

Module: Phase Transition Basics

We present some basic equilibrium statistical mechanics models (i.e., the binary alloy, the mean field Ising Model, the spin glass, magnetic thin films) as examples of systems which exhibit phase transitions. Using a concept map we outline the various ways one can investigate phase transitions (e.g., through the micro-canonical ensemble, Gibbs-Bogoliubov Inequality, Method of Steepest Descent) and then we list and define terms associated with the theory of phase transitions.

- **What is the Topic:** The purpose of this module is to review some basics of phase transitions in statistical mechanics. I'll use two (or three) of Kardar's problems in [1] as examples of soluble models of phase transitions. Specifically, it seems that a simple way to investigate whether a system shows a phase transition is to first compute the free energy as a function of the order parameter; next compute the order parameter from this free energy to obtain a self-consistent equation for order parameter; finally, if this self-consistent equation yields multiple solutions for the order parameter in certain temperature regimes then the system exhibits a phase transition. This document only covers second-order phase transitions.
- **What questions does it answer?**
(Hopefully) This document will allow you to determine whether statistical mechanics systems exhibit phase transitions, how to compute the critical temperature for such system, and possibly how to calculate the critical exponents for mean field theory models.
- **Why are these questions important?**
It's difficult for me to answer this conclusively. For the longest time I didn't think phase transitions were that interesting. Generally, understanding the phase behavior of a system allows us to understand how order parameters in a system change.

1 Model of a Binary Alloy

The first model we will look at comes from problem 1.1 in [1]. It concerns a model of a so called binary alloy. But it seems the atoms of the alloy can transmute from one kind to the other (seeing as the difference between their quantities is the order parameter), so I'm not sure how physical this model is. In the model we assume we have atoms of type A and type B arranged in a lattice. The when like atoms are next to each other they interact with a coupling $-J$ and when unlike atoms are next to each other they interact with a coupling $+J$. We have N_A atoms of type A and N_B atoms of type B .

One physical question we may ask first, is what might the lowest energy configuration of the system look like? Given our coupling structure, the energy of the system is lowest if all of our lattice sites are filled with the same type of atom, that is all A atoms or all B atoms. Ignoring the lower order edge effects of the system, the energy of this lowest state is

$$E_0 = -\frac{N}{2}6J = -3NJ \quad (1)$$

where the 6 is for the fact we are considering a 3D lattice (and that each atom has 6 nearest neighbors) and the $1/2$ is for double counting of atoms.

For a more general system we could say that there is a probability p_A that a single lattice site will have an atom A and a probability p_B that a single lattice site will have an atom B . We will also look at the system

under the unphysical assumption that all atoms interact with all other atoms. The total energy of the system is such a scenario is then

$$\begin{aligned}
E &= \sum_{p_i=p_A, p_B} \sum_{p_j=p_A, p_B} \frac{1}{2} \sum_{i,j} E(i,j) p_i p_j \\
&= \frac{1}{2} \sum_i E(i,i) p_i p_i + \sum_{i<j} E(i,j) p_i p_j \\
&= \frac{1}{2} N(-6Jp_A^2 - 6Jp_B^2) + N 6Jp_A p_B \\
&= -3NJ(p_A - p_B)^2
\end{aligned} \tag{2}$$

(This derivation is not clear. Re do). When we take these probabilities to in turn be defined by the relative proportion of the atoms (with $N = N_A + N_B$), we find

$$E = -3NJ \left(\frac{N_A - N_B}{N} \right)^2 = -3NJx^2 \tag{3}$$

where we defined $x \equiv (N_A - N_B)/N$.

The larger goal is to investigate the equilibrium thermodynamics of this system, which boils down to finding the free energy and then from the free energy, determining whether the system exhibits phase transitions. Eq.(3) gives us the energy part of the free energy, so we need only compute the entropy. We are completing our calculation in the microcanonical ensemble, so computing the entropy is a counting problem. The foundational question is given N lattice sites, how many ways can we arrange N_A type A atoms and N_B type B atoms (with $N_A + N_B = N$). The answer is a N choose N_A (or N_B)

$$\Omega = \frac{N!}{N_A! N_B!} \tag{4}$$

and the entropy is

$$S = k_B \ln \Omega. \tag{5}$$

We can put this entropy in a form more amenable to a phase transition analysis by taking certain approximations. If we take $N, N_A, N_B \gg 1$ then we can apply Stirling's approximation to Eq.(4) to find

$$\begin{aligned}
\Omega &\simeq \frac{1}{\sqrt{2\pi}} \left(\frac{N}{N_A N_B} \right)^{\frac{1}{2}} \frac{N^N}{N_A^{N_A} N_B^{N_B}} e^{-N} e^{N_A} e^{N_B} \\
&\simeq \frac{1}{\sqrt{2\pi}} \left(\frac{N}{N_A} \right)^{N_A} \left(\frac{N}{N_B} \right)^{N_B}.
\end{aligned} \tag{6}$$

With the definitions $N = N_A + N_B$ and $Nx = N_A - N_B$, we find

$$\frac{N}{N_A} = \frac{2}{1+x} \tag{7}$$

$$\frac{N}{N_B} = \frac{2}{1-x}. \tag{8}$$

Thus the entropy is

$$\begin{aligned}
S/k_B &\simeq -\frac{1}{2} \ln 2\pi + \frac{1}{2} \ln \frac{N}{N_A N_B} + N_A \ln \frac{N}{N_A} + N_B \ln \frac{N}{N_B} \\
&= -\frac{1}{2} \ln 2\pi + \frac{N}{2} (1+x) \ln \frac{2}{1+x} + \frac{N}{2} (1-x) \ln \frac{2}{1-x}
\end{aligned}$$

$$= -\frac{N}{2}(1+x) \left[-\ln 2 + \ln(1+x) \right] - \frac{N}{2}(1-x) \ln \left[-\ln 2 + \ln(1-x) \right] \quad (9)$$

Now we take make an approximation which is not at all general. We will assume N_A and N_B are relatively close in number so that $x \ll 1$. We can then expand the logarithms in Eq.(9) to find

$$\begin{aligned} S/k_B &= -\frac{N}{2}(1+x) \left[-\ln 2 + x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \mathcal{O}(x^5) \right] \\ &\quad - \frac{N}{2}(1-x) \left[-\ln 2 - x - \frac{x^2}{2} - \frac{x^3}{3} - \frac{x^4}{4} - \mathcal{O}(x^5) \right] \\ &= -\frac{N}{2} \left[-2\ln 2 - x^2 - \frac{x^4}{2} + \mathcal{O}(x^6) \right] - \frac{N}{2} x \left[2x + \frac{2}{3}x^3 + \mathcal{O}(x^5) \right] \\ &= -\frac{N}{2} \left[-2\ln 2 + x^2 + \frac{x^4}{6} + \mathcal{O}(x^5) \right]. \end{aligned} \quad (10)$$

We now have all the necessary pieces to write our free energy. Given Eq.(3) and Eq.(10) we find

$$\begin{aligned} F &= E - TS \\ &= -3NJx^2 - \frac{N}{\beta} \left(\ln 2 - \frac{x^2}{2} - \frac{x^4}{12} \right) + \mathcal{O}(x^6), \end{aligned} \quad (11)$$

where we defined $\beta = 1/k_B T$. For future simplicity, we will drop the higher order terms and the constant and simply define the free energy as

$$F(x) \equiv \left(\frac{1}{2\beta} - 3J \right) Nx^2 + \frac{N}{\beta} \frac{x^4}{12} \quad (12)$$

The next step is to find the value of x which minimizes Eq.(12), and then analyze this x to see if it admits multiple values for the same temperature. We follow the standard minimization algorithm. First, computing the critical points

$$F'(x) = \left(\frac{1}{\beta} - 6J \right) Nx + \frac{N}{\beta} \frac{x^3}{3} = 0 \implies \bar{x} = \begin{cases} 0, \\ \pm \sqrt{3(6J\beta - 1)}. \end{cases} \quad (13)$$

For notational simplicity we will define x_0 as the critical point at $x = 0$, and we'll define the other two critical points as x_{\pm} . Now, computing the second derivative of the free energy

$$F''(x) = \left(\frac{1}{\beta} - 6J \right) N + \frac{N}{\beta} x^2, \quad (14)$$

and checking the the stability of each point

$$F''(x = x_0) = N(k_B T - 6J) > 0 \quad (\text{for } T > 6J/k_B) \quad (15)$$

$$F''(x = x_{\pm}) = 2N(6J - k_B T) > 0 \quad (\text{for } T < 6J/k_B). \quad (16)$$

Thus we see we have a phase transition in our system at $T = 6J/k_B$. The order parameter is \bar{x} , the lowest energy state of the free energy, and it has the value

$$\bar{x}(T) = \begin{cases} 0 & (\text{for } T > 6J/k_B) \\ \pm \sqrt{3(6J\beta - 1)} & (\text{for } T < 6J/k_B) \end{cases}. \quad (17)$$

(It would be worth drawing a phase diagram in the (T, x) plane to demonstrate this difference.)

