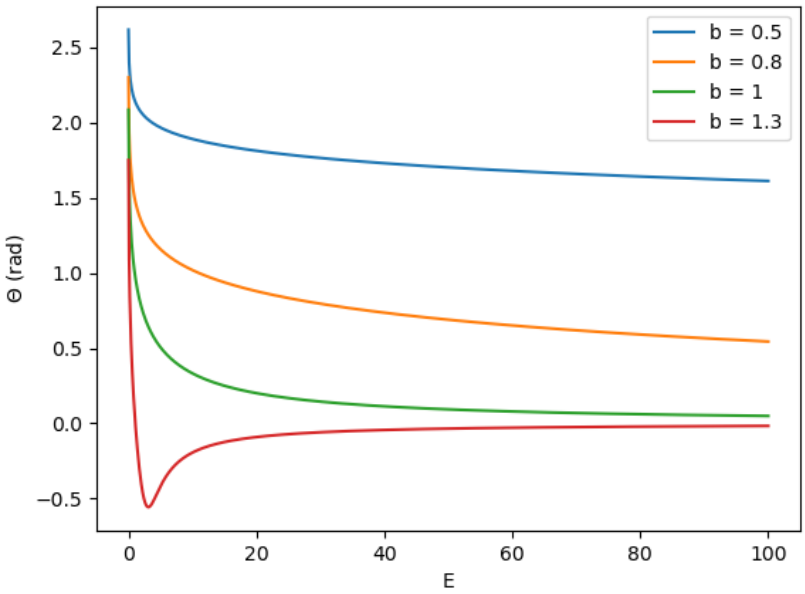


Figure 3: Solution for a Lennard-Jones potential.

It was also deemed interesting to plot the angle to the impact parameter b, as in project 1. The results for different values of the energy can be seen in figure 4.

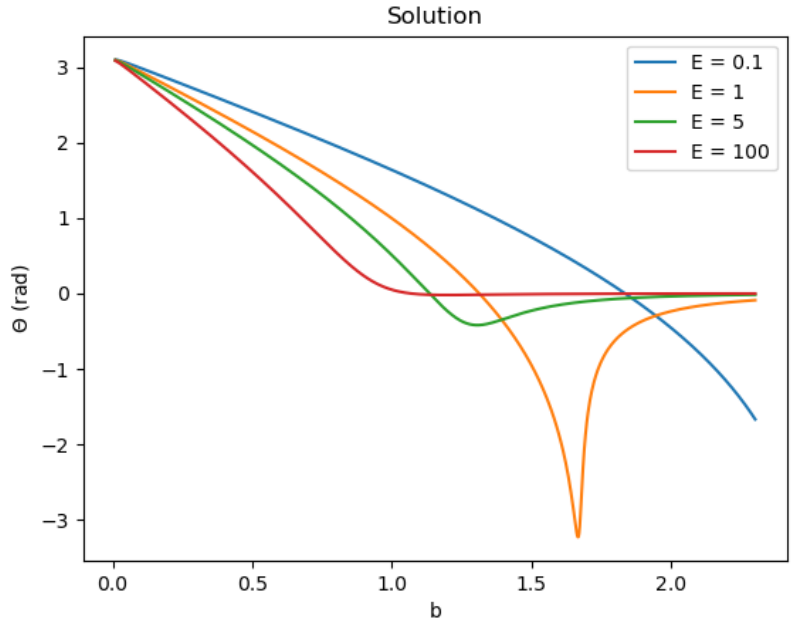


Figure 4: Solution for a Lennard-Jones potential.

Lastly, the differential cross section was to be computed. This experimental property

is defined as:

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\Theta}\right| \tag{6}$$

This property was calculated using the results from figure 4, since a simple approximate derivative can be achieved by calculating $\frac{dy}{dx}$ for every point. The results can be seen in figure 5.

