PHYS 5640 - Project 2

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1 Critical Exponents from Landau's Theory

We aim to obtain the following critical exponents using Landau's theory of continuous phase transitions: $\alpha = 0$, $\beta = 1/2$, $\gamma = 1$, and $\nu = 1$.

Near the critical temperature of the system T_c the following quantities are defined to scale as

$$c \sim \frac{1}{|T - T_c|^\alpha} \tag{1}$$

$$m \sim (T_c - T)^\beta \sim H^{1/\delta}\big|_{T=T_c} \tag{2}$$

$$\chi = \left.\frac{\partial m}{\partial H}\right|_{H=0} \sim \frac{1}{|T - T_c|^\gamma} \tag{3}$$

$$\xi \sim \frac{1}{|T - T_c|^\nu} \tag{4}$$

where c is the specific heat, m is the magnetic order parameter, χ is the magnetic susceptibility, and ξ is the correlation length of the system. The exponents α, β, δ, γ, and ν are known as critical exponents.

First, we write the Landau free energy expansion as

$$F(m) = am^2 + bm^4 + ... \tag{5}$$

with $a = \frac{A}{2}(T - T_c)$. This free energy neglects all odd powers of m, since the system has time-reversal symmetry ($m \to -m$ leaves the Hamiltonian $\mathcal{H}$ unchanged). In minimizing Eq. 5 with respect to m we can find

$$\frac{\partial F}{\partial m} = 0 = 2am + 4bm^3$$
$$0 = m\left(2a + 4bm^2\right)$$

therefore we have two options

$$m = \begin{cases} 0, & T > T_c \\ \sqrt{-\frac{a}{2b}} = \sqrt{\frac{A(T_c - T)}{4b}}, & T < T_c \end{cases}$$

From Eq. 2, we find that for low-temperature, ordered states

$$\boxed{\beta = 1/2.}$$

Next, we consider the free energy with the time reversal symmetry broken due to a magnetic field of strength H:

$$F(m) = -Hm + am^2 + bm^4 \tag{6}$$

Again if we minimize with respect to the magnetization we find

$$\frac{\partial F}{\partial m} = 0 = -H + 2am + 4bm^3$$

Using Eq. 3, we know that the magnetic susceptibility is the derivative of the magnetization w.r.t. the magnetic field strength. Thus if we take the derivative of the above equation, we find

$$0 = -1 + 2a\frac{\partial m}{\partial H} + 12bm^2\frac{\partial m}{\partial H} = -1 + 2a\chi + 12bm^2\chi.$$

Thus, we have

$$\chi = \frac{1}{2a + 12bm^2}$$

substituting in the scaling we found for m we obtain

$$\chi = \begin{cases} \frac{1}{2a} = \frac{1}{A(T-T_c)}, & T > T_c \\ \frac{1}{6a} = \frac{1}{3A(T-Tc)}, & T < T_c \end{cases}$$

Using the known scaling for χ given by Eq. 3 we obtain

$$\boxed{\gamma = 1.}$$

Now we wish to obtain the value of α. We can do this by using the universal scaling relationship among critical exponents[1]

$$2 - \alpha = \gamma\frac{\delta+1}{\delta-1}$$

First, we need to find δ, which can be found by considering the free energy with a magnetic field (Eq. 6). At $T = T_c$ we have that $a = A(T - T_c)/2 = 0$, thus we obtain for the free energy

$$F(m) = -Hm + bm^4$$

which is minimized with respect to m when

$$0 = -H + 4bm^3$$

$$\to H \sim m^3 \to m \sim H^{1/3} \to \delta = 3.$$

Now we can use the fact that $\gamma = 1$ and $\delta = 1$ and plug into the universal relationship among the critical exponents:

$$2 - \alpha = 1\frac{3+1}{3-1} = 2 \to \alpha = 0$$

Therefore we have

$$\boxed{\alpha = 0.}$$

Finally, we can find ν by examining the correlation length ξ of the system. First we write the correlation function as