A related question to ask is for what values of x is $F''(x)$ zero. From Eq.(14), we find

$$x_{\text{sp}}(T) = \pm \sqrt{6J\beta - 1} \quad (\text{for } T < 6J/k_B) \quad (18)$$

[1] states that $x_{\text{sp}}(T)$ is called the spinodal line and defines the onset of hysteresis effects and metastability. I do not see how such an interpretation is apparent from $x_{\text{sp}}(T)$ and its relationship to $\bar{x}(T)$.

2 Mean Field Theory of Ising Model

The Ising model is a canonical model in statistical mechanics. Here we explore how the mean field theory solution of the Ising Model predicts phase transitions within the model. The prediction is incorrect for the one-dimensional case, but becomes progressively more accurate as we increase in dimensionality¹.

The local environment of an electron in a crystal can lead the electron's spin to lie either parallel or anti-parallel to a specific lattice direction. We denote the direction of the i th spin by σ_i and for a collection of such spins which interact with each other and are subject to an external magnetic field the Hamiltonian can be written as

$$\mathcal{H}_N(\{\sigma_i\}) = \frac{1}{2} \sum_{i,j} J_{ij} \sigma_i \sigma_j - h \sum_i \sigma_i, \quad (19)$$

where h is the external magnetic field and J_{ij} is the interaction energy between spins i and j . For N spins we make the exceedingly physically imprecise approximation that all spins interact with each other with the same coupling $J_{ij} = -J/N$. For this system this amounts to a mean field approximation. The Hamiltonian for this system then becomes

$$\begin{aligned} \mathcal{H}_N(\{\sigma_i\}) &= -\frac{J}{2N} \sum_{i,j} \sigma_i \sigma_j - h \sum_i \sigma_i \\ &= -N(Jm^2/2 + hm) \equiv E(m, h) \end{aligned} \quad (20)$$

where we defined $m \equiv \sum_i \sigma_i / N = M/N$. To study the equilibrium properties of such a system, we must compute the partition function. We have

$$\begin{aligned} Z_N(h, T) &= \sum_{\{\sigma_i\}} \exp[-\beta \mathcal{H}(\{\sigma_k\})] \\ &= \sum_{M=-N}^N \Omega_N(M) e^{-\beta E(M/N, h)} \end{aligned} \quad (21)$$

$$= \sum_{M=-N}^N e^{-\beta F(M/N, h, \beta)}, \quad (22)$$

where $F = E - \ln \Omega / \beta$ is the free energy (as it is written in the microcanonical ensemble) where $\Omega_N(M)$ is the number of ways to specify N binary valued (+1 or -1) spins so that the sum of all the spins is M . Labeling the number of + spins and the number of - spins as M_+ and M_- respectively, we then have

$$\Omega_N(M) = \frac{N!}{M_+! M_-!}. \quad (23)$$

¹I haven't computed this. I remember Manoharan mentioning it last semester

By definition we must have $M_+ - M_- = Nm$. So if we study Eq.(23) in the limit of $N \gg 1$ and $m \ll 1$, we can transfer wholesale our computation of the entropy from the previous section. The free energy is then found to be

$$F(m, h, \beta) = -N(Jm^2/2 + hm) + (N/2\beta)(m^2 + m^4/6), \quad (24)$$

where we dropped the constant term and the higher order terms. Within this limit the discrete partition function definition Eq.(22) can be replaced with a continuous integral and we can employ the steepest descent approximation. Doing so we have

$$\begin{aligned} Z_N(h, T) &= \sum_{M=-N}^N \exp\left(-\beta F(M/N, h, \beta)\right) \\ &\simeq \int_{-N}^N dM \exp\left(-\beta F(M/N, h, \beta)\right) \\ &= \int_{-1}^{+1} dm \exp\left(-\beta F(m, h, \beta)\right) \\ &\simeq \exp\left(-\beta \min[F(m, h, \beta)]_{m=\bar{m}}\right). \end{aligned} \quad (25)$$

where $\min[F(m, h, \beta)]_{m=\bar{m}}$ is the free energy evaluated at $m = \bar{m}$ with \bar{m} being the value of m at which Eq.(24) satisfies is at a local minimum. The Helmholtz free energy of this system is then

$$F(h, T) = -\frac{1}{\beta} \ln Z_N(h, T) \simeq \min[F(m, h, \beta)]_{m=\bar{m}}. \quad (26)$$

Computing the derivative of Eq.(24), we find

$$\frac{\partial}{\partial m} F(m, h, \beta) = -N(Jm + h) + (N/\beta)(m + m^3/3) = 0 \quad (27)$$

and so the constraint equation for \bar{m} is

$$\frac{1}{3\beta} \bar{m}^3 - \left(J - \frac{1}{\beta}\right) \bar{m} - h = 0 \quad (28)$$

This equation determines $\bar{m}(h, T)$, the value of m which defines thermal equilibrium.

In [1], Kardar states “ $F(m, h, \beta)$ is an analytic function but not convex for $T < T_c$.” This means that while $F(m, h, \beta)$ is an analytic function for its entire domain in m , it is only convex (i.e, it only has a local minimum near $m = 0$) when $T > T_c$ because below T_c the expansion of $m \ll 1$ leads to a $F(m, h, \beta)$ with a local maximum (i.e., a concave function) near $m = 0$.

Kardar also states that “the true free energy $F(h, T)$ is convex but becomes non-analytic due to the minimization”. This means, given that $F(h, T)$ is determined from $F(h, T) \simeq \min[F(m, h, \beta)]_{m=\bar{m}}$, the function $F(h, T)$ is always defined according to a local minimum and is therefore always convex. However, for finite field h , there is a discontinuity in $\bar{m}(h, T)$ at the critical temperature, and so $F(h, T)$ is non-analytic at this temperature.²

Next, we would like to make the phase behavior more explicit by finding precisely the critical temperature for this system. Physically, for spin systems in particular, this is the temperature (at zero external field) below which spontaneous magnetization occurs (i.e., the value of T below which $\bar{m}(0, T)$ is non-zero). We

²I'm actually not sure if there is a discontinuity at finite h . I think Kardar has a diagram showing why this is the case, but I need to check it.

can compute this temperature using Eq.(28). With $h = 0$, we have

$$\bar{m} \left[\frac{1}{3\beta} \bar{m}^2 - J + k_B T \right] = 0. \quad (29)$$

A similar equation was derived (from a similar free energy) in the previous section. Thus we can state that the equilibrium values of the magnetization are

$$\bar{m}(0, T) = \begin{cases} 0 & T \geq J/k_B \\ \pm \sqrt{\frac{3}{k_B T} (J - k_B T)} & T < J/k_B. \end{cases} \quad (30)$$

Thus $T = J/k_B$ is the critical temperature.

We can demonstrate the existence of this phase transition in a different way by computing the near-critical-temperature scaling behavior of the heat capacity and the susceptibility, both at zero field.

To compute the heat capacity, we first must compute the energy. We have

$$\begin{aligned} E &= -\frac{\partial}{\partial \beta} \ln Z(h, T) \\ &= \frac{\partial}{\partial \beta} [\beta \min[F(m, h, \beta)]_{m=\bar{m}}] \\ &= -\frac{\partial}{\partial \beta} [N\beta(J\bar{m}^2/2 + h\bar{m}) - (N/2)(\bar{m}^2 + \bar{m}^4/6)] \\ &= -N(J\bar{m}^2/2 + h\bar{m}) - N\beta(J\bar{m} + h) \frac{\partial \bar{m}}{\partial \beta} + N(\bar{m} + \bar{m}^3/3) \frac{\partial \bar{m}}{\partial \beta} \\ &= -N(J\bar{m}^2/2 + h\bar{m}) + N[\bar{m} + \bar{m}^3/3 - \beta(J\bar{m} + h)] \frac{\partial \bar{m}}{\partial \beta}. \end{aligned} \quad (31)$$

And given that the heat capacity we're looking for is

$$C_T = -k_B \beta^2 \frac{\partial E}{\partial \beta} \Big|_{h=0}, \quad (32)$$

we obtain

$$\begin{aligned} \frac{\partial E}{\partial \beta} \Big|_{h=0} &= -NJ\bar{m} \frac{\partial \bar{m}}{\partial \beta} + N[1 + \bar{m}^2 - \beta J] \left(\frac{\partial \bar{m}}{\partial \beta} \right)^2 \\ &\quad + N[\bar{m} + \bar{m}^3/3 - \beta J\bar{m}] \frac{\partial^2 \bar{m}}{\partial \beta^2} \\ &= -NJ\bar{m} \frac{\partial \bar{m}}{\partial \beta} + N[1 + \bar{m}^2 - \beta J] \left(\frac{\partial \bar{m}}{\partial \beta} \right)^2, \end{aligned} \quad (33)$$

where we used Eq.(28) in the last line. Now, let's evaluate this expression within the temperature range $T < J/k_B$ (because above this temperature \bar{m} is temperature independent). From Eq.(30), we find

$$\begin{aligned} \bar{m} &= \pm \sqrt{3(\beta J - 1)} \\ \frac{\partial \bar{m}}{\partial \beta} &= \pm \frac{1}{2} \frac{3J}{\sqrt{3(\beta J - 1)}} \\ \bar{m} \frac{\partial \bar{m}}{\partial \beta} &= \frac{1}{2} 3J. \end{aligned} \quad (34)$$

