Computational Physics II 5640 Spring 2018

Project Assignment 2

Due: Wednesday March 21

1. Critical exponents from Landau's theory (50%). Obtain the following critical exponents based on Landau's theory of continuous phase transitions: $\alpha = 0$, $\beta = 1/2$, $\gamma = 1$, and $\nu = 1/2$. (this is a pen and paper problem).

2. Scaling relation (50%). In the vicinity of a second-order phase transition, the magnetization and susceptibility satisfy the following relation for a finite system:

$$m \sim L^a \, \Phi(\xi/L), \qquad \chi \sim L^b \, \Upsilon(\xi/L). \tag{1}$$

where ξ is the correlation length, L is the linear size of the system, and $\Phi(x)$ and $\Upsilon(x)$ are universal functions. Close to the phase transition temperature T_c, the correlation length diverges as $\xi \sim 1/|T - T_c|^\nu$. (i) What is the asymptotic behavior of these two functions at small x? (ii) Use these asymptotic functional form to determine the exponents a and b.

3. Critical exponents from finite size scaling of Monte Carlo simulations (100%). We consider again the ferromagnetic Ising model on a square lattice $\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j$, $(J > 0)$. To analyze the critical behaviors, we need to compute various physical quantities. The first one is specific heat:

$$c = \frac{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}{T^2 L^2}, \tag{2}$$

Here $\beta = 1/T$ is the inverse temperature, $\langle \cdots \rangle$ means sample averages in simulations. The order parameter of the phase transition is given by

$$m = \langle |M| \rangle / L^2 = \Big\langle \Big| \sum_i \sigma_i \Big| \Big\rangle / L^2, \tag{3}$$

It is important to use the absolute value $|M|$ in computing m, otherwise the total magnetization M oscillates between the two time-reversal equivalent ordered states in different runs, giving rise to a vanishing sample average. $m = 1$ in the perfectly ordered state. The spin susceptibility is

$$\chi = \frac{\langle M^2 \rangle - \langle |M| \rangle^2}{T L^2}. \tag{4}$$

And finally we are also interested in the fourth-order Binder cumulant:

$$B_4 = 1 - \frac{\langle M^4 \rangle}{3 \langle M^2 \rangle^2}. \tag{5}$$

The critical temperature (or transition temperature) is determined by the crossing of various $B_4(T)$ curves as demonstrated in Fig. 1. For 2D Ising model, the critical temperature is $T_c = 2J/\ln(1+\sqrt{2}) \approx 2.269J$ from Onsager's exact solution. Next the scaling relation $B_4 = f(\xi/L)$, where $\xi \sim |T - T_c|^{-\nu}$ is the correlation length allows us to extract the critical exponent ν. This can be done by plotting B_4 verse $|T - T_c| \, L^{1/\nu}$; the different B_4 curves should collapse onto a single universal curve $f(x)$ with the right choice of ν. Again, Onsager's exact solution gives $\nu = 1$. Note the combination $|T - T_c| \, L^{1/\nu}$ is simply $(L/\xi)^{1/\nu}$.

The scaling relation $m(T) \sim (T_c - T)^\beta$ indicates that $mL^{\beta/\nu}$ vs $(L/\xi)^{1/\nu}$ should collapse on another universal curve as demonstrated in Fig. 2. This allows us to extract the exponent β which is 1/8 for 2D Ising model. The exponent γ can be similarly obtained by plotting $\chi L^{\gamma/\nu}$ vs $(L/\xi)^{1/\nu}$; see Fig. 3. The divergence of specific heat is governed by critical exponent α: $c \sim |T - T_c|^{-\alpha}$. However, the exponent $\alpha = 0$ for 2D Ising model, but there is a logarithmic correction to specific heat, i.e. $c_{\max} \sim \log(L)$ when $T \sim T_c$. To test the logarithmic divergence of c, one can plot $c/\ln(L)$ vs $(L/\xi)^{1/\nu}$; the data points from different curves should collapse on yet another universal curve; see Fig. 4.

Use your Monte Carlo codes to produce the various curves for at least three different lattice sizes L. Then perform the finite-size scaling analysis outlined above to obtain critical exponents.

