Ising Model

1. Magnetization:

Copy into your working directory the sample program `~kvollmay/classes.dir/capstone_s2005.dir/ising.dir/ising_sample1.cc`. Familiarize yourself with the program and add to it a function which determines $M(s) = \frac{1}{N} \sum_{i=1}^{N} s_i$. Print out t, E, M. Check your result.

2. Monte Carlo Step

2a. As preparation for the Monte Carlo step with the Metropolis Algorithm, make a sketch of the possible scenarios for a flip of spin s_i. What is ΔE in each case? When do you flip for sure and when do you flip with probability p? What is p in the latter case?

2b. Implement the Monte Carlo step. Have a look at $M(t)$ and $E(t)$ (for $T = 2.0$).

2c. Determine $M(t)$ for $T = 5.0, 3.0, 2.0, 1.0$. Save your data and plot $M(t)$ for the different temperatures all in one graph.

3. $\langle M(T) \rangle$:

3a. Get me before you start with this part so that we can discuss your results from 2c. and its consequences.
Determine $< M >$ for $T = 2.0$. Check your result by comparing with your result for 2b.

3b. Determine $M(T)$ (make sure to record only equilibrated averages). Get me after this part, so that we can discuss your result.

3c. Next we check if we find the expected powerlaw for $\langle M(T) \rangle$. Rerun your program from 3b. but for $1.0 \leq T \leq 3.0$ in steps of $\Delta T = 0.05$ and redirect your output into a file (`MEofT`). Then use gnuplot to fit the expected powerlaw: On the commandline type `gnuplot`. Within gnuplot first look at your data with `plot "MEofT"`. We expect $M(T) = A(T_c - T)^\beta$. Do a fit on your data with the following steps:

1. `f(x) = A*(Tc-x)**beta`
2. `A=1`
3. `Tc=2.5`
4. `beta=0.5`
5. `fit [1.5:2.5] f(x) "MEofT" via A,Tc,beta`

Play with the fitting range. Get me to discuss your results.

Ising Model: Magnetization & Susceptibility

3. Magnetization $\langle M(T) \rangle$:

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3c. (if time permits): Next we check if we find the expected powerlaw for $\langle M(T) \rangle$. Rerun your program from 3b. but for $1.0 \leq T \leq 3.0$ in steps of $\Delta T = 0.05$ and redirect your output into a file (`MEofT`). Then use gnuplot to fit the expected powerlaw: On the commandline type `gnuplot`. Within gnuplot first look at your data with `plot "MEofT"`. We expect
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Play with the fitting range. Get me to discuss your results.

4. Susceptibility:

4a. If one includes an external magnetic field H then $E = -\sum J s_i s_j - H \sum s_i$. Similar to the fluctuation dissipation relation for the specific heat one can find a relation for the susceptibility $\chi = \lim_{H \to 0} \frac{\partial \langle M \rangle}{\partial H}$, where $\langle M \rangle = \frac{1}{Z} \sum_{\{s\}} M \exp(-\beta E)$, $M = \sum s_i$, and $\beta = \frac{1}{kT}$. Find the fluctuation dissipation relation for the susceptibility.

4b. Add to your program from 3b. the measurement of $\langle M^2 \rangle$ and print out $\chi(T)$. For better statistics use `L=16`, equilibrate for `1000*L`^{2} MC steps and run your simulation for `3000*L`^{2} MC steps.

4c. Similarly determine $C(T)$.

4d. (if time permits): Let us determine the critical exponent γ. Theoretically we expect for $T \approx T_c$ that $\chi \sim |T - T_c|^{-\gamma}$. To be able to fit your data redo 4b for $1.5 \leq T \leq 3.5$ in steps of $\Delta T = 0.05$ and redirect your output into a file (`ChiofT`). Then use gnuplot to fit the expected χ to your data.
(`f(x) = A * abs(x-Tc)**(- alpha)`
`fit [2.41:3.51] f(x) "ChiofT" via A,Tc,alpha`)

Project III: Ising Model

Get together in groups of two or three. You will work today on further analysis of the Ising model. Pick one of the projects described below. Each group will present in class for about 7 min what they have worked on and what their results are.
Work with your group until about 10:20am on your analysis. From 10:20 – 10:35 work as a group on your presentation. You may use the transparencies and pens provided in class. From 10:35 until the end of the class each group will give their presentation.