And so Eq.(33) becomes

$$\begin{aligned}\left.\frac{\partial E}{\partial \beta}\right|_{h=0} &= 3NJ^2 + N[1 + 3\beta J - 3 - \beta J]\frac{3J^2}{4(\beta J - 1)} \\ &= 3NJ^2 - N(\beta J + 1)\frac{3J^2}{2(\beta J - 1)}\end{aligned}\quad (35)$$

By Eq.(32), we then find

$$\begin{aligned}C_T\Big|_{h=0} &= -\frac{3}{2}Nk_B\beta^2J^2\left[2 - \frac{(\beta J + 1)}{\beta J - 1}\right] \\ &= -\frac{3}{2}Nk_B\beta^2J^2\left[\frac{\beta J - 3}{\beta J - 1}\right],\end{aligned}\quad (36)$$

which implies the singular behavior of the heat capacity is

$$C_T\Big|_{h=0} \sim |T_c - T|^{-1}. \quad (37)$$

The susceptibility is much easier to compute. Given Eq.(28), we compute the field derivative to obtain

$$\begin{aligned}0 &= \frac{1}{\beta}\bar{m}^2\frac{\partial \bar{m}}{\partial h} - (J - 1/\beta)\frac{\partial \bar{m}}{\partial h} - 1 \\ \frac{\partial \bar{m}}{\partial h} &= \frac{\beta}{\bar{m}^2 - (\beta J - 1)},\end{aligned}\quad (38)$$

and thus given the solution of Eq.(30), we obtain

$$\chi\Big|_{h=0} = \frac{\beta}{2(\beta J - 1)}. \quad (39)$$

Thus similar to the heat capacity, the zero-field susceptibility has the critical temperature behavior

$$\chi\Big|_{h=0} \sim |T - T_c|^{-1}. \quad (40)$$

3 SK Spin Glass

As a more involved mathematical model of phase transitions we consider the phase properties of a spin glass in the Sherrington Kirkpatrick model [3]. To do so we compute the free energy using the method of steepest descents, and analyze how the order parameters of change with temperature or interaction parameters.

We have a system of N spins s_i which interact through the Hamiltonian

$$H = -\frac{1}{2}\sum_{i \neq j} J_{ij}s_i s_j, \quad (41)$$

where J_{ij} is drawn from the distribution

$$p(J_{ij}) = \frac{1}{\sqrt{2\pi J^2}}e^{-(J_{ij}-J_0)^2/2J^2}. \quad (42)$$

In order for our final expression for the free energy to be extensive, we take $J \equiv \tilde{J}/\sqrt{N}$ and $J_0 = \tilde{J}_0/N$ with

\tilde{J} and \tilde{J}_0 as intensive parameters.

In this system, disorder is represented by Eq.(42). Spin glasses have a type of disorder termed *quenched* disorder which requires the free energy for the spin-glass Hamiltonian Eq.(41) to be averaged over Eq.(42). First, we write the non-averaged partition function for Eq.(41) in a more useful form:

$$\begin{aligned} Z &= \sum_{\{s_i\}} \exp \left(\frac{\beta}{2} \sum_{i \neq j} J_{ij} s_i s_j \right) \\ &= \sum_{\{s_i\}} \prod_{i \neq j} \exp \left(\frac{\beta}{2} J_{ij} s_i s_j \right). \end{aligned} \quad (43)$$

The quantity we want to compute (the disorder averaged free energy) is then

$$\begin{aligned} \langle \ln Z \rangle &= \int_{-\infty}^{\infty} \prod_{i \neq j} dJ_{ij} p(J_{ij}) \ln Z \\ &= \int_{-\infty}^{\infty} \prod_{i \neq j} dJ_{ij} p(J_{ij}) \ln \left\{ \sum_{\{s_i\}} \prod_{i \neq j} \exp \left(\frac{\beta}{2} J_{ij} s_i s_j \right) \right\}, \end{aligned} \quad (44)$$

where the product of differentials is understood to be a wedge product and the integration operates on $\ln Z$. This integral is intractable, so to reduce it something we can compute we use identity (which can be obtained from $e^x = \lim_{n \rightarrow \infty} (1 + x/n)^n$)

$$\ln x = \lim_{n \rightarrow 0} \frac{x^n - 1}{n}. \quad (45)$$

With this identity $\ln Z$ becomes

$$\begin{aligned} \ln Z &= \lim_{n \rightarrow 0} n^{-1} \left[\left(\sum_{\{s_i\}} \prod_{i \neq j} \exp \left(\frac{\beta}{2} J_{ij} s_i s_j \right) \right)^n - 1 \right] \\ &= \lim_{n \rightarrow 0} n^{-1} \left[\sum_{\{s_i^1\}} \cdots \sum_{\{s_i^n\}} \prod_{i \neq j} \exp \left(\frac{\beta}{2} J_{ij} (s_i^1 s_j^1 + \cdots + s_i^n s_j^n) \right) - 1 \right] \\ &= \lim_{n \rightarrow 0} n^{-1} \left[\sum_{\{s_i^\alpha\}} \prod_{i \neq j} \exp \left(\frac{\beta}{2} J_{ij} \sum_{\alpha} s_i^\alpha s_j^\alpha \right) - 1 \right], \end{aligned} \quad (46)$$

where the sum over α runs from 1 to n . Thus Eq.(44) is

$$\langle \ln Z \rangle = \lim_{n \rightarrow 0} n^{-1} \left[\sum_{\{s_i^\alpha\}} \prod_{i \neq j} \int_{-\infty}^{\infty} dJ_{ij} p(J_{ij}) \exp \left(\frac{\beta}{2} J_{ij} \sum_{\alpha} s_i^\alpha s_j^\alpha \right) - 1 \right]. \quad (47)$$

Computing this integral therefore comes down to a calculation of

$$\int_{-\infty}^{\infty} dJ_{ij} p(J_{ij}) \exp \left(\frac{\beta}{2} J_{ij} \sum_{\alpha} s_i^\alpha s_j^\alpha \right). \quad (48)$$

Defining $\Omega \equiv \sum_{\alpha} s_i^{\alpha} s_j^{\alpha}$ and $v \equiv J_{ij}$ for notational simplicity, we have

$$\frac{1}{\sqrt{2\pi J^2}} \int_{-\infty}^{\infty} dv e^{-(v-J_0)^2/2J^2} e^{\beta v \Omega/2}. \quad (49)$$

Key to calculating this integral is completing the square. The completion is as follows

$$\begin{aligned} -\frac{1}{2J^2} (v - J_0)^2 + \frac{\beta}{2} v \Omega &= -\frac{v^2}{2J^2} + \frac{J_0 v}{J^2} + \frac{\beta v \Omega}{2} - \frac{J_0^2}{2J^2} \\ &= -\frac{1}{2J^2} \left[v^2 - 2vJ^2 \left(\frac{J_0}{J^2} + \frac{\beta \Omega}{2} \right) \right] - \frac{J_0^2}{2J^2} \\ &= -\frac{1}{2J^2} \left(v - \left(J_0 + \frac{J^2 \beta \Omega}{2} \right) \right)^2 + \frac{1}{2J^2} \left(J_0 + \frac{\beta J^2 \Omega}{2} \right)^2 - \frac{J_0^2}{2J^2} \\ &= -\frac{u^2}{2J^2} + \frac{\beta J_0}{2} \Omega + \frac{\beta^2 J^2}{8} \Omega^2 \end{aligned} \quad (50)$$

We therefore find

$$\int_{-\infty}^{\infty} dJ_{ij} p(J_{ij}) \exp \left(\frac{\beta}{2} J_{ij} \sum_{\alpha} s_i^{\alpha} s_j^{\alpha} \right) = \exp \left(\frac{\beta J_0}{2} \sum_{\alpha} s_i^{\alpha} s_j^{\alpha} + \frac{\beta^2 J^2}{8} \sum_{\alpha, \beta} s_i^{\alpha} s_j^{\alpha} s_i^{\beta} s_j^{\beta} \right), \quad (51)$$

and thus $\langle \ln Z \rangle$ becomes

$$\begin{aligned} \langle \ln Z \rangle &= \lim_{n \rightarrow 0} n^{-1} \left[\sum_{\{s_i^{\alpha}\}} \prod_{i \neq j} \exp \left(\frac{\beta J_0}{2} \sum_{\alpha} s_i^{\alpha} s_j^{\alpha} + \frac{\beta^2 J^2}{8} \sum_{\alpha, \beta} s_i^{\alpha} s_j^{\alpha} s_i^{\beta} s_j^{\beta} \right) - 1 \right] \\ &= \lim_{n \rightarrow 0} n^{-1} \left[\sum_{\{s_i^{\alpha}\}} \exp \left\{ \sum_{i \neq j} \left(\frac{\beta J_0}{2} \sum_{\alpha} s_i^{\alpha} s_j^{\alpha} + \frac{\beta^2 J^2}{8} \sum_{\alpha, \beta} s_i^{\alpha} s_j^{\alpha} s_i^{\beta} s_j^{\beta} \right) \right\} - 1 \right]. \end{aligned} \quad (52)$$