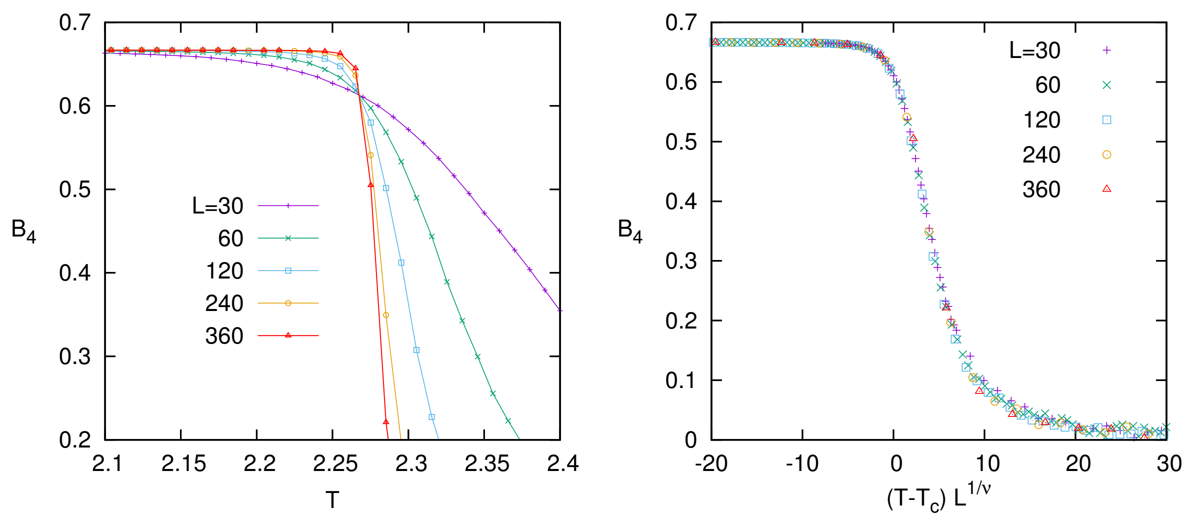

Figure 1: (Left) Binder's 4th-order cumulant vs temperature for varying lattice sizes. The crossing of the different curves gives the critical temperature $T_c \approx 2.269$. (Right) Finite-size scaling plot of Binder's cumulant; the exponent $\nu = 1$ is used in this plot.

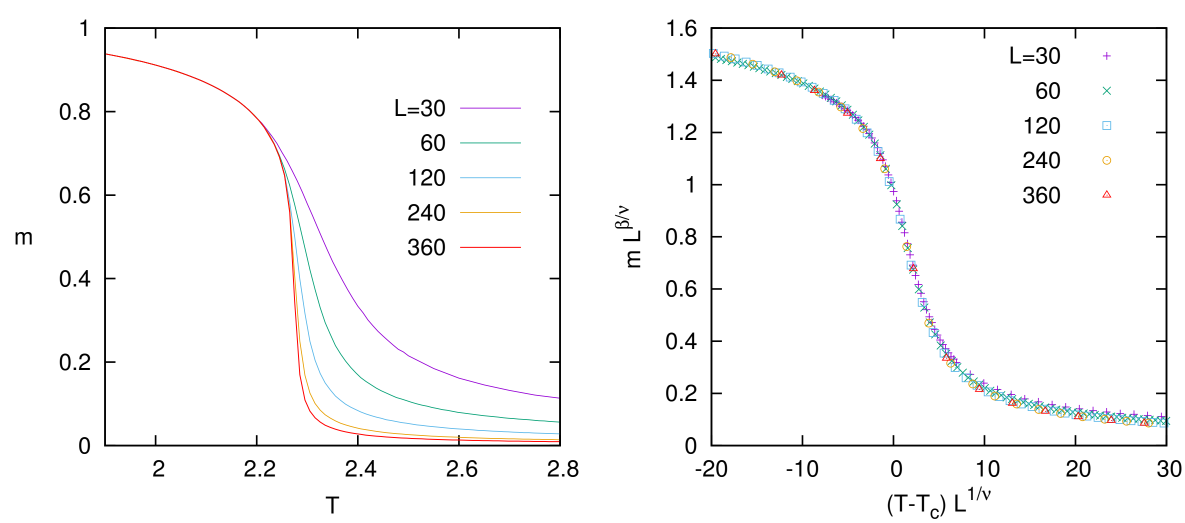

Figure 2: (Left) Magnetic order parameter m as a function of temperature with different L. (Right) Finite-size scaling plot of m with $\beta = 1/8$.