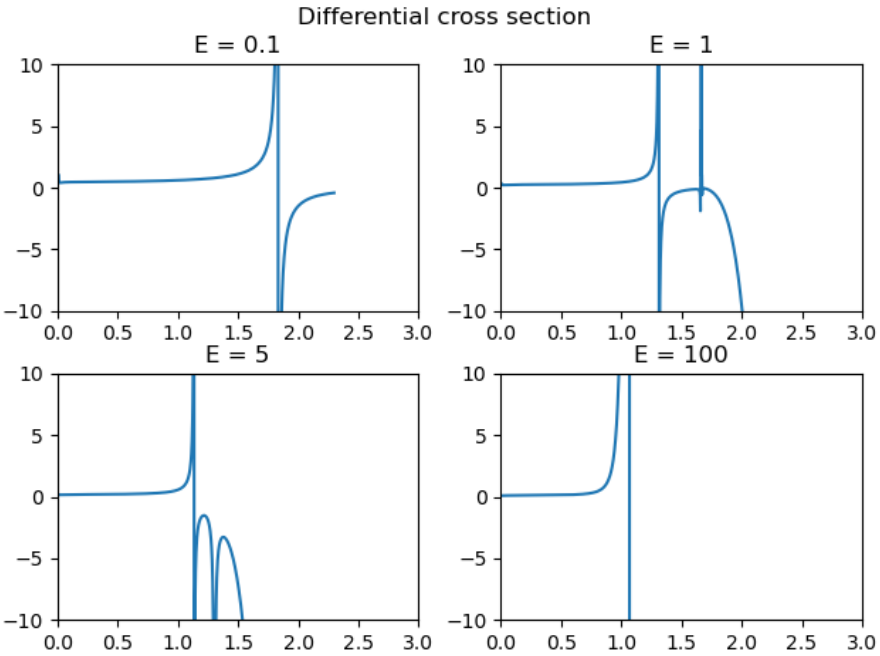


Figure 5: Differential cross section plots for different E.

Conclusion

The solutions in project 1 seems to be very accurate, by comparing the numerical and analytical solution. A thing to note is that figure 1b only goes to ≈ 2.7. arcsin is undefined when the argument is > 1. By looking at equation 3, this is the case when:

$$1 < \frac{b}{3\sqrt{1-\frac{1}{6}}} \implies b > 2.7386... \tag{7}$$

This seems to be very accurate with the plot. Also, when looking at figure 2, the plot is essentially flipped. This is to be expected since the potential is now of different sign. Physically, it also makes sense. For the first plot, the particle completely turns around for small b. For bigger b, the particle is less affected. For the second case, it goes straight through for small b. Otherwise, it bends.
In project 2, we no longer have a analytical solution to compare the numerical to. However, plot 3 and 4 seem reasonable. In figure 3, the solutions with lower impact parameter b are more affected by the potential. This makes sense, since they are further away. However, for the intermediate $b = 1.3$, we see a dip. This is because the nature of Lennard-Jones potential, its got both an attractive and repulsive force. Figure 4 is also expected, with the same reasoning. Figure 5 unfortunately does not say very much, because they have several divergences. These are because of division by zero. By looking at equation 6, it has division by $\sin\Theta$. The solutions in figure 4 is clearly zero for some values.

Part B - Ising model using Monte Carlo Methods

The second half of this paper involves simulating a two dimensional lattice of particles with spin. The specific model is called the Ising model and we will predominantly use the Metropolis algorithm, which is a stochastic model. The Hamiltonian for the total energy of the system is:

$$H = -J \sum_i \sum_{NN} S_i S_{NN} - B \sum_i S_i, \tag{8}$$

where the i ranges over the entire lattice and the NN notation mean the four nearest neighbours to the particle i. $S_i = \pm 1$ is the spin of the particle and B is a potential external magnetic field. For an exact solution, one needs to calculate the partition function and the canonical ensemble. However this proves difficult or even impossible for lattices, since one needs to account for every single possible set of spins in the lattice. For example, this means that a 8x8 lattice has 2^64 possible sets, which is impossible to calculate efficiently. The Metropolis algorithm simulates whether a particles spin will flip, depending on if the energy would be lower, but also randomness introduced by higher temperatures. The thermal properties we are interested in is the order parameter, susceptibility, specific heat and the 4^{th} order cumulant. The latter is used to obtain the phase transition. The order parameter is calculated by taking an average of all the spins and taking the absolute value, i.e.