From here we simplify the summations in order to extract terms which will eventually lead us to the order parameters of this system. We have

$$\begin{aligned} \sum_{i \neq j} \sum_{\alpha} s_i^{\alpha} s_j^{\alpha} &= \sum_{\alpha} \left(\sum_{i, j} s_i^{\alpha} s_j^{\alpha} - \sum_{i=j} 1 \right) \\ &= \sum_{\alpha} \left(\sum_i s_i^{\alpha} \right)^2 - Nn \end{aligned} \quad (53)$$

and

$$\begin{aligned} \sum_{i \neq j} \sum_{\alpha, \beta} s_i^{\alpha} s_j^{\alpha} s_i^{\beta} s_j^{\beta} &= \sum_{\alpha, \beta} \left(\sum_{i, j} s_i^{\alpha} s_i^{\beta} s_j^{\alpha} s_j^{\beta} - \sum_{i=j} 1 \right) \\ &= \sum_{\alpha, \beta} \left(\sum_i s_i^{\alpha} s_i^{\beta} \right)^2 - Nn^2 \\ &= \sum_{\alpha, \beta} \left(\sum_i s_i^{\alpha} s_i^{\beta} \right)^2 - Nn^2 \end{aligned}$$

$$\begin{aligned}
&= \sum_{\alpha \neq \beta} \left(\sum_i s_i^\alpha s_i^\beta \right)^2 - \sum_{\alpha = \beta} \left(\sum_i 1 \right)^2 - Nn^2 \\
&= \sum_{\alpha \neq \beta} \left(\sum_i s_i^\alpha s_i^\beta \right)^2 + nN^2 - Nn^2.
\end{aligned} \tag{54}$$

The result for the dimensionless free energy is therefore

$$\begin{aligned}
\langle \ln Z \rangle &= \lim_{n \rightarrow 0} n^{-1} \left[\exp \left(-\frac{\beta J_0}{2} Nn + \frac{\beta^2 J^2}{8} nN^2 - \frac{\beta^2 J^2}{8} Nn^2 \right) \right. \\
&\quad \times \sum_{\{s_i^\alpha\}} \exp \left\{ \frac{\beta J_0}{2} \sum_\alpha \left(\sum_i s_i^\alpha \right)^2 + \frac{\beta^2 J^2}{8} \sum_{\alpha \neq \beta} \left(\sum_i s_i^\alpha s_i^\beta \right)^2 \right\} - 1 \Big].
\end{aligned} \tag{55}$$

In the thermodynamic limit we have $N \gg 1$, and given the intensive definitions of J_0 and J we have (for $n \rightarrow 0$) $J^2 Nn^2 \ll J_0 Nn \ll J^2 N^2 n$, and so this result reduces to

$$\begin{aligned}
\langle \ln Z \rangle &= \lim_{n \rightarrow 0} n^{-1} \left[\exp \left(\frac{\beta^2 J^2}{8} N^2 n \right) \right. \\
&\quad \times \sum_{\{s_i^\alpha\}} \exp \left\{ \frac{\beta J_0}{2} \sum_\alpha \left(\sum_i s_i^\alpha \right)^2 + \frac{\beta^2 J^2}{8} \sum_{\alpha \neq \beta} \left(\sum_i s_i^\alpha s_i^\beta \right)^2 \right\} - 1 \Big].
\end{aligned} \tag{56}$$

Now, we employ the Hubbard Stratonovich identity [4]

$$e^{\lambda a^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-\frac{1}{2}x^2 + a\sqrt{2\lambda}x} \tag{57}$$

twice to write

$$\begin{aligned}
\exp \left\{ \frac{\beta J_0}{2} \sum_\alpha \left(\sum_i s_i^\alpha \right)^2 \right\} &= \prod_\alpha \int_{-\infty}^{\infty} dx_\alpha \sqrt{\frac{N}{2\pi}} \exp \left\{ -\frac{N}{2} \sum_\alpha x_\alpha^2 + \sum_\alpha x_\alpha \sqrt{\beta \tilde{J}_0} \sum_i s_i^\alpha \right\} \\
\exp \left\{ \frac{\beta^2 J^2}{8} \sum_{\alpha \neq \beta} \left(\sum_i s_i^\alpha s_i^\beta \right)^2 \right\} &= \prod_{\alpha \neq \beta} \int_{-\infty}^{\infty} dy_{\alpha\beta} \sqrt{\frac{N}{2\pi}} \exp \left\{ -\frac{N}{2} \sum_{\alpha \neq \beta} y_{\alpha\beta}^2 + \sum_{\alpha \neq \beta} y_{\alpha\beta} \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} \sum_i s_i^\alpha s_i^\beta \right\},
\end{aligned} \tag{58}$$

and where we used $\tilde{J}_0 = J_0 N$ and $\tilde{J}^2 = J^2 N$ to eliminate the factors of N in the exponential's argument. So the free energy becomes

$$\begin{aligned}
\langle \ln Z \rangle &= \lim_{n \rightarrow 0} n^{-1} \left[\exp \left(\frac{\beta^2 J^2}{8} N^2 n \right) \right. \\
&\quad \int_{-\infty}^{\infty} \prod_\alpha dx_\alpha \sqrt{\frac{N}{2\pi}} \prod_{\alpha \neq \beta} dy_{\alpha\beta} \sqrt{\frac{N}{2\pi}} \exp \left\{ -\frac{N}{2} \sum_\alpha x_\alpha^2 - \frac{N}{2} \sum_{\alpha \neq \beta} y_{\alpha\beta}^2 \right\} \\
&\quad \sum_{\{s_i^\alpha\}} \exp \left\{ \sqrt{\beta \tilde{J}_0} \sum_\alpha x_\alpha \sum_i s_i^\alpha + \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} \sum_{\alpha \neq \beta} y_{\alpha\beta} \sum_i s_i^\alpha s_i^\beta \right\} - 1 \Big]
\end{aligned}$$

$$\begin{aligned}
&= \lim_{n \rightarrow 0} n^{-1} \left[\exp \left(\frac{\beta^2 J^2}{8} N^2 n \right) \right. \\
&\quad \int_{-\infty}^{\infty} \prod_{\alpha} dx_{\alpha} \sqrt{\frac{N}{2\pi}} \prod_{\alpha \neq \beta} dy_{\alpha\beta} \sqrt{\frac{N}{2\pi}} \exp \left\{ -\frac{N}{2} \sum_{\alpha} x_{\alpha}^2 - \frac{N}{2} \sum_{\alpha \neq \beta} y_{\alpha\beta}^2 \right\} \\
&\quad \left. \exp \ln \sum_{\{s_i^{\alpha}\}} \exp \left\{ \sqrt{\beta \tilde{J}_0} \sum_{\alpha} x_{\alpha} \sum_i s_i^{\alpha} + \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} \sum_{\alpha \neq \beta} y_{\alpha\beta} \sum_i s_i^{\alpha} s_i^{\beta} \right\} - 1 \right]. \quad (60)
\end{aligned}$$

We are close to a free energy which can be analyzed by steepest descents. First, given the symmetry between different replicas (i.e., different values of α) we can predict that the critical values \bar{x}_{α} and $\bar{y}_{\alpha\beta}$ have constant values \bar{x} and \bar{y} as functions of α and β . This allows us to remove them from the summations. Doing so for the sum over $y_{\alpha\beta}$ and putting the spin sum in a more useful form we have

$$\begin{aligned}
\sum_{\alpha \neq \beta} y_{\alpha\beta} \sum_i s_i^{\alpha} s_i^{\beta} &= y \sum_{\alpha \neq \beta} \sum_i s_i^{\alpha} s_i^{\beta} \\
&= y \left[\sum_{\alpha, \beta} \sum_i s_i^{\alpha} s_i^{\beta} - \sum_{\alpha=\beta} \sum_i s_i^{\alpha} s_i^{\alpha} \right] \\
&= y \left[\sum_i \left(\sum_{\alpha} s_i^{\alpha} \right)^2 - Nn \right], \quad (61)
\end{aligned}$$

and so the free-energy becomes

$$\begin{aligned}
\langle \ln Z \rangle &= \lim_{n \rightarrow 0} n^{-1} \left[\exp \left(\frac{\beta^2 J^2}{8} N^2 n \right) \right. \\
&\quad \int_{-\infty}^{\infty} dx \left(\sqrt{\frac{N}{2\pi}} \right)^n dy \left(\sqrt{\frac{N}{2\pi}} \right)^n \exp \left\{ -\frac{N}{2} n x^2 - \frac{N}{2} (n^2 - n) y^2 - y N n \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} \right\} \\
&\quad \left. \exp \ln \sum_{\{s_i^{\alpha}\}} \exp \left\{ \sqrt{\beta \tilde{J}_0} x \sum_i \sum_{\alpha} s_i^{\alpha} + \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} y \sum_i \left(\sum_{\alpha} s_i^{\alpha} \right)^2 \right\} - 1 \right] \quad (62)
\end{aligned}$$

and using the identity

$$\ln \sum_{\{s_{i,j}\}} \exp \left(\sum_i \sum_j f_{i,j} \right) = \ln \prod_i \sum_{\{s_j\}} \exp \left(\sum_j f_{i,j} \right) = N \ln \sum_{\{s_j\}} \exp \left(\sum_j f_j \right), \quad (63)$$

where we were able to drop the index i because it was just a label. We thus have

$$\begin{aligned}
\langle \ln Z \rangle &= \lim_{n \rightarrow 0} n^{-1} \left[\exp \left(\frac{\beta^2 J^2}{8} N^2 n \right) \int_{-\infty}^{\infty} dx \left(\sqrt{\frac{N}{2\pi}} \right)^n dy \left(\sqrt{\frac{N}{2\pi}} \right)^n \right. \\
&\quad \left. \exp \left\{ -\frac{N}{2} n x^2 - \frac{N}{2} (n^2 - n) y^2 - y N n \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} \right\} \right]
\end{aligned}$$

$$+N \ln \sum_{\{s^\alpha\}} \exp \left\{ \sqrt{\beta \tilde{J}_0} x \sum_{\alpha} s^\alpha + \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} y \left(\sum_{\alpha} s^\alpha \right)^2 \right\} - 1 \right]. \quad (64)$$