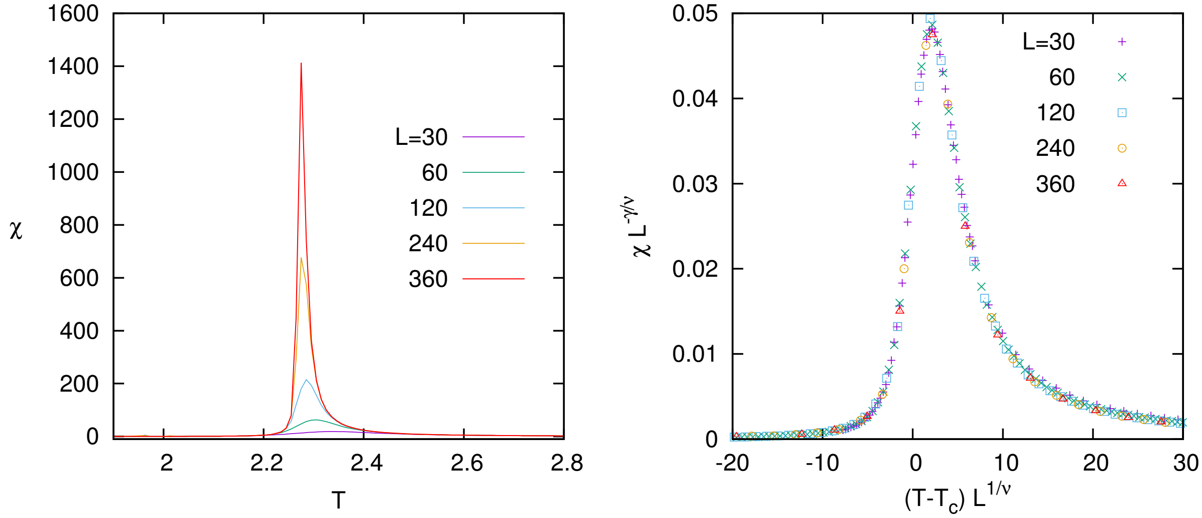

Figure 3: (Left) Magnetic susceptibility χ as a function of temperature with different L. (Right) Finite-size scaling plot of χ with $\gamma = 7/4$.

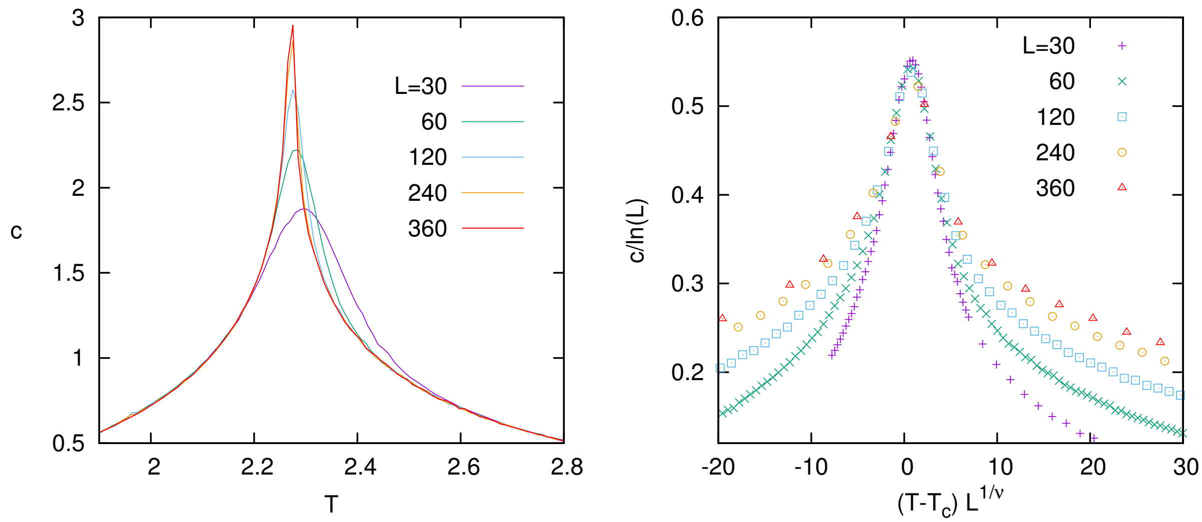

Figure 4: (Left) Specific heat c versus temperature for different lattice size L. (Right) Finite-size scaling plot of c with logarithmic correction included.