$$|M| = \frac{1}{N} \Big| \sum_i^N S. \Big| \tag{9}$$

The susceptibility is given by:

$$\chi = \sum_i^N S_i - M^2. \tag{10}$$

Specific heat is:

$$C_B = \sum_i^N H^2 - E^2, \tag{11}$$

where E is the energy. Lastly, the 4^{th} order cumulant is given by:

$$U_L = 1 - \frac{\langle M^4 \rangle}{3 \langle M^2 \rangle^2}. \tag{12}$$

Project 3

Firstly, we consider constant ferromagnetic interactions between all particles ($J > 0$ and constant) and no external field B. There are periodic boundary conditions and three different lattice sizes were used: 8x8, 16x16 and 32x32. The results of the simulation can be seen in figure 6-9

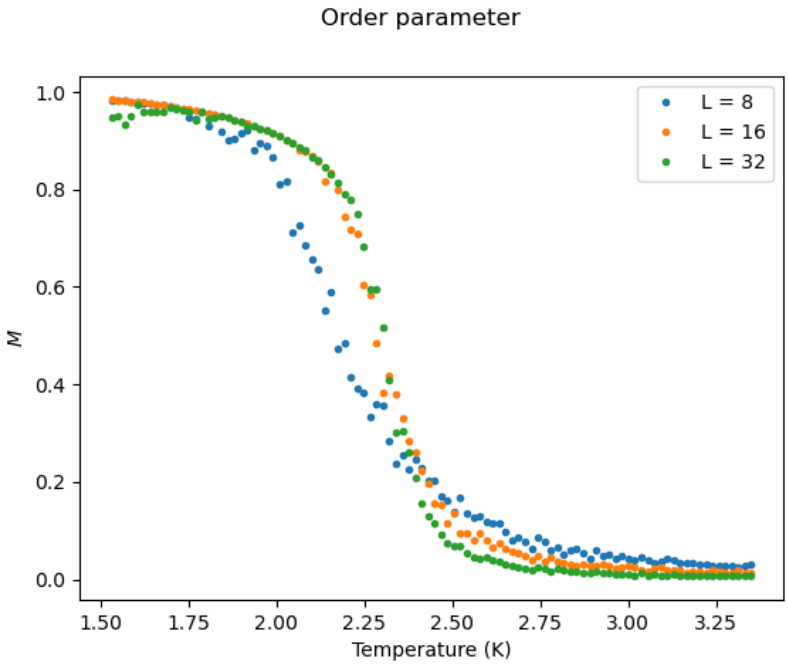


Figure 6: Order parameter of the simulation.