Now comes some tricky mathematics. In order to perform the sum over spins (i.e., $\sum_{\{s_i^\alpha\}}$), we need to eliminate the quadratic term in the exponential. We can do this by using Eq.(57) to write

$$\exp \left\{ \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} y \left(\sum_{\alpha} s^\alpha \right)^2 \right\} = \int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} \exp \left[\left(2y \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} \right)^{1/2} z \sum_{\alpha} s^\alpha \right], \quad (65)$$

and so the exponential in the logarithm becomes

$$\begin{aligned} \sum_{\{s^\alpha\}} \exp \left\{ \sqrt{\beta \tilde{J}_0} x \sum_{\alpha} s^\alpha + \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} y \left(\sum_{\alpha} s^\alpha \right)^2 \right\} \\ = \int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} \sum_{\{s^\alpha\}} \exp \left[z \sqrt{y \beta \tilde{J}} \sum_{\alpha} s^\alpha + x \sqrt{\beta \tilde{J}_0} \sum_{\alpha} s^\alpha \right] \\ = \int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} 2^n \cosh^n \left[z \sqrt{y \beta \tilde{J}} + x \sqrt{\beta \tilde{J}_0} \right]. \end{aligned} \quad (66)$$

We want to take the logarithm of this and then take the $n \rightarrow 0$ limit. This is tantamount to expanding the logarithm of this quantity about $n = 0$. Schematically we have

$$\begin{aligned} \ln \left[\int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} (2 \cosh A(z))^n \right] &= \ln \left[\int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} \left(1 + n \frac{d}{dn} (2 \cosh A(z))^n \Big|_{n=0} + \mathcal{O}(n^2) \right) \right] \\ &= \ln \left[1 + n \int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} \ln(2 \cosh A(z)) + \mathcal{O}(n^2) \right] \\ &= n \int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} \ln(2 \cosh A(z)). \end{aligned} \quad (67)$$

So we have

$$\begin{aligned} \ln \sum_{\{s^\alpha\}} \exp \left\{ \sqrt{\beta \tilde{J}_0} x \sum_{\alpha} s^\alpha + \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} y \left(\sum_{\alpha} s^\alpha \right)^2 \right\} \\ = n \int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} \ln \left(2 \cosh \left[z \sqrt{y \beta \tilde{J}} + x \sqrt{\beta \tilde{J}_0} \right] \right), \end{aligned} \quad (68)$$

and the free energy is

$$\begin{aligned} \langle \ln Z \rangle &= \lim_{n \rightarrow 0} n^{-1} \left[\int_{-\infty}^{\infty} dx \left(\sqrt{\frac{N}{2\pi}} \right)^n dy \left(\sqrt{\frac{N}{2\pi}} \right)^n \right. \\ &\quad \left. \exp \left\{ \frac{\beta^2 J^2}{8} N^2 n - \frac{N}{2} n x^2 - \frac{N}{2} (n^2 - n) y^2 - y N n \sqrt{\frac{\beta^2 \tilde{J}^2}{4}} \right\} \right] \end{aligned}$$

$$+Nn \int_{-\infty}^{\infty} dz \frac{e^{-z^2/2}}{\sqrt{2\pi}} \ln \left(2 \cosh \left[z \sqrt{y \beta \tilde{J}} + x \sqrt{\beta \tilde{J}_0} \right] \right) \Big\} - 1 \Big]. \quad (69)$$

Finally, employing steepest descents, expanding the exponential and only keeping the terms which are linear in n , we find

$$\begin{aligned} \langle \ln Z \rangle / N &= \frac{\beta^2 \tilde{J}^2}{8} - \frac{1}{2} \bar{x}^2 + \frac{1}{2} \bar{y}^2 - \bar{y} \frac{\beta \tilde{J}}{2} + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz e^{-z^2/2} \ln \left(2 \cosh \left[z \sqrt{\bar{y} \beta \tilde{J}} + \bar{x} \sqrt{\beta \tilde{J}_0} \right] \right) \\ &= -\frac{1}{2} \bar{x}^2 + \frac{1}{2} \left(\bar{y} - \beta \tilde{J}/2 \right)^2 + \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz e^{-z^2/2} \ln \left(2 \cosh \left[z \sqrt{\bar{y} \beta \tilde{J}} + \bar{x} \sqrt{\beta \tilde{J}_0} \right] \right) \end{aligned} \quad (70)$$

(I'm missing a factor of 2 somewhere.) Defining

$$\bar{x} \sqrt{\beta \tilde{J}_0} \equiv m \beta \tilde{J}_0, \quad \sqrt{\bar{y} \beta \tilde{J}} \equiv \beta \tilde{J} (q/2)^{1/2} \quad (71)$$

We find with $F = -\ln Z / \beta$

$$F(q, m) \beta N^{-1} = \frac{\beta \tilde{J}_0}{2} m^2 - \frac{\beta^2 \tilde{J}^2}{8} (q-1)^2 - (2\pi)^{-1/2} \int_{-\infty}^{\infty} dz e^{-z^2/2} \ln \left(2 \cosh \left[z \beta \tilde{J} \sqrt{q/2} + \beta \tilde{J}_0 m \right] \right). \quad (72)$$

Now the equilibrium conditions for this free energy are determined by computing the free energy derivatives of m and q and setting both to zero. The free energy derivative for m clearly yields

$$m = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dz e^{-z^2/2} \tanh \left[z \beta \tilde{J} (q/2)^{1/2} + \beta \tilde{J}_0 m \right]. \quad (73)$$

The free energy derivative for q is less transparent. Computing it we find

$$\frac{\partial}{\partial q} F(q, m) \beta N^{-1} = -\frac{\beta^2 \tilde{J}^2}{4} (q-1) - (2\pi)^{-1/2} \frac{\beta \tilde{J}}{2\sqrt{2q}} \int_{-\infty}^{\infty} dz e^{-z^2/2} z \tanh \left[z \beta \tilde{J} (q/2)^{1/2} + \beta \tilde{J}_0 m \right] = 0. \quad (74)$$

Applying integration by parts to the second term we have

$$\begin{aligned} &\frac{\beta \tilde{J}}{2\sqrt{2q}} \int_{-\infty}^{\infty} dz e^{-z^2/2} z \tanh \left[z \beta \tilde{J} (q/2)^{1/2} + \beta \tilde{J}_0 m \right] \\ &= \frac{\beta \tilde{J}}{2\sqrt{2q}} e^{-z^2/2} \tanh \left[z \beta \tilde{J} (q/2)^{1/2} + \beta \tilde{J}_0 m \right] \Big|_{z=-\infty}^{z=\infty} \\ &\quad + \frac{\beta^2 \tilde{J}^2}{4} \int_{-\infty}^{\infty} dz e^{-z^2/2} \text{sech}^2 \left[z \beta \tilde{J} (q/2)^{1/2} + \beta \tilde{J}_0 m \right]. \end{aligned} \quad (75)$$

The first term is zero and so Eq.(74) yields the value for q of

$$\begin{aligned} q &= 1 - (2\pi)^{-1/2} \int_{-\infty}^{\infty} dz e^{-z^2/2} \text{sech}^2 \left[z \beta \tilde{J} (q/2)^{1/2} + \beta \tilde{J}_0 m \right] \\ &= (2\pi)^{-1/2} \int_{-\infty}^{\infty} dz e^{-z^2/2} \tanh^2 \left[z \beta \tilde{J} (q/2)^{1/2} + \beta \tilde{J}_0 m \right] \end{aligned} \quad (76)$$

where we used $\text{sech}^2 x = 1 - \tanh^2 x$. To determine the phase behavior of the spin glass we need to find the solutions to Eq.(73) and Eq.(76). We also need to determine what these quantities correspond to physically to understand how this phase behavior is reflected in the original spin system.