$$G(r_1, r_2) = \langle m(r_1)m(r_2)\rangle \sim e^{-|r_1-r_2|/\xi}$$

Next, we will us the fact that

$$\langle m(r_1)m(r_2)\rangle = \sum_m m(r_1)m(r_2)\pi(m)$$

where

$$\pi(m) = \frac{1}{Z}e^{-\beta F(m)}$$

with

$$F(m) \approx \int dx(c|\nabla m|^2 + am^2)$$

[1] https://en.wikipedia.org/wiki/Critical_exponent#Scaling_relations

We can express the m and ∇m in terms of its Fourier Transform:

$$m(x) = \frac{1}{2\pi}\int \tilde{m}(k)e^{ikx}dk$$

and

$$\nabla m(x) = \frac{ik}{2\pi}\int \tilde{m}(k)e^{ikx}dk$$

which tells us that

$$\int dx m(x)^2 = \frac{1}{(2\pi)^2}\int\int\int dx dk_1 dk_2 \tilde{m}(k_1)\tilde{m}(k_2)e^{ix(k_1+k_2)}.$$

Since

$$\int dx e^{ix(k_1+k_2)} = 2\pi\delta(k_1+k_2)$$

we have that

$$k_1 = -k_2$$

in our Fourier Transforms of m^2 and $|\nabla m|^2$. Thus

$$\int dx|\nabla m|^2 = k^2\int\int\int dx dk_1 dk_2 \tilde{m}(k_1)\tilde{m}(k_2)e^{ix(k_1+k_2)} = k^2\int dk\tilde{m}(k)^2$$

This then gives us a new expression for $F(m)$ in terms of the Fourier modes of m:

$$F(m) = \int dk(ck^2+a)|\tilde{m}(k)|^2$$

which then tells us that

$$\pi(m) = \frac{1}{Z}e^{-\beta\int dk(ck^2+a)|\tilde{m}(k)|^2}$$

which is a normal distribution of the form

$$\pi(x) = \frac{1}{Z}e^{-\frac{x^2}{2\sigma^2}}$$

with

$$\sigma^2 = \frac{1}{2(ck^2+a)}.$$

Normal distributions have the property that for $\pi(x)$, $\langle x^{2n+1}\rangle = 0$ for n an integer and $\langle x^2\rangle = \sigma^2$. This tells us that

$$\langle\tilde{m}(k)\rangle = 0, \quad \langle\tilde{m}(k)\tilde{m}(k')\rangle = 0 \ \ (k \neq k').$$

and

$$\langle|\tilde{m}(k)|^2\rangle = \sigma^2 = \frac{1}{2(ck^2+a)} = \frac{1}{2c}\frac{1}{k^2+a/c}$$

Plugging this back into the form of the correlation function

$$G(r_1,r_2) = \langle m(r_1)m(r_2)\rangle = \int\int dk dk'\langle\tilde{m}(k)\tilde{m}(k')\rangle e^{ikr_1+ik'r_2}$$

using $\langle\tilde{m}(k)\tilde{m}(k')\rangle = 0 \ \ (k \neq k')$ we obtain

$$\begin{aligned} G(r_1,r_2) &= \int dk\langle m(k)^2\rangle e^{ik(r_1-r_2)} \\ &= \frac{1}{2c}\int dk\frac{1}{k^2+a/c}e^{ik(r_1-r_2)} \end{aligned}$$

