Exercise 1

Model

The Ising model is represented by a 3-dimensional lattice of L^3 integer values σ_{ijk}. For a given temperature $N_S \cdot L^3$ single spin flips at random positions are performed. The temperature of the system is raised in steps of $\delta T = (T_e - T_s)/N_T$. The program takes L, T_s, T_e, N_T, N_S as parameters.

Energy and magnetization are measured as $\frac{E_{tot}^{(T)}}{J} = \sum_n n\sigma_a\sigma_b$ and $M_{tot}^{(T)} = \sum_{ijk} \sigma_{ijk}$ respectively. Those quantities are measured after each L^3 single spin flips (a "system sweep") and subsquently averaged over all N_S sweeps of a timestep giving $\langle E_{tot} \rangle_T$ and $\langle M_{tot} \rangle_T$.

Utilizing the same scheme $\left\langle E_{tot}^2 \right\rangle_T$ and $\left\langle M_{tot}^2 \right\rangle_T$ are retrieved. Using these quantities $\chi(T) = \frac{\left\langle M_{tot}^2 \right\rangle_T - \langle M_{tot} \rangle_T^2}{T}$ as well as $C_V(T) = \frac{\left\langle E_{tot}^2 \right\rangle_T - \langle E_{tot} \rangle^2}{T^2}$ can be computed.

All four quantities are then given out per system size L^3.

Code

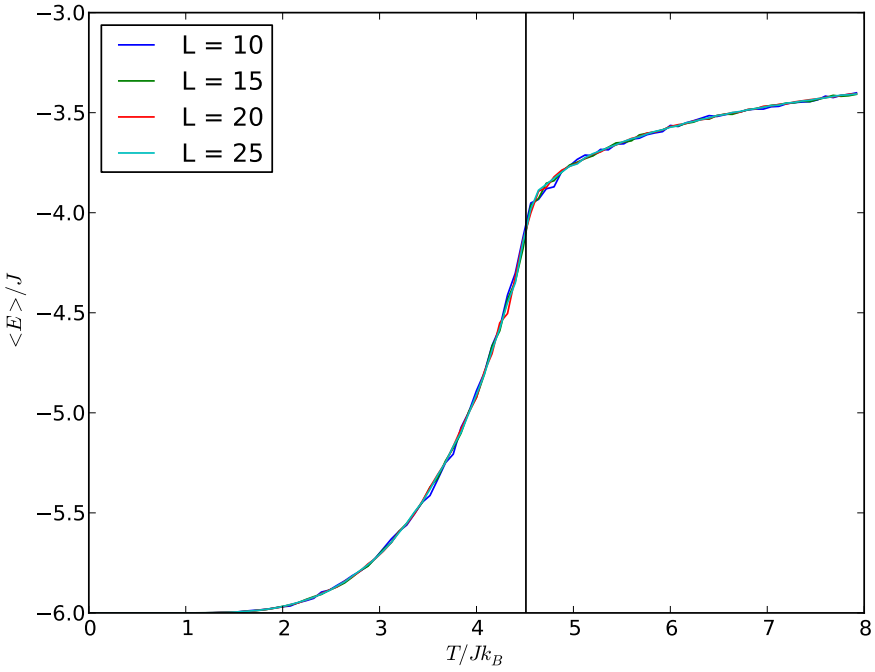
The code can easily be built using cmake. run `$ cmake . && make` in the directory ex01_ricoh/src/Ex1/. Or run the script run_experiments.sh which builds the code, writes the parameter files and starts the program.