The interpretation provided in [5] is that m and q respectively are the disorder-averaged mean spin and

mean spin squared, respectively. That is

$$m = \langle \langle s \rangle_T \rangle_J \quad (77)$$

$$q = \langle \langle s \rangle_T^2 \rangle_J. \quad (78)$$

where $\langle \cdots \rangle_T$ is the standard Boltzmann average and $\langle \cdots \rangle_J$ is the disorder average over values of J . The various phases in this system are distinguished by the values of m and q . These phases are

$$m = 0, q = 0 : \quad (\text{paramagnetic phase}) \quad (79)$$

$$m \neq 0, q \neq 0 : \quad (\text{ferromagnetic phase}) \quad (80)$$

$$m = 0, q \neq 0 : \quad (\text{spin glass phase}) \quad (81)$$

We note that by Eq.(73) and Eq.(76), if $m \neq 0$ we must have $q \neq 0$. We can explore the thermal properties which relate the paramagnetic and spin glass phases by setting $J_0 = 0$. Doing so we find for m

$$m = (2\pi)^{-1/2} \int_{-\infty}^{\infty} dz e^{-z^2/2} \tanh \left[z\beta\tilde{J}(q/2)^{1/2} \right] = 0. \quad (82)$$

To compute q we assume $q \ll 1$ and expand employ the expansion $\tanh^2 x = x^2 - 2x^4/3 + 17x^6/45 + \cdots$. We obtain

$$\begin{aligned} q &= (2\pi)^{-1/2} \int_{-\infty}^{\infty} dz e^{-z^2/2} \left(z^2 \lambda^2 q - \frac{2}{3} z^4 \lambda^4 q^2 + \frac{17}{45} z^6 \lambda^6 q^3 + \cdots \right) \\ &= \lambda^2 q - 2\lambda^4 q^2 + \frac{17}{3} \lambda^6 q^3 + \mathcal{O}(q^4), \end{aligned} \quad (83)$$

where we defined $\lambda \equiv \beta\tilde{J}$. Dividing by q and then solving for q^2 gives us

$$q^2 = \frac{1}{2\lambda^4} (\beta^2 \tilde{J}^2 - 1) + \mathcal{O}(q^3). \quad (84)$$

The result Eq.(84) indicates that for $\beta^{-1} < \tilde{J}$ we have $q \neq 0$ (spin glass phase), and for $\beta^{-1} > \tilde{J}$ we have $q = 0$ (paramagnetic phase). Thus we see we have a phase transition.

This discussion (grounded as it is in [3]) is actually not correct. This solution for $J_0 = 0$, qualitatively reproduces the appropriate spin glass behavior for q but it turns out this solution is an unstable one for the free energy of this system. The correct solution is apparently due to Parisi and involves replica-symmetry breaking and the concept of ultrametricity. See [5] and [6] for references.

4 Magnetic Thin Films

Following problem 6 in Chapter 1 of [1], we employ the Gibbs-Bogoliubov inequality to investigate the phase behavior of a generalized spin system. The system consists of n layers with N spin sites on each layer. The spins interact with nearest neighbor spin within the same layer, and with the spins directly above and below them in different layers. The Hamiltonian for this system is

$$\mathcal{H} = -J_H \sum_{\alpha=1}^n \sum_{\langle i,j \rangle} \vec{s}_i^\alpha \cdot \vec{s}_j^\alpha - J_V \sum_{\alpha=1}^{n-1} \sum_i \vec{s}_i^\alpha \cdot \vec{s}_i^{\alpha+1}, \quad (85)$$

where Roman indices denote the spin site in a single layer and Greek indices denote the layer. To investigate the phase behavior of the system governed by this Hamiltonian we will employ the mean field theory

approach represented by the use of the inequality

$$F[\mathcal{H}] \leq F[\mathcal{H}_0] + \langle \mathcal{H} - \mathcal{H}_0 \rangle_{\mathcal{H}_0}. \quad (86)$$

First we posit a simple variational Hamiltonian:

$$\mathcal{H}_0 = - \sum_{\alpha=1}^n \sum_i \vec{h}^\alpha \cdot \vec{s}_i^\alpha, \quad (87)$$

where \vec{h}^α are the set of variational fields whose value will be chose as to minimize the RHS of Eq.(86). The partition function corresponding to this Hamiltonian is then

$$\begin{aligned} Z_0(\{h^\alpha\}) &= \left[\prod_{\alpha,i} \int d\Omega(\vec{s}_i^\alpha) \right] \exp \left(\beta \sum_{\alpha,i} \vec{h}^\alpha \cdot \vec{s}_i^\alpha \right) \\ &= \prod_{\alpha,i} \left[\int_0^{2\pi} d\phi_i^\alpha \int_0^\pi d\theta_i^\alpha \sin \theta_i^\alpha \exp \left(\beta \vec{h}^\alpha \cdot \vec{s}_i^\alpha \right) \right] \\ &= \prod_{\alpha,i} \left[2\pi \int_0^\pi d\theta_i^\alpha \sin \theta_i^\alpha e^{\beta h^\alpha \cos(\theta_i^\alpha - \theta_h^\alpha)} \right], \end{aligned} \quad (88)$$

where we used the fact \vec{s}_i^α has unit norm, and θ_h^α and θ_i^α are the angles that the field \vec{h}^α and the spin site \vec{s}_i^α respectively make with a chosen \hat{z} direction. As an assumption (which does not contradict our eventual variational results) we can expect all the variational fields \vec{h}^α to be in the same direction \hat{z} . Taking this assumption, the partition function then becomes

$$\begin{aligned} Z_0(\{h^\alpha\}) &= \prod_{\alpha,i} \left[2\pi \int_0^\pi d\theta_i^\alpha \sin \theta_i^\alpha e^{\beta h^\alpha \cos \theta_i^\alpha} \right] \\ &= \prod_{\alpha,i} 2\pi \int_{-1}^1 du e^{\beta h^\alpha u} \\ &= \prod_{\alpha,i} \frac{4\pi}{\beta h^\alpha} \sinh(\beta h^\alpha). \end{aligned} \quad (89)$$

Now we can start computing the quantities on the RHS of Eq.(86). The free energy associated with our variational Hamiltonian is

$$\beta F[\mathcal{H}_0] = -\ln Z_0 = -N \sum_{\alpha} (\ln \sinh(\beta h^\alpha) - \ln(\beta h^\alpha)), \quad (90)$$

where we dropped a thermodynamically irrelevant constant. The average energy for this Hamiltonian is

$$\begin{aligned} \langle \beta \mathcal{H}_0 \rangle_0 &= -\beta \frac{\partial}{\partial \beta} \ln Z_0 \\ &= -N \sum_{\alpha} (\beta h^\alpha \coth(\beta h^\alpha) - 1) = -N \sum_{\alpha} \beta h^\alpha \mathcal{L}(\beta h^\alpha) \end{aligned} \quad (91)$$

where we introduced the Langevin function $\mathcal{L}(h) = \coth(h) - 1/h$. Next we compute $\langle \vec{s}_i^\alpha \rangle$ (the average spin at a single site) because it will serve as the order parameter for this system. By definition we can write $\vec{s}_i^\alpha = \sin \theta_i^\alpha \cos \phi_i^\alpha \hat{x} + \sin \theta_i^\alpha \sin \phi_i^\alpha \hat{y} + \cos \theta_i^\alpha \hat{z}$. Averaging the x and y components of this spin over the

auxiliary angle ϕ_i^α yields zero, so we have simply

$$\langle \vec{s}_i^\alpha \rangle = \hat{z} \langle \cos \theta_i^\alpha \rangle = \hat{z} \frac{\partial}{\partial (\beta h^\alpha)} \ln Z_0 = \hat{z} \mathcal{L}(\beta h^\alpha). \quad (92)$$

Defining $m_\alpha = |\langle \vec{s}_i^\alpha \rangle|$, we in turn have

$$m_\alpha = \mathcal{L}(\beta h^\alpha). \quad (93)$$

Lastly computing the average energy of Eq.(85) we find

$$\begin{aligned} \langle \beta \mathcal{H} \rangle_0 &= -\beta J_H \sum_{\alpha=1}^n \sum_{\langle i,j \rangle} \langle \vec{s}_i^\alpha \cdot \vec{s}_j^\alpha \rangle - \beta J_V \sum_{\alpha=1}^{n-1} \sum_i \langle \vec{s}_i^\alpha \cdot \vec{s}_i^{\alpha+1} \rangle \\ &= -\beta J_H \sum_{\alpha=1}^n \sum_{\langle i,j \rangle} \langle \vec{s}_i^\alpha \rangle \cdot \langle \vec{s}_j^\alpha \rangle - \beta J_V \sum_{\alpha=1}^{n-1} \sum_i \langle \vec{s}_i^\alpha \rangle \cdot \langle \vec{s}_i^{\alpha+1} \rangle \\ &= -\beta J_H N_q \sum_{\alpha=1}^n \mathcal{L}(\beta h^\alpha)^2 - \beta J_V N \sum_{\alpha=1}^{n-1} \mathcal{L}(\beta h^\alpha) \mathcal{L}(\beta h^{\alpha+1}) \end{aligned} \quad (94)$$