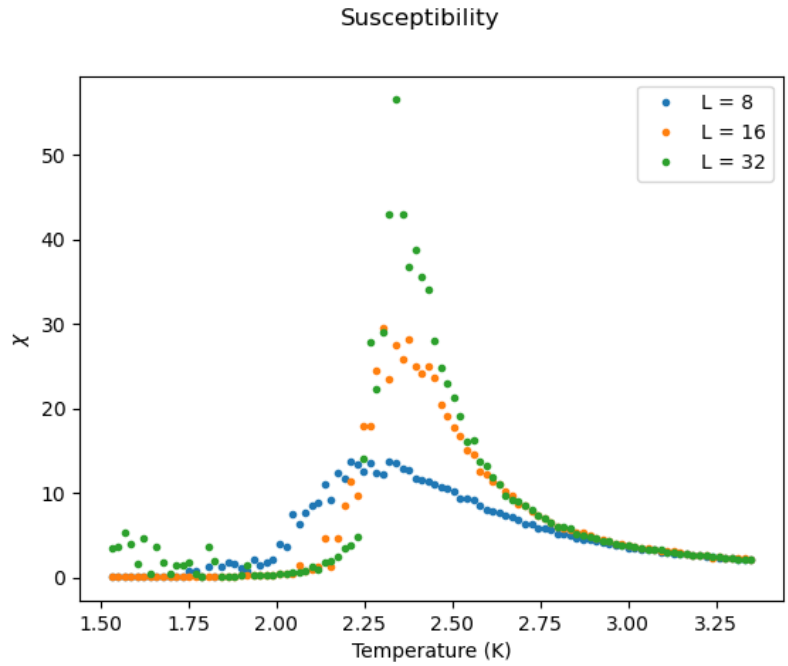


Figure 7: Susceptibility of the simulation.

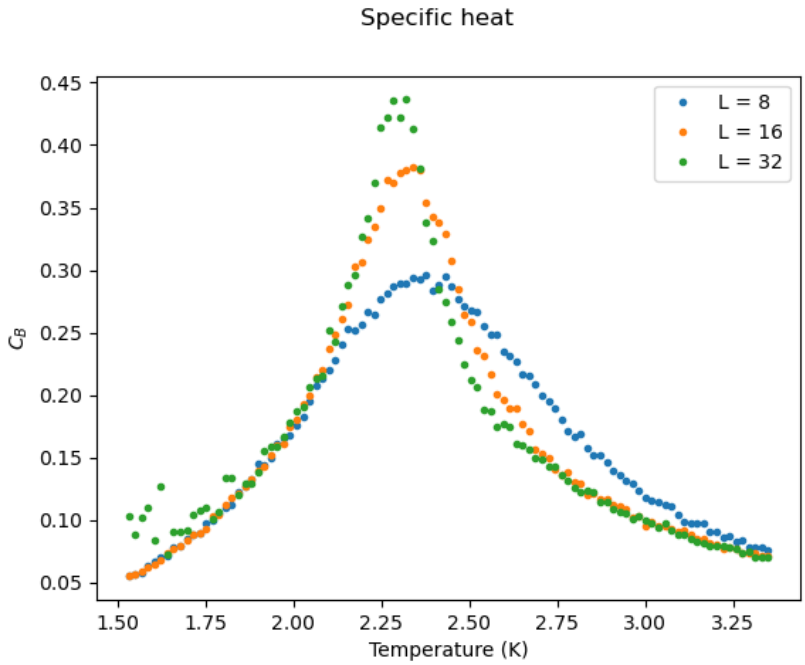


Figure 8: Order parameter of the simulation.

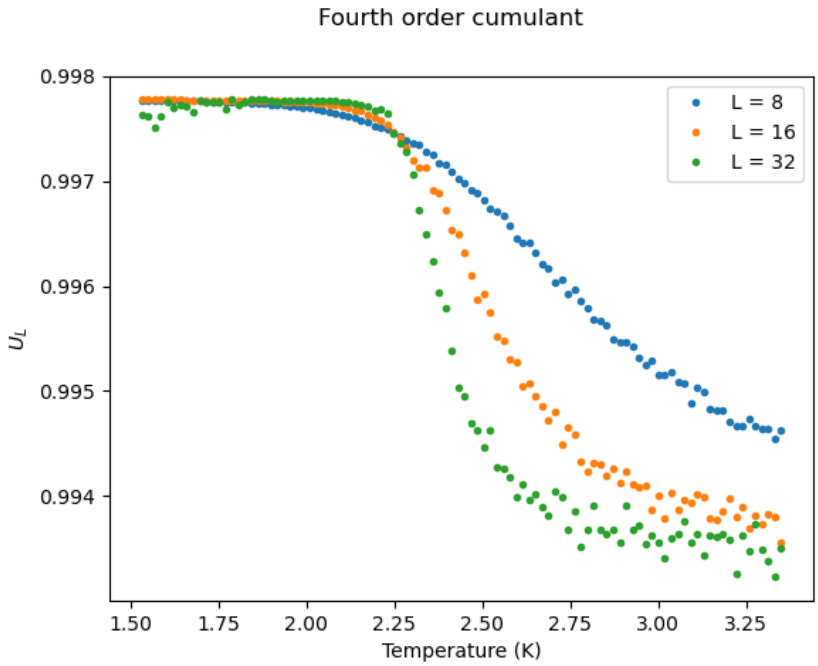


Figure 9: Order parameter of the simulation.

