Assignment 6

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1 Harden Problem 1

Let K be the coupling and h the external field in a 1D Ising model. From the lectures these can be transformed into effective coupling and fields K' and h' respectively. Unfortunately, the transformation is iterative and takes the form

$$x' = \frac{x\,(1+y)^2}{(x+y)\,(1+xy)} \tag{1}$$

$$y' = \frac{y\,(x+y)}{1+xy} \tag{2}$$

where $x = e^{-4K}$ and $y = e^{-h}$.

We can show that this iterative scheme has two fixed points by asking ourselves what are fixed points? They are points when the iterative scheme has arrived at some value and won't change no matter how many more times we iterate *i.e.* when $x' = x$ and $y' = y$ we call these value x_*, y_*. Let's start with y. At the fixed point

$$\begin{aligned}
y' &= \frac{y\,(x+y)}{1+xy} \\
y_* &= \frac{y_*\,(x+y_*)}{1+xy_*} \\
y_*\,(1+xy_*) &= y_*\,(x+y_*) \\
0 &= y_*\,(x+y_*) - y_*\,(1+xy_*) \\
&= y_*\,(x+y_*-1-xy_*) \\
&= y_*\,(1-y_*)\,(1-x)
\end{aligned}$$

$$\boxed{y_* = 0, 1} \tag{3}$$

For x we are only asked about one fixed point $x_* = 0$. But that's obvious when we set $x' = x = x_*$:

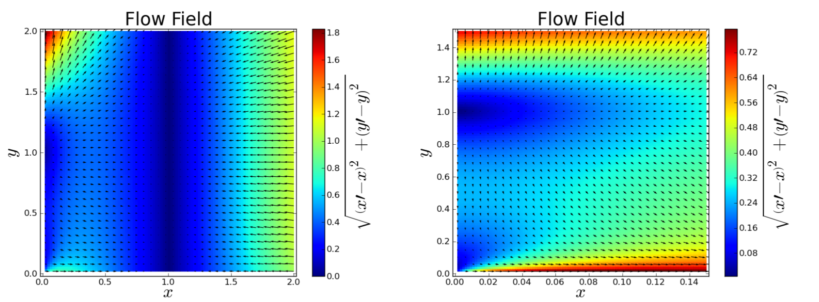
$$\begin{aligned} x' &= \frac{x\,(1+y)^2}{(x+y)\,(1+xy)} \\ x_* &= \frac{x_*\,(1+y)^2}{(x_*+y)\,(1+x_*y)} \\ 0 &= x_*\left(1-\frac{(1+y)^2}{(x_*+y)\,(1+x_*y)}\right) \\ &= x_*\left[(x_*+y)\,(1+x_*)-(1+y)^2\right] \\ &= x_*\left[x_*-1+y^2x_*-y^2+x_*^2y-y\right] \\ &= x_*\,(x_*-1)\left[1+y\,(x_*+1)+y^2\right] \end{aligned}$$

$$\boxed{x_* = 0, 1} \tag{4}$$

We can show that $x_* = 1$ is a fixed line by substituting it into the iterative scheme and seeing that the left over y terms cancel out. Therefore, the left over combinations give the fixed points

$$(x_*, y_*) = (0,0)\,,(0,1)\,. \tag{5}$$

To see these, we switch to a graphical represenation. Fig. 1 is a plot of the difference between x and x', and y and y'. The total data is in the flow diagram of the vectors but since I sometimes find it hard to judge the magnitude of these arrows when there are so many of them, I plotted the magnitude as a color plot in the background (the color scale is normalized in each one, see the color legends to the right of each figure). From Fig. 1a the $x_* = 1$ fixed line is clear as a dark blue stripe.



(a) Renormalization flow diagram.

(b) Renormalization flow diagram zoomed into the fixed points.

Figure 1: Normalized difference between x, x' and y, y'. Colour gives the magnitude while arrows give the entire vector.

The fixed points aren't as obvious from Fig. 1a so we zoom into small x to get Fig. 1b which shows the fixed points very clearly. Notice one thing about these figures is that y only techniqually exists between $[0, 1]$ by $y = e^{-h}$. The range in Fig. 1 was just to help you visualize. The truely acceptable range is shown in Fig. 2 .