If we perform this complex integral around the singularity $k = \pm i\sqrt{a/c}$, we obtain

$$G(r_1, r_2) \sim e^{-|r_1 - r_2|/\sqrt{c/a}}$$

Comparing to the ideal form of the correlation function

$$G(r_1, r_2) \sim e^{-|r_1 - r_2|/\xi}$$

we see that the correlation length is

$$\xi = \sqrt{c/a} = \sqrt{\frac{2c}{A(T - T_c)}}$$

From the finite scaling for ξ from Eq. 3 we then know that $\nu = 1/2$. Thus, we've found

$$\boxed{\nu = 1/2.}$$

2 Scaling Relation

The magnetization m and the magnetic susceptibility χ follow the following relationships for a finite system

$$m \sim L^a \Phi(\xi/L), \qquad \xi \sim L^b \Upsilon(\xi/L) \tag{7}$$

where ξ is the correlation length of the system and L is the linear system size. At small x ($x << 1$) we know that the universal function $\Phi(x)$ follows

$$\Phi(x) \sim x^b.$$

Plugging the above into Eq. 7 we obtain

$$m \sim L^a \left(\xi/L\right)^b = L^{a-b}\xi^b.$$

Since $x << 1$ we know that $L \to \infty$, and we know that as $L \to \infty$ the magnetization should become independent of the system size L. Therefore we have

$$m \sim \xi^b$$

for small x. Pairing this with the previous equation we have

$$m \sim L^{a-b}\xi^b \sim \xi^b$$

$$\to a = b$$

Using a similar argument that $m \sim \xi^b$ as x becomes small, we can find the values of a and b. We can use the fact that

$$m \sim (T_c - T)^\beta$$

and

$$\xi \sim \frac{1}{|T - T_c|^\nu}$$

to state

$$m \sim (T_c - T)^\beta \sim \xi^b \sim (T_c - T)^{-\nu b}$$

which tells us that

$$\beta = -\nu b \to b = -\frac{\beta}{\nu}.$$

Given $a = b$ and $\beta = \nu = 1/2$ we then have

$$\boxed{\to a = b = -1}$$

3 Critical exponents from finite size scaling of Monte Carlo simulations

I performed a Monte Carlo simulation of the ferromagnetic Ising model on a square lattice of length L. The Hamiltonian of this system is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

where $\langle i, j\rangle$ corresponds to the nearest neighbors j of spin i. The system was simulated using a Monte Carlo code that considers spin flips on the lattice. The probability of acceptance of a spin flip is a function of the change in energy that the spin flip causes. Performing a chain of spin flips provides one with a distribution over states of the system. Thus, computing observables at every state computed provides a distribution over the observable. The specific heat c, the magnetic order parameter m, the magnetic susceptibility χ, and the 4^{th}-order Binder's cumulant B_4 are computable through measurement of the energy of the system $\mathcal{H}$ (given by the Hamiltonian) and the magnetization of the system M given by

$$M = \sum_i \sigma_i.$$

Measuring both $\mathcal{H}$ and M at each step provides a distribution over these observables. The quantities of interest (c, m, χ, and B_4) are the moments of and cumulants of these distributions:

$$c = \frac{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}{T^2 L^2} \tag{8}$$

$$m = \frac{\langle |M| \rangle}{L^2} \tag{9}$$

$$\chi = \frac{\langle M^2 \rangle - \langle |M| \rangle^2}{T L^2} \tag{10}$$

$$B_4 = 1 - \frac{\langle M^4 \rangle}{3 \langle M^2 \rangle^2} \tag{11}$$

The point where the B_4 vs temperature curves of all system sizes cross is known as the critical temperature T_c (Fig. 1) and it is given analytically as $T_c = 2J/\left(\ln(1+\sqrt{2})\right)$ for a 2D Ising model. The correlation length ξ can be compute from the critical temperature T_c and the critical exponent ν: $\xi \sim |T - T_c|^{-\nu}$. The scaling relationship $B_4 = f(\xi/L)$ tells us that the B_4 should collapse onto a single when plotted versus $(T - T_c)L^{1/\nu}$ for $\nu = 1$ (Fig. 1). Similarly, $mL^{\beta/\nu}$ should collapse onto a universal curve when plotted versus $(T - T_c)L^{1/\nu}$ for $\beta = 1/8$ (Fig. 2). Again, $\xi L^{\gamma/\nu}$ should collapse when plotted versus $(T - T_c)L^{1/\nu}$ for $\gamma = 7/4$ (Fig. 3). Finally, the specific heat (with a logarithmic correction) $c/\ln(L)$ should collapse when plotted versus $(T - T_c)L^{1/\nu}$ (Fig. 4).