Project 4

Now, we look at antiferromagnetic interactions with the presence of a external magnetic field $B \neq 0$. Otherwise, the solution is essentially the same. J was set to $-k_B$ and $B = k_B/2$ where k_B is Boltzmanns konstant.

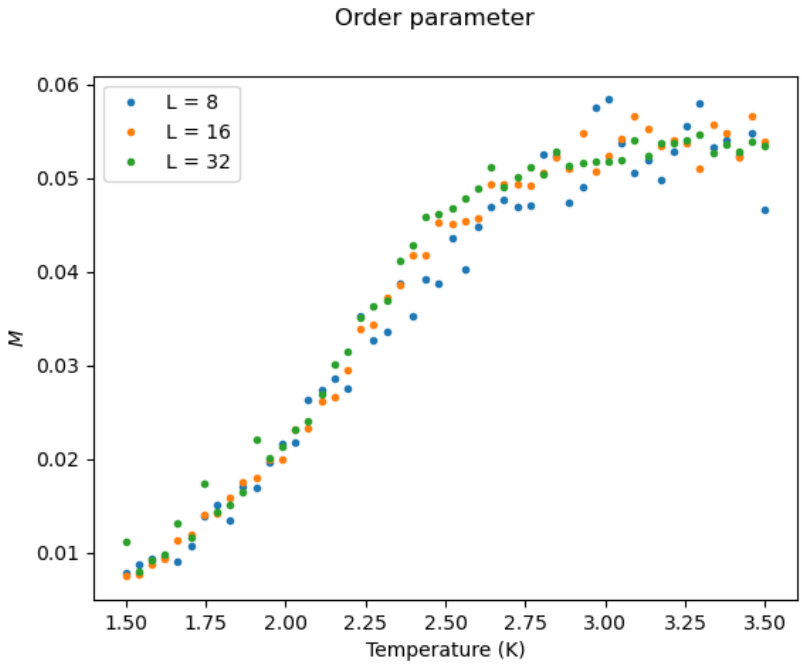


Figure 10: Order parameter of the simulation.

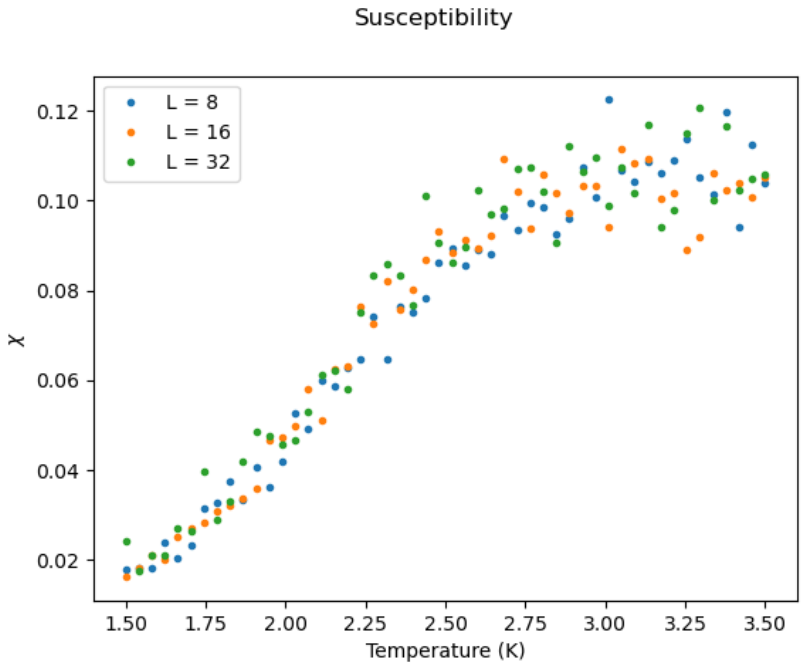


Figure 11: Susceptibility of the simulation.