Where we defined $N_q \equiv \sum_{\langle i,j \rangle} 1$ as the number of unique spin site combinations. With these results, our total variational free energy is consequently

$$\begin{aligned} \beta F[\mathcal{H}_0] + \beta \langle \mathcal{H} - \mathcal{H}_0 \rangle_{\mathcal{H}_0} &= -N \sum_{\alpha} \left(\ln \sinh(\beta h^\alpha) - \ln(\beta h^\alpha) \right) - \beta J_H N_q \sum_{\alpha=1}^n \mathcal{L}(\beta h^\alpha)^2 \\ &\quad - \beta J_V N \sum_{\alpha=1}^{n-1} \mathcal{L}(\beta h^\alpha) \mathcal{L}(\beta h^{\alpha+1}) + N \sum_{\alpha} \beta h^\alpha \mathcal{L}(\beta h^\alpha). \end{aligned} \quad (95)$$

Towards minimizing this expression we differentiate with respect to h^γ and set the result to zero to obtain

$$\begin{aligned} 0 &= -N \beta \mathcal{L}(\beta h^\gamma) - 2\beta^2 J_H N_q \mathcal{L}(\beta h^\gamma) \mathcal{L}'(\beta h^\gamma) - \beta^2 J_V N [\mathcal{L}(\beta h^{\gamma+1}) + \mathcal{L}(\beta h^{\gamma-1})] \mathcal{L}'(\beta h^\gamma) \\ &\quad + N \beta \mathcal{L}(\beta h^\gamma) + N \beta^2 h^\gamma \mathcal{L}'(\beta h^\gamma) \\ &= -2\beta^2 J_H N_q \mathcal{L}(\beta h^\gamma) - \beta^2 J_V N [\mathcal{L}(\beta h^{\gamma+1}) + \mathcal{L}(\beta h^{\gamma-1})] + N \beta 2h^\gamma, \end{aligned} \quad (96)$$

which yields the self-consistency condition

$$h^\gamma = 2J_H \frac{N_q}{N} \mathcal{L}(\beta h^\gamma) + J_V [\mathcal{L}(\beta h^{\gamma+1}) + \mathcal{L}(\beta h^{\gamma-1})] \quad (97)$$

or, with Eq.(93),

$$\frac{1}{\beta} \mathcal{L}^{-1}(m_\gamma) = 2J_H \frac{N_q}{N} m_\gamma + J_V (m_{\gamma-1} + m_{\gamma+1}). \quad (98)$$

To look at the magnetization at the surface layer, we take $\gamma = n$. In the limit of $n \rightarrow \infty$ we can take $\lim_{n \rightarrow \infty} m_n = m$, and, using the inverse expansion of the Langevin function $\mathcal{L}^{-1}(m) = 3m + 9m^3/5 + \mathcal{O}(m^5)$, Eq.(98) becomes

$$\frac{1}{\beta} (3m + 9m^3/5) = 2\Omega m + \frac{1}{\beta} \mathcal{O}(m^5), \quad (99)$$

where we defined $\Omega \equiv J_H N_q/N + J_V$. Upon solving for m , this equation gives

$$m_{\pm} = \pm \frac{\sqrt{10}}{3} \sqrt{\beta \Omega - 3/2}. \quad (100)$$

The result Eq.(100) indicates that the “top” layer of this infinite system exhibits a second-order phase transition at $k_B T_c = 2\Omega/3$.

Returning to Eq.(98), we can write the equation as

$$3m_\gamma + \frac{9}{5}m_\gamma^3 + \mathcal{O}(m^5) = 2\beta\Omega m_\gamma + \beta J_V (m_{\gamma-1} - 2m_\gamma + m_{\gamma+1}), \quad (101)$$

which implies a natural continuum limit of

$$3m(x) + \frac{9}{5}m(x)^3 = 2\beta\Omega m(x) + \beta J_V \frac{d^2 m}{dx^2}, \quad (102)$$

where we dropped the higher order term and defined J_V as the continuum version of J_V . Guessing a solution of $m(x) = \tanh(kx)$ yields

$$\begin{aligned} -2k^2 J_V \text{sech}^2(kx) \tanh(kx) &= (3 - 2\beta) \tanh(kx) + \frac{9}{5} \tanh^3(kx) \\ -2k^2 J_V \text{sech}^2(kx) &= 3 - 2\beta + \frac{9}{5} (1 - \text{sech}^2(kx)). \end{aligned} \quad (103)$$

This final equation is only valid so long as

$$2k^2 J_V = \frac{9}{5} = 2\beta - 3. \quad (104)$$

Which tells us that at $k_B T_c = 5/12$, the solution to is Eq.(102) is $m(x) = \tanh(3x/\sqrt{10J_V})$.

5 Concept Map

We provide a concept map summarizing the various ways to investigate phase behavior in a thermal system in equilibrium.

6 Ising Model in Three Acts - July 2, 2016

We give an example of utilizing the concept map above to analyze a physical system by applying it to the all-interacting Ising model. Namely, we will consider the all-interacting Ising Model from three perspectives of equilibrium thermodynamics:

- Microcanonical Ensemble
- Hubbard-Stratonovich Approach and Steepest Descent
- Gibbs-Bogoliubov (GB) Inequality

and show that all the perspectives yield consistent equilibrium conditions for an order parameter in the thermodynamic limit of $N \gg 1$. The fundamental Hamiltonian for this system is

$$\mathcal{H}(\{s_k\}) = -\frac{J}{2N} \sum_{i,j} s_i s_j. \quad (105)$$

6.1 Microcanonical Ensemble

To analyze the all-interacting Ising model with the microcanonical ensemble, we must first write the free energy for the system. We have N spins, of which we assume an arbitrary M_+ are pointed “up” and M_-

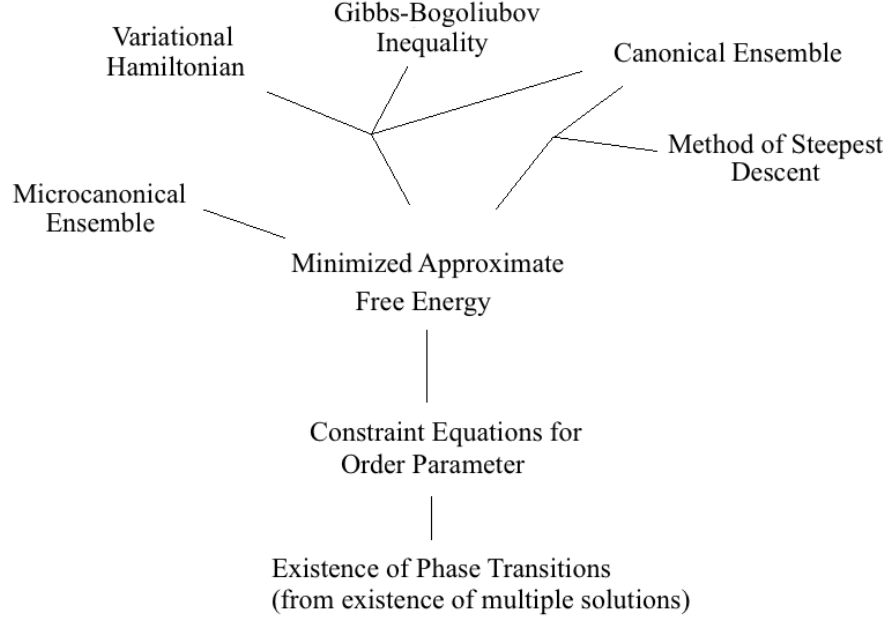


Figure 1: How the existence of phase transitions in a thermal system is established through the canonical ensemble and the microcanonical ensemble. The map is read from top-to-bottom.

are pointed down. The total magnetization is then $\sum_i s_i = M = M_+ - M_-$. Thus the free energy

$$\mathcal{F}(M) = \mathcal{E}(M) - \frac{1}{\beta} \mathcal{S}(M) = -\frac{J}{2N} M^2 - \frac{1}{\beta} \ln \Omega_N(M), \quad (106)$$

where

$$\Omega_N(M) = \binom{N}{M_+} = \frac{\Gamma(N+1)}{\Gamma\left(\frac{N+M}{2}+1\right) \Gamma\left(\frac{N-M}{2}+1\right)}. \quad (107)$$

Writing this free energy again, we have

$$\mathcal{F}(M) = -\frac{J}{2N} M^2 + \frac{1}{\beta} \left[\ln \Gamma\left(\frac{N+M}{2}+1\right) + \ln \Gamma\left(\frac{N-M}{2}+1\right) \right] + \mathcal{F}_0, \quad (108)$$

and differentiating with respect to M gives us

$$\mathcal{F}'(M) = -\frac{J}{N} M + \frac{1}{2\beta} \left[\psi_0\left(\frac{N+M}{2}+1\right) - \psi_0\left(\frac{N-M}{2}+1\right) \right] = 0 \quad (109)$$

where ψ_0 is the digamma function. Next we employ the approximation

$$\psi_0(x+1) = \ln(x+1/2) + \mathcal{O}((x+1)^{-2}) \quad (110)$$

to reduce the second term to³.

$$\begin{aligned}
\psi_0\left(\frac{N+M}{2}+1\right) - \psi_0\left(\frac{N-M}{2}+1\right) &= \ln \frac{(N+M)/2+1/2}{(N-M)/2+1/2} + \mathcal{O}(N^{-2}) \\
&= \ln \frac{1+M/(1+N)}{1-M/(1+N)} + \mathcal{O}(N^{-2}) \\
&= 2 \tanh^{-1}(M/(1+N)) + \mathcal{O}(N^{-2}).
\end{aligned} \tag{111}$$

The free energy is then

$$\mathcal{F}'(Nm) = -Jm + \frac{1}{\beta} \tanh^{-1}(m/(1+1/N)) + \mathcal{O}(N^{-2}), \tag{112}$$

where we defined $m \equiv M/N$. Solving for m , Eq.(112) gives us the equilibrium condition

$$\tanh(\beta Jm) = \frac{m}{1+1/N} + \mathcal{O}(N^{-2}). \tag{113}$$

Differentiating Eq.(112) once more, we have that the solution to Eq.(113) yields a stable equilibrium if

$$-\beta J + \frac{1}{1+1/N} \frac{1}{1-m^2} > 0. \tag{114}$$

This equation is valid for $m = 0$ up until $\beta J < 1$ is violated; beyond this value $m \neq 0$ is the stable equilibrium.