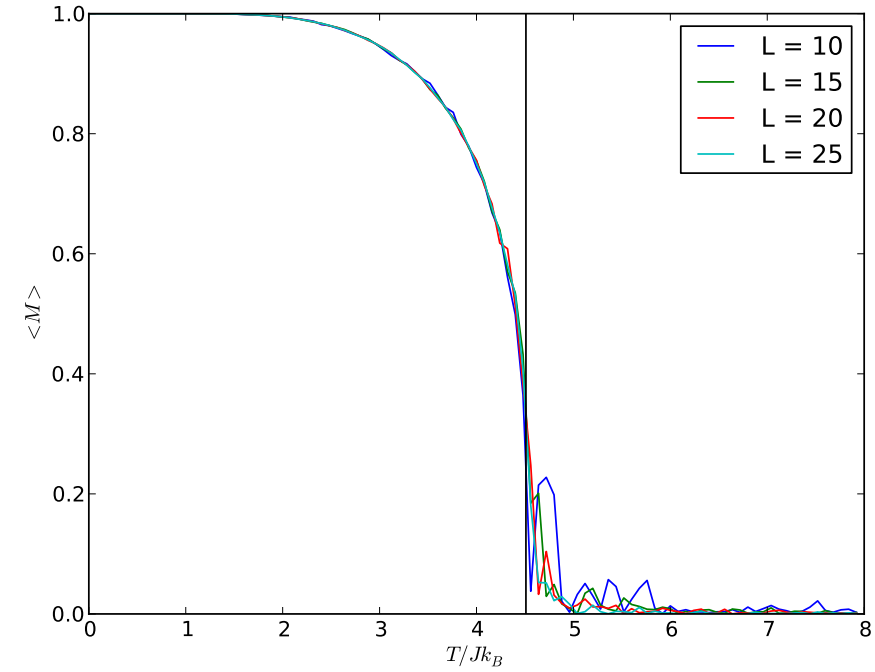
Simulations

The following value was found to lead to converging simulations: $N_S = 200$. Temperature was varied from $T_s = 0$ to $T_e = 8$ in $N_T = 100$ steps. The experiment was run for systems of the size $L = \{10, 15, 20, 25\}$.

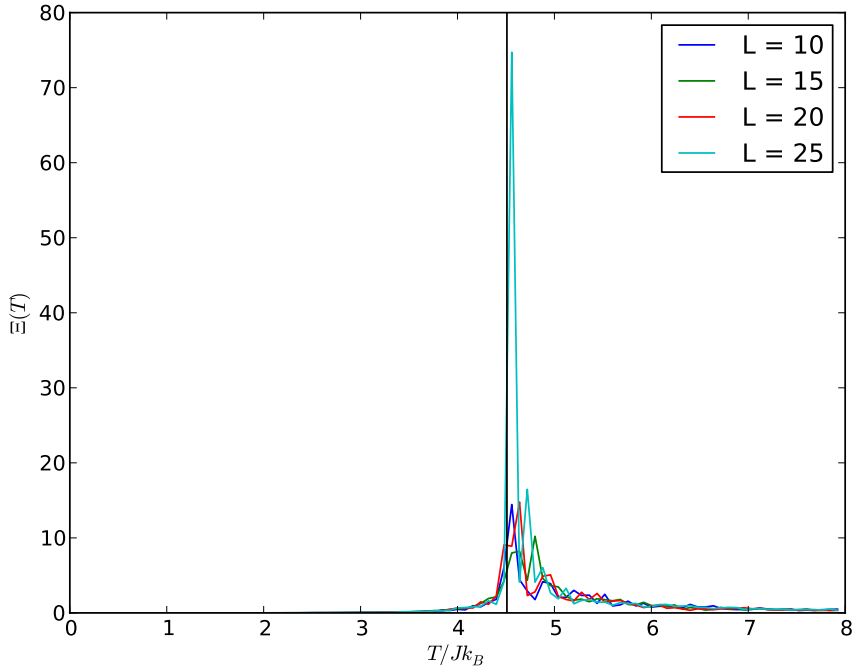
Results

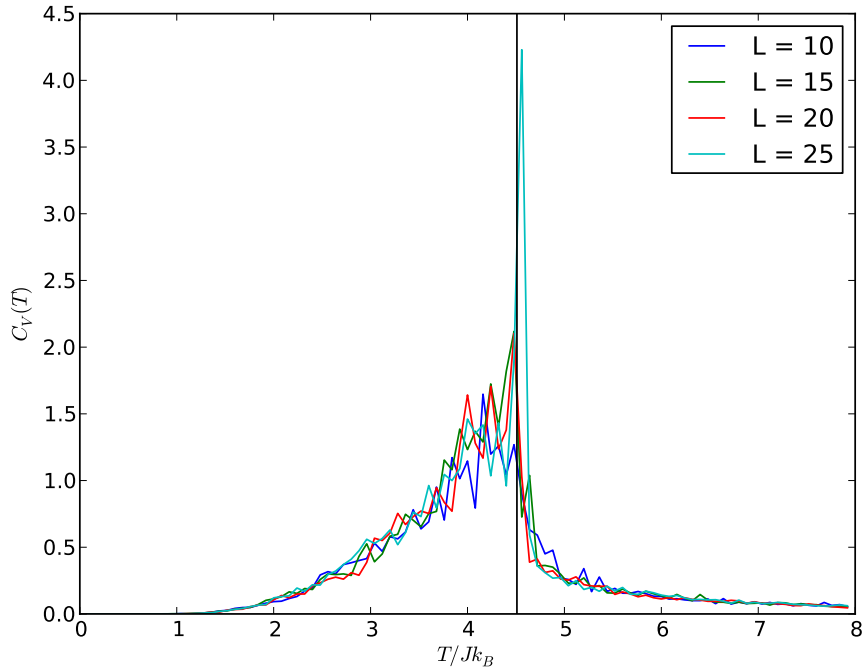
All quantities were plotted vs. T for all system sizes. Additionaly the theoretical value for $T_c = 4.51$ was plotted as a vertical line.





The Energy increase flattens after $T = T_c$. Magnetization should decrease exponentially until reaching 0 at T_c. The higher L gets the less $\langle M \rangle$ will fluctuate after T_c.





These two quantities should display a pole at T_c which they do for high enough L.