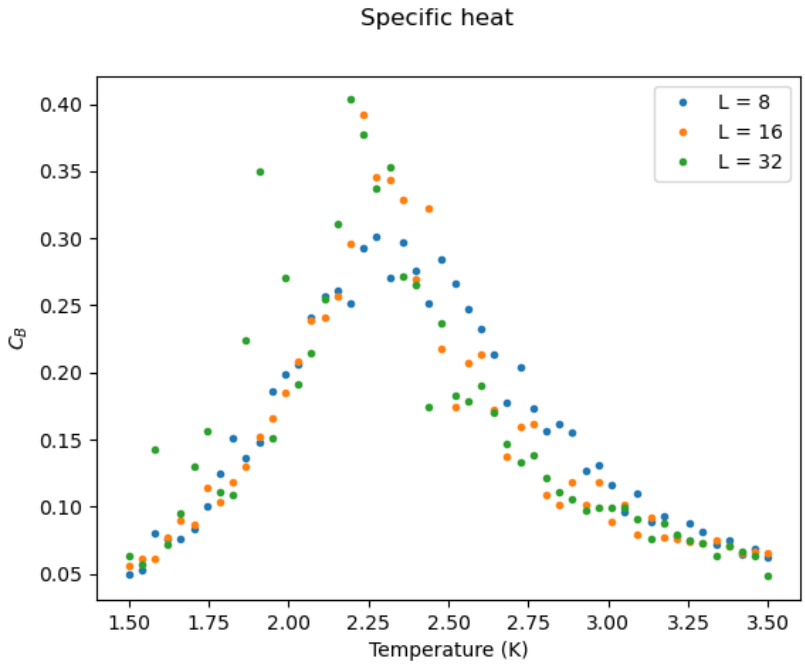


Figure 12: Specific heat of the simulation.

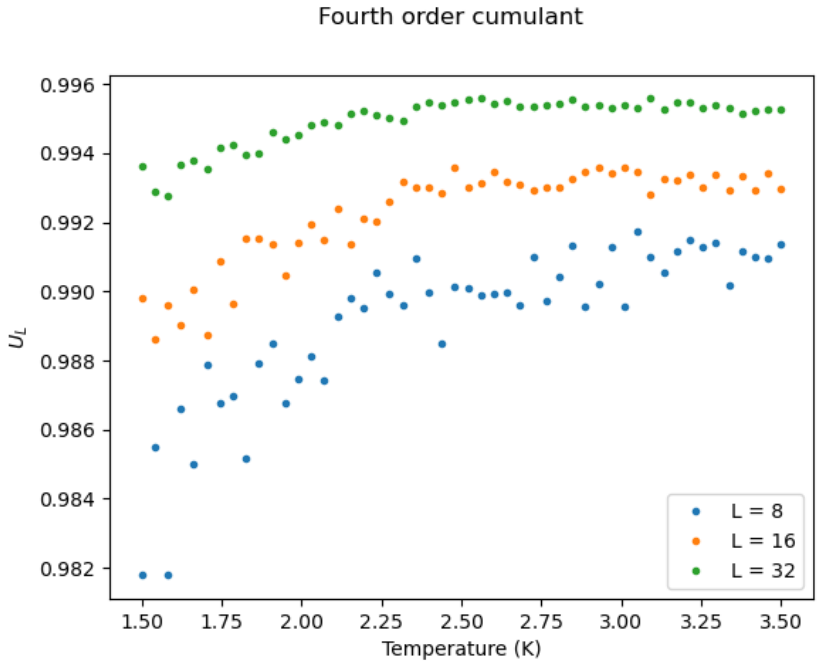


Figure 13: Order parameter of the simulation.