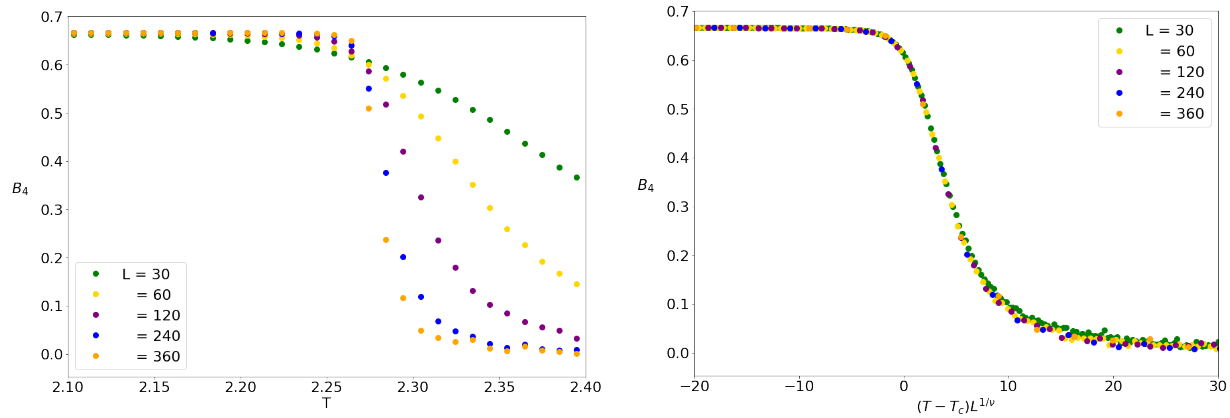

Figure 1: Binder's 4^{th}-order cumulant (B_4) as a function of temperature T (left) and the finite-size scaling plot for B_4 using $\nu = 1$ (right) for various lattice sizes.

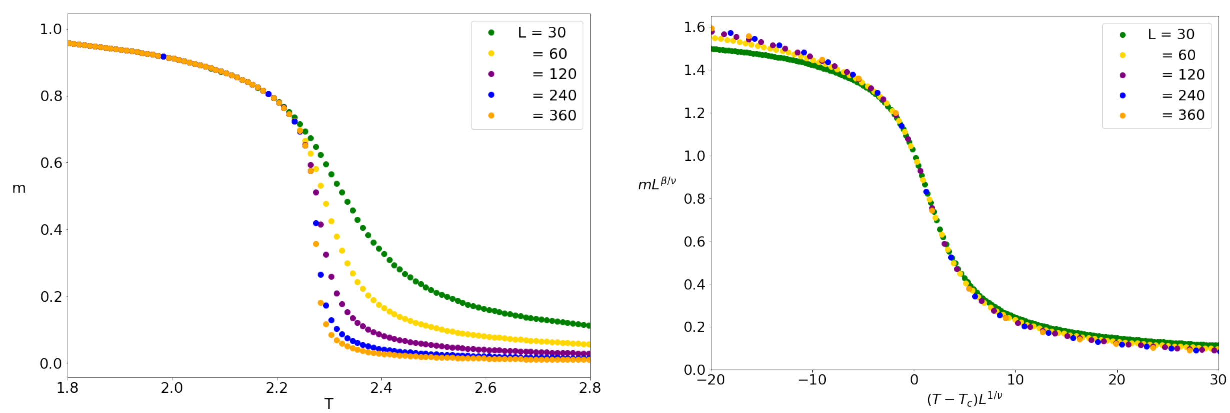

Figure 2: Magnetic order parameter m as a function of temperature T (left) and the finite-size scaling plot for m using $\nu = 1$ and $\beta = 1/8$ (right) for various lattice sizes.