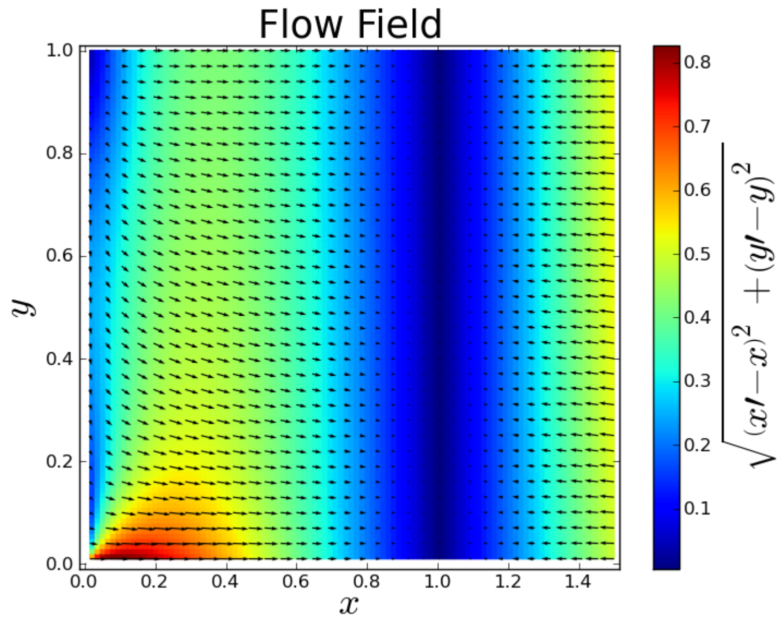


Figure 2: Normalized difference between x, x' and y, y' over physically acceptable range.

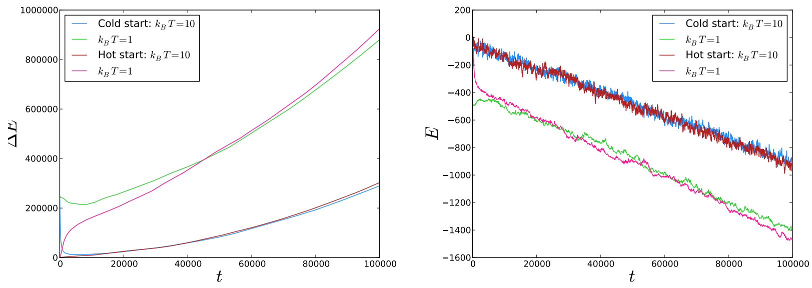
2 Shendruk Problem 2

2.1 1-D

2.1.1 Problem 2.1.a

The Ising model is conceptually simple but that doesn't mean that it is always easy to get good data out of it. For instance, consider a 1-D ferromagnet of $N = 500$ spins with no external field present. From Fig. 3a, very rapidly the hot and cold starts agree when $k_{\rm B}T/J = 10$. But when $k_{\rm B}T/J = 1$ far longer is required. An equilibration time of 20,000 seems sufficient since the hot start and the cold start agree, even for such cold temperatures (the colder it is the slower it equilibrates). But there is clearly a problem: Neither the energy fluctuations in Fig. 3a nor the energy itself in Fig. 3b have plateaued. Obviously, this is not equilibrated properly.

The rate of change with time of energy and energy fluctuations is not due to too short of an equilibrium time. The system is just too small or the temperature is too large. Let's keep all other parameters fixed and increase the number of spins to $N = 10000$. This is shown in Fig. 4. After long times (about $t = 10000$ time steps for $k_{\rm B}T/J = 10$ and say $t \approx 300000$ for $k_{\rm B}T/J = 1$), the energy and



(a) Energy fluctuations.

(b) Instantaneous energy.

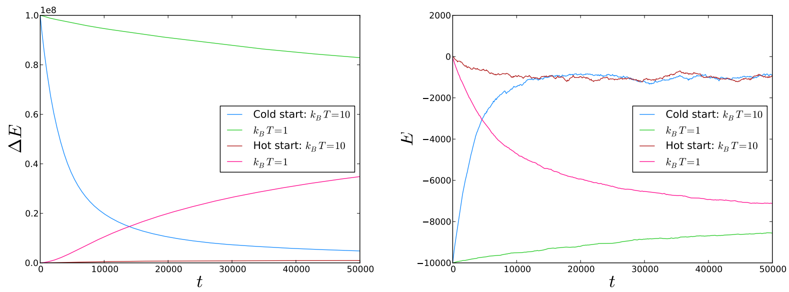
Figure 3: Equilibration for 1-D chain of $N = 500$ spins forming a ferromagnet ($J = 1$) in no external field ($B = 0$).

it's fluctuations have reached a point we might reasonably say their values are not rapidly evolving. The larger the system the more stable it is.