Lastly, we study another algorithm, namely the "heat bath" algorithm. This algorithm gives the probability for p_i spin = 1 and $1 - p_i$ spin = -1 by

$$p_i = \frac{e^{\frac{2j\sum_j S_j}{k_B}}}{1 + e^{\frac{2j\sum_j S_j}{k_B}}}, \tag{13}$$

where, S_j is the spins of the nearest neighbours. The results can be seen below.

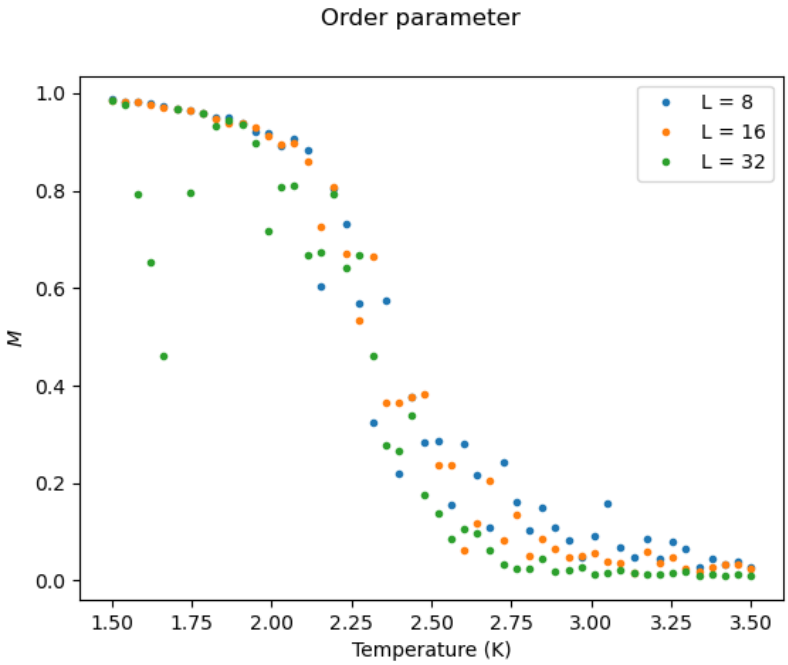


Figure 14: Order parameter of the simulation.

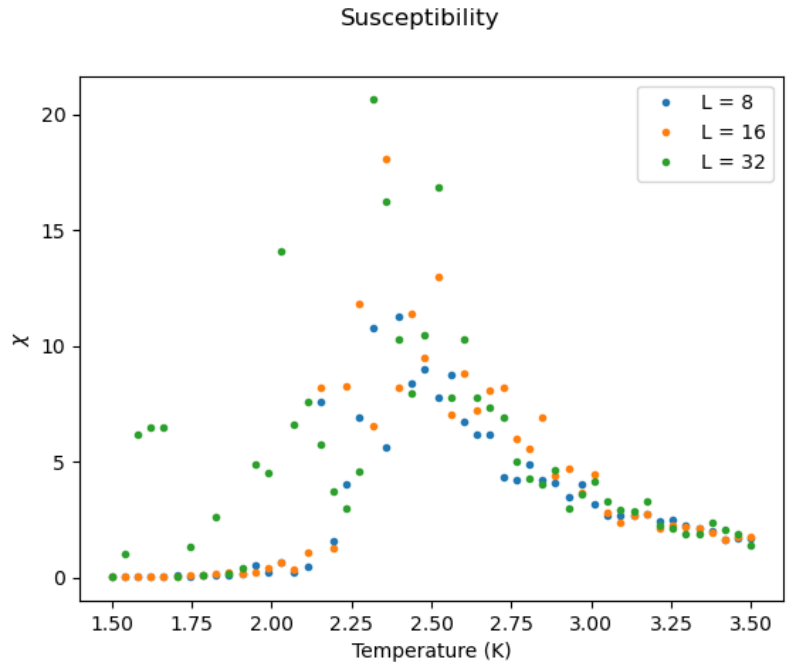


Figure 15: Susceptibility of the simulation.