Project III.1

4. Susceptiblity

4a. Use the fluctuation dissipation relation for the susceptibility $\chi = \lim_{H\to 0} \frac{\partial \langle M \rangle}{\partial H}$

$$\chi = \frac{1}{kT} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \tag{4}$$

where we choose energy and temperature units such that $k = 1$. Use your program from 3b. of last class, or use the sample file
`~kvollmay/classes.dir/capstone_s2005.dir/ising.dir/ising_sample4.cc`.
For better statistics use `L=16`, equilibrate for `1000*L`^{2} MC steps and run your simulation for `3000*L`^{2} MC steps. Use $0.25 \le T \le 5.0$ in temperature steps of $\Delta T = 0.25$. Add to the program the measurement of $\langle M^2 \rangle$ and print out $\chi(T)$. Interpret your result.

4b. (if time permits) Refine your measurement to check your interpretation. For $1.5 \le T \le 3.5$ in steps of $\Delta T = 0.1$ equilibrate for `3000*L`^{2} steps and run your simulation for `5000*L`^{2} MC steps.

5. Specific Heat

Add to your program the measurement of $C(T)$ using the fluctuation dissipation relation from last class. Use the same parameters as in 4a. Interpret your result.

6. Critical Exponents (if time permits)

Let us determine the critical exponent γ. Theoretically we expect for $T \approx T_c$ that $\chi \sim |T - T_c|^{-\gamma}$. If you have done 4b then combine your data from 4a and 4b, by copying both into the same file and taking the data from 4b for the temperature range $1.5 \le T \le 3.5$. If you have not done 4b then use your data from 4a. In the following I assume that your data are in file named `ChiofT`. Use gnuplot to fit the expected χ to your data.

```
gnuplot
f(x) = A * abs(x-Tc)**(- gamma)
```

```
Tc=2.4
A=1
gamma=1
```
using 4a data: `fit [2.25:5.0] f(x) "ChiofT" via A,Tc,gamma`
using 4a and 4b combined data: `fit [2.4:3.5] f(x) "ChiofT" via A,Tc,gamma`

Project III.2

7. Relaxation

Use your program from 2b. or use the sample file
`~kvollmay/classes.dir/capstone_s2005.dir/ising.dir/ising_sample7.cc`.
Our goal is to observe the relaxation of the system.

7a. Relaxation Time $\tau(T)$

Our goal is to get the relaxation time τ as a function of temperature T. To get an estimate for τ, we
(i) first run the program at a specific temperature, e.g. $T = 1.5$ for `NSTEPMAX=500*L`^{2} MC steps.
(ii) Have a look at $M(t)$ with `xgraph -m MEoft.data` to decide from which time on `NEQUILSAVE` it is save to measure $\langle M \rangle$.
(iii) Then determine $\langle M \rangle$ by using gawk (for example):
```
gawk 'BEGIN{Mav=0;count=0;NEQUILSAVE=100}{if($1>NEQUILSAVE) {Mav +=
$2;count++}}END{print Mav/count}' MEoft.data
```
The resulting number is `Mav`$= \langle M \rangle$. (If $\langle M \rangle < 0$ use `Mav=0`.)
(iv) Then look again at $M(t)$ to determine the first crossing point of $M(t)$ with `Mav`. (v) Record your resulting $\tau(T)$ in a file `thetaofT.data`.
Repeat (i)-(v) for temperatures $1.5 \le T \le 4.0$. You will have to adjust for each temperature `NSTEPMAX`. First use $\Delta T = 0.5$, then fill in more detailed points to get a nice graph of $\tau(T)$.

7b. Relaxation $M(t)$ (if time permits)

Let's next see how the system relaxes to its equilibrium. To do so, rerun your simulation for $T = 2.2$ for `NSTEPMAX=500*L`^{2} MC steps. Then fit the resulting $M(t)$ to the function $M(t) =$`Mav` $+(1 - \exp(-t/\tau)$. We use gnuplot. Type in
```
gnuplot
f(x) = Mav+(1-Mav)*exp(-x/tau)
fit [0:100] f(x) "MEoft.data" via tau,Mav
plot "MEoft.data",f(x)
set xrange [0:50] replot
```