Another (often easier) way to do this is to add a field. A small magnetic field will help stabilize the system and in fact we will find that it is essential to getting good data in 2-D but it's a trade off since it will change some of the analytic results.

2.1.2 Problem 2.1.b

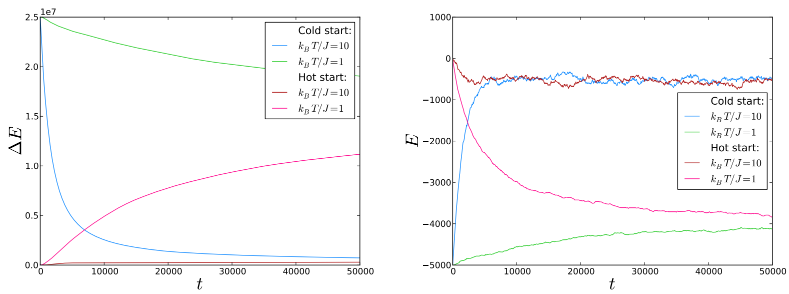
But we have a new problem! The values of E and ΔE for the hot and cold start pretty much agree in Fig. 4 but the systems for which $k_B T/J = 1$ do not have agreeing hot and cold starts. Therefore, we must conclude that one of (or both) haven't reached their equilibrium. $t = 50000$ time steps is not huge for one or two simulations but once we start plotting thermodynamic variables as a function of temperature we are going to need many, many simulations to get acceptable resolution. We must comprimise.



(a) Energy fluctuations. (b) Instantaneous energy.

Figure 4: Equilibration for 1-D chain of $N = 10000$ spins forming a ferromagnet ($J = 1$) in no external field ($B = 0$).

Fig. 5 shows the time evolution of a 1-D ferromagnet Ising chain of $N = 5000$ spins with no external field applied. The energy and it's fluctuations do not descend or climb as they did for the smaller system shown in Fig. 3 and the differences between hot and cold starts are not as pronounced as in Fig. 4. The ΔE agreement between hot and cold starts for low temperatures is still not great but this tells us to expect greater uncertainty of our thermodynamic functions at lower temperatures.



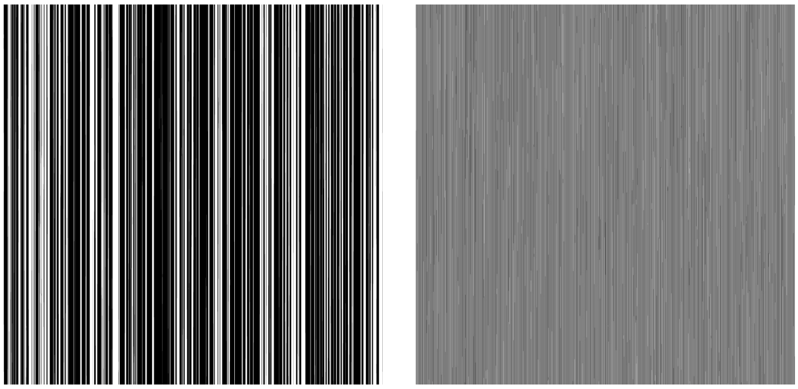
(a) Energy fluctuations. (b) Instantaneous energy.

Figure 5: Equilibration for 1-D chain of $N = 5000$ spins forming a ferromagnet ($J = 1$) in no external field ($B = 0$).

From our discussion and Fig. 5, we assert that $N = 5000$ with an equilibration time of $t_{eq} = 30000$ is reasonable.

2.1.3 Problem 2.1.c

I look at $N = 5000$ at $k_B T/J = 0.75$ with a tiny $B = 0.01$ after equilibration in Fig. 6 . The ferromagnet in Fig. 6a has clear domains of correlated spin up or down regions while Fig. 6b is almost grey since the black and the white are so anti-correlated.



(a) Ferromagnetic system of $J = 1$ (b) Ferromagnetic system of $J = -1$

Figure 6: Visual comparision between ferromagnetic (left) and antiferromagnetic (right) systems. Time is represented by the y-axis. The temperature is low enough that few changes happen over the viewing time.