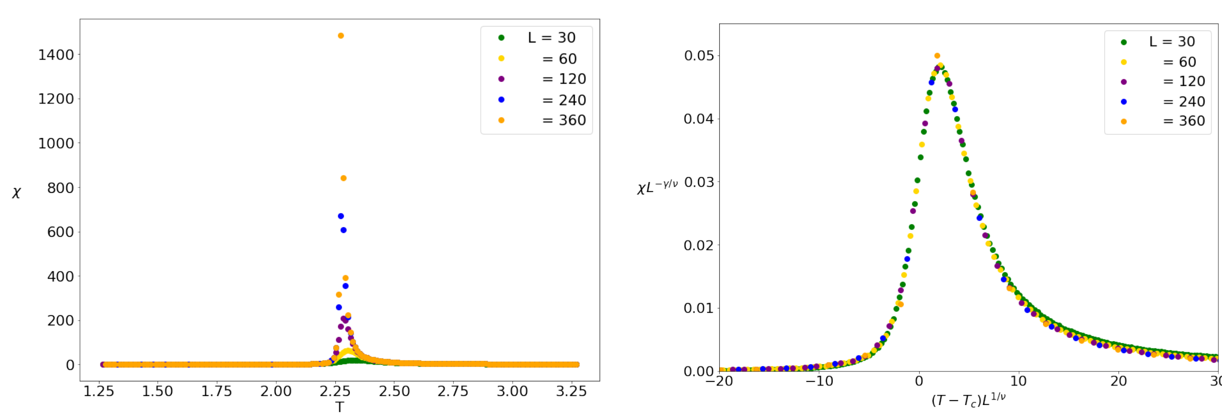

Figure 3: Magnetic susceptibility χ as a function of temperature T (left) and the finite-size scaling plot for χ using $\nu = 1$ and $\gamma = 7/4$ (right) for various lattice sizes.

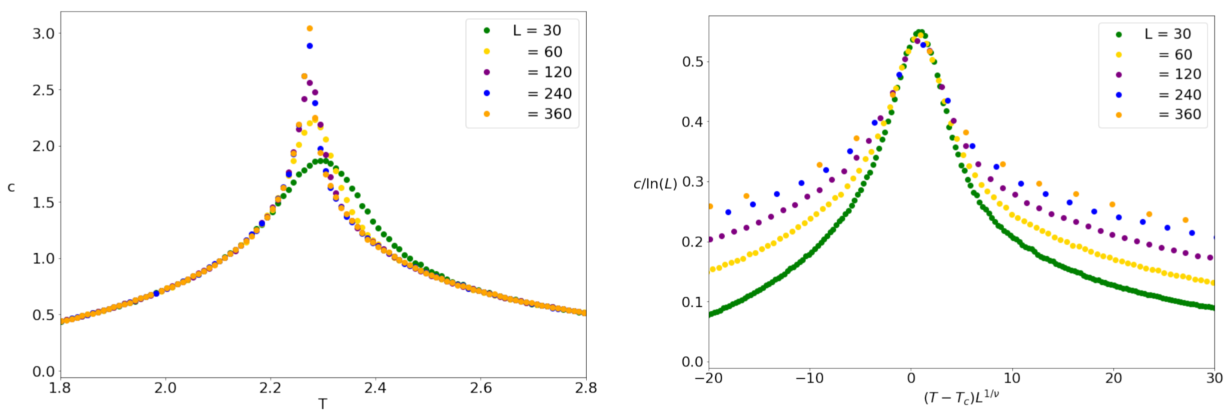

Figure 4: Specific heat c as a function of temperature T (left) and the finite-size scaling plot for c with the logarithmic correction included using $\nu = 1$ (right) for various lattice sizes.