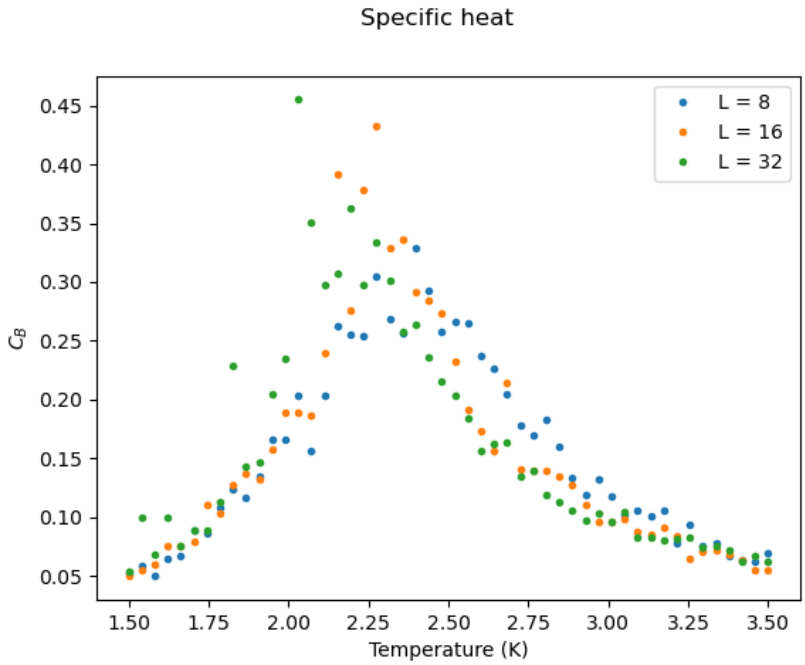


Figure 16: Specific heat of the simulation.

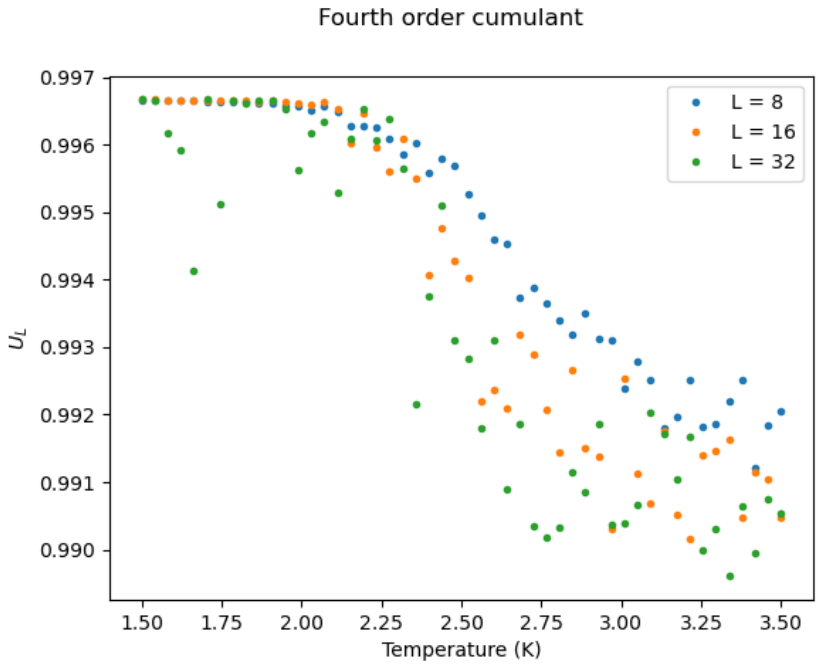


Figure 17: Order parameter of the simulation.

Conclusion

The plots for project 3 seems to work well. There seems to be a clear phase transition at around $T \approx 2.3$ K. It can be seen most clearly in figure 9, where the plots cross.
In project 2, the external field and and antiferromagnetic coupling plays a clear role. The magnetization in figure 10 is essentially flipped along the phase transition temperature. The fourth order cumulant in plot 13 does no longer meet, so the phase transition cannot

be extracted from that plot. The heat bath algorithm does not seem as efficient as the metropolis.