2.1.4 Problem 2.1.d

We plot the energy, the magnetization, the heat capacity, and the susceptibility (which is found very similarily to the heat capacity and I should have asked you to plot). We do this for a ferromagnet with an exchange energy J, with periodic boundary conditions, in a weak external field $B = 0.05$. We initialize with a hot start and equilibrate for $t_{eq} = 30000$ time steps. We do a hundred simulations from $k_\mathrm{B}T/J = 0$ to 10.

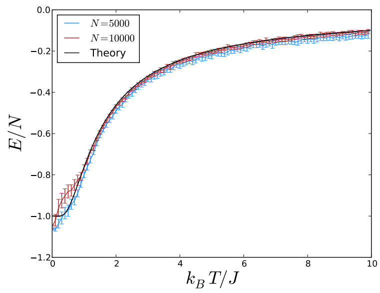
The expectation values I'll compare against are

$$\frac{E}{J} = -N \tanh\left(\frac{J}{k_\mathrm{B}T}\right)$$

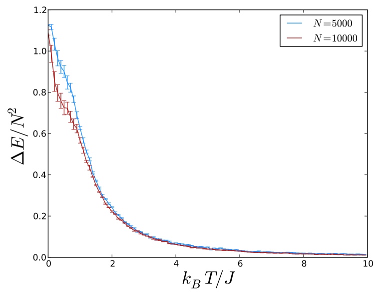
$$C = \frac{(J/k_\mathrm{B}T)^2}{\cosh^2 (J/k_\mathrm{B}T)}$$

$$M = \frac{N e^{J/k_\mathrm{B}T} \sinh (B/k_\mathrm{B}T)}{\sqrt{e^{2J/k_\mathrm{B}T} \sinh^2 (B/k_\mathrm{B}T) + e^{-2J/k_\mathrm{B}T}}}.$$

To start with we use $N = 5000$ spins as suggested in one of the previous sections but to improve the agreement we redo all simulations for twice as many spins ($N = 10000$). To compare between the two we can just scale by N.



(a) Energy as a function of $k_\mathrm{B}T$.



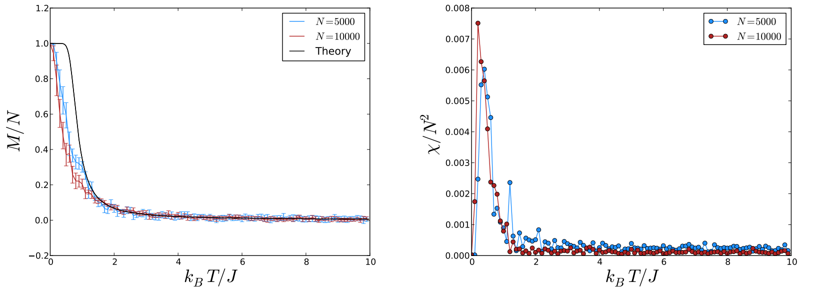
(b) Energy fluctuations as a function of $k_\mathrm{B}T$.

It is fairly evident that increasing N beyond $N = 5000$ does not significantly increase the accuaracy. In Fig. 7a we sort of capture some of the levelling off at small temperatures but otherwise the data don't differ. Furthermore, the poor agreement of specific heat C at low temperatures indicates that we do need some improvement. Let's increase the field to $B = 0.5$ which is pretty large by not huge. We will get worse agreement with theory; however, the data shouldn't be as noisy. According to Fig. 9 the noise is much better (Look at the C/N scale) but still not great.

3 Shendruk Problem 2

3.1 1-D

For 2-D we use a system of $N = 22500$ spins in a small magnetic field of $B = 0.05$ compared to the exchange energy $J = 1$. Speaking of which we know that all



(a) Magnetization.

(b) Susceptibility is the variance of the average of the magnetization.

Figure 7: Magnetization and susceptibility as a function of $k_{\mathrm{B}}T$.

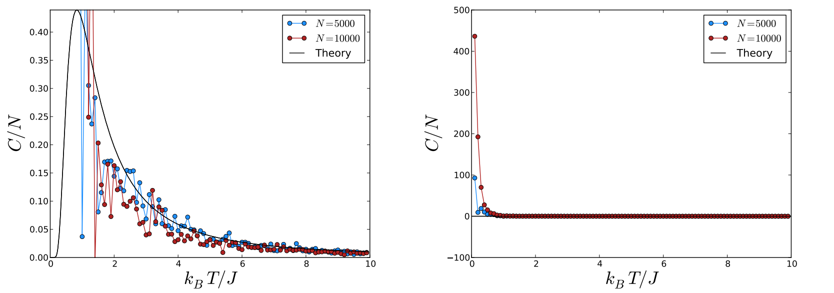


Figure 8: Specific heat as a function of $k_{\mathrm{B}}T$.

the interesting stuff happens below $k_{\mathrm{B}}T/J = 5$ so we simulate over a smaller range of $k_{\mathrm{B}}T/J$ than we did in 1-D.

We expect there to be a phase transition at a critical temperature of

$$\boxed{\frac{k_{\mathrm{B}}T_c}{J} = \frac{2}{\ln\left(1+\sqrt{2}\right)} \approx 2.27}. \tag{6}$$

The critical temperature T_c comes into the theoretical expectation value of the magnetization and the specific heat

$$M = \left(1 - \left[\sinh\left(\ln\left(1+\sqrt{2}\right)\frac{T_c}{T}\right)\right]^{-4}\right)^{1/8}$$

$$C = \frac{8}{\pi T_c}\ln\left(\frac{T_c}{1-T/T_c}\frac{e^{-(1+\pi/4)}}{2}\right).$$

I've included Fig. 10 , a picture of the domains near the critical temperature T_c. Near the critical temperature there is no characteristic size to the domains *i.e.* tiny domains and huge domains are equally likely. In a manner of speaking it's fractal in nature.

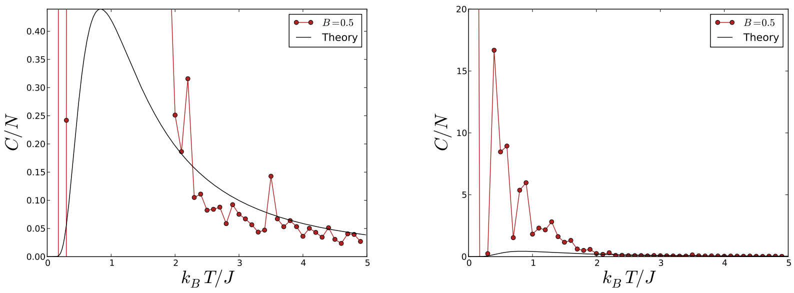


Figure 9: Specific heat as a function of $k_{\mathrm{B}}T$ but now with an applied field of $B = 0.5$.

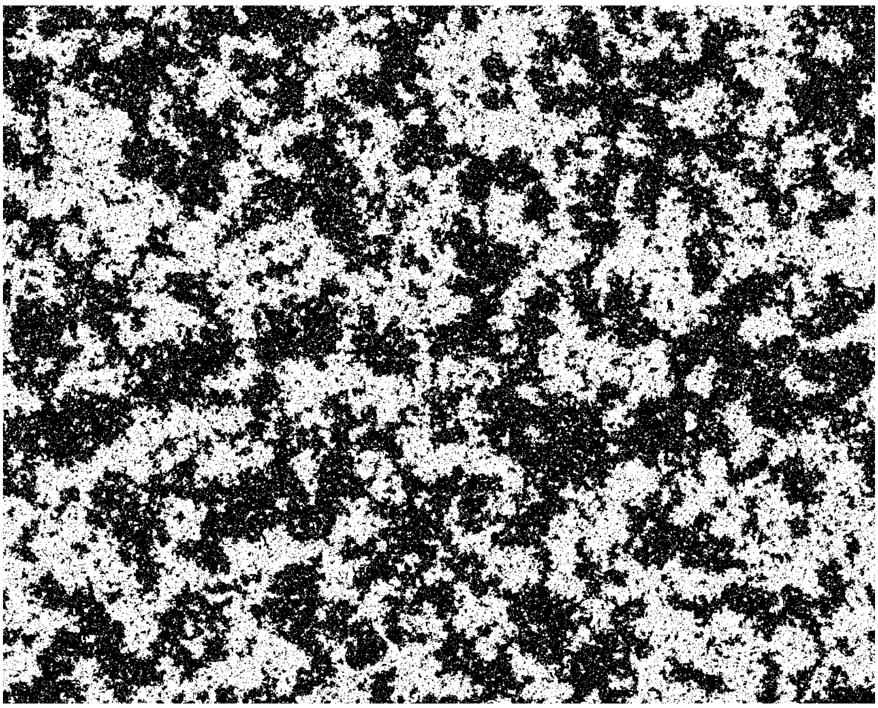


Figure 10: Domains for a 2-D Ising model near the transition temperature. Notice the fractal nature.