6.2 Hubbard-Stratonovich and Steepest Descent

For the Hubbard Stratonovich approach to this problem we begin the the partition function for the hamiltonian Eq.(105):

$$Z_N(\beta J) = \sum_{M=-N}^{M=+N} \Omega_N(M) e^{\beta J M^2 / 2N}. \tag{115}$$

We then use the integral identity

$$e^{\beta J M^2 / 2N} = \sqrt{\frac{N}{2\pi\beta J}} \int_{-\infty}^{\infty} du e^{-Nu^2/2\beta J + Mu}, \tag{116}$$

To obtain

$$\begin{aligned}
Z_N(\beta J) &= \sqrt{\frac{N}{2\pi\beta J}} \int_{-\infty}^{\infty} du e^{-Nu^2/2\beta J} \sum_{M=-N}^{M=+N} \Omega_N(M) e^{Mu} \\
&= \sqrt{\frac{N}{2\pi\beta J}} \int_{-\infty}^{\infty} du e^{-Nu^2/2\beta J} \sum_{M_+=0}^N \binom{N}{M_+} e^{(2M_+-N)u} \\
&= \sqrt{\frac{N}{2\pi\beta J}} \int_{-\infty}^{\infty} du e^{-Nu^2/2\beta J} e^{-Nu} (1 + e^{2u})^N \\
&= \sqrt{\frac{N}{2\pi\beta J}} \int_{-\infty}^{\infty} du e^{-Nu^2/2\beta J} (2 \cosh u)^N
\end{aligned} \tag{117}$$

³To be precise the error terms below are not precisely consistent with Eq.(110) but we will consider them in the $M \ll N$ limit

Defining $\beta J y \equiv u$, we then apply steepest descent to obtain the approximate free energy

$$-\frac{1}{\beta} \ln Z_N(\beta J) \simeq F(\bar{y}) = \frac{N}{2} J \bar{y}^2 - \frac{N}{\beta} \ln \cosh(\beta J \bar{y}) + F_0. \quad (118)$$

Differentiating this free energy with respect to \bar{y} gives the condition

$$F'(\bar{y})/NJ = \bar{y} - \tanh(\beta J \bar{y}) = 0, \quad (119)$$

or

$$\bar{y} = \tanh(\beta J \bar{y}). \quad (120)$$

From Eq.(119) the condition for stable equilibrium is

$$1 - \beta J \text{sech}(\beta J m) > 0, \quad (121)$$

which plots can show is only valid at $m = 0$ if $\beta J < 1$.

6.3 GB Inequality

The GB inequality is

$$F[\mathcal{H}] \leq F[\mathcal{H}_0] + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \equiv F_{\text{approx.}} \quad (122)$$

where $F[\mathcal{H}]$ is the free energy of our desired system with hamiltonian

$$\mathcal{H} = -\frac{J}{2N} \sum_{i,j}^N s_i s_j \quad (123)$$

and $F[\mathcal{H}_0]$ is the free energy associated with the trial Hamiltonian and

$$\langle \mathcal{O} \rangle = \text{Tr } \mathcal{O} e^{-\beta \mathcal{H}_0}. \quad (124)$$

We begin with the trial Hamiltonian

$$\mathcal{H}_0 = -h_0 \sum_{i=1}^N s_i. \quad (125)$$

The associated partition function is

$$Z_0 = \sum_{\{s_k\}} e^{\beta h_0 \sum_i s_i} = (2 \cos(\beta h_0))^N. \quad (126)$$

The moments relevant for this analysis are then

$$\sum_{i=1}^N \langle s_i \rangle_0 = -\frac{\partial}{\partial(\beta h_0)} \ln Z_0 = N \tanh(\beta h_0) = N \langle s_i \rangle_0 \quad (127)$$

$$\begin{aligned} \sum_{i,j}^N \langle s_i s_j \rangle_0 &= \sum_{i < j} \langle s_i s_j \rangle_0 + \sum_{i=j} \langle s_i s_i \rangle_0 \\ &= 2 \frac{N(N-1)}{2} \langle s_i \rangle_0 \langle s_j \rangle_0 + N \\ &= N(N-1) \tanh^2(\beta h_0) + N \end{aligned} \quad (128)$$

We note we could have also computed the second moment by using the derivative identity

$$\frac{1}{Z_0} \frac{\partial^2 Z_0}{\partial(\beta h_0)^2} = \frac{\partial^2}{\partial(\beta h_0)^2} \ln Z_0 + \left(\frac{\partial}{\partial(\beta h_0)} \ln Z_0 \right)^2. \quad (129)$$

Now, computing the free energy in Eq.(122) gives us

$$\begin{aligned} F_{\text{approx.}}(h_0) &= F[\mathcal{H}_0] + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0 \\ &= -\frac{N}{\beta} \ln \cosh(\beta h_0) + N h_0 \tanh(\beta h_0) - \frac{J}{2} (N-1) \tanh^2(\beta h_0) + F_{\text{approx. } 0}. \end{aligned} \quad (130)$$

Differentiating this expression with respect to h_0 and setting the result to zero for some $h_0 = \bar{h}_0$ gives us the condition

$$\begin{aligned} 0 &= F'_{\text{approx.}}(\bar{h}_0) = N \beta \bar{h}_0 \text{sech}^2(\beta \bar{h}_0) - \beta J (N-1) \tanh(\beta \bar{h}_0) \text{sech}^2(\beta \bar{h}_0) \\ &= \text{sech}^2(\beta \bar{h}_0) (N \beta \bar{h}_0 - \beta J (N-1) \tanh(\beta \bar{h}_0)). \end{aligned} \quad (131)$$

Setting the quantity in the parentheses to zero and given Eq.(127), we find

$$N \bar{h}_0 = J (N-1) \tanh(\beta \bar{h}_0) = J (N-1) \overline{\langle s_i \rangle}_0, \quad (132)$$

where we defined $\overline{\langle s_i \rangle}_0$ as the value of $\langle s_i \rangle_0$ which minimizes Eq.(130). Given that h_0 is proportional to $\langle s_i \rangle_0$, the equilibrium condition is established by Eq.(131). Now with Eq.(132), we find the order parameter is given by the equation

$$\overline{\langle s_i \rangle}_0 = \tanh \left(\beta J \overline{\langle s_i \rangle}_0 (1 - 1/N) \right), \quad (133)$$

Inserting Eq.(133) into Eq.(130), gives us the free energy

$$F_{\text{approx.}} \Big|_{\langle s_i \rangle_0 = \overline{\langle s_i \rangle}_0} = -\frac{N}{\beta} \ln \left[\cosh \beta J \overline{\langle s_i \rangle}_0 (1 - 1/N) \right] + \frac{J(N-1)}{2} \overline{\langle s_i \rangle}_0^2 + F_{\text{approx. } 0} \quad (134)$$

or equivalently

$$F_{\text{approx.}} \Big|_{\langle s_i \rangle_0 = \overline{\langle s_i \rangle}_0} = \frac{N}{2\beta} \ln(1 - \overline{\langle s_i \rangle}_0^2) + \frac{J(N-1)}{2} \overline{\langle s_i \rangle}_0^2 + F_{\text{approx. } 0} \quad (135)$$

where we used

$$\tanh^{-1} \overline{\langle s_i \rangle}_0 = \beta J \overline{\langle s_i \rangle}_0 (1 - 1/N). \quad (136)$$

Note: Although Eq.(134) and Eq.(135) are equivalent, they do not yield the same value of $\langle s_i \rangle_0$ when we differentiate them with respect to $\langle s_i \rangle_0$ and set the associated results to zero. This is because Eq.(134) and Eq.(135) are the values of the minimum free energy Eq.(130), and hence differentiating as a function of their parameter values and setting the corresponding result to zero doesn't correspond to any physical constraint (as far as I can tell).

6.4 Summary

Reviewing our previous results it is clear they are all consistent if we are careful how we consider the $\mathcal{O}(N^{-1})$ corrections. It is important to note this consistency is apparent primarily in the derived equilibrium conditions rather than the free energies. In any case we summarize these free energies and conditions below

- Microcanonical Ensemble:

$$F(m) = -\frac{NJ}{2} m^2 + \frac{1}{\beta} [\ln \Gamma(N(1+m)/2 + 1) - \ln \Gamma(N(1-m)/2 + 1)] \quad (137)$$

$$F'(\bar{m}) = 0 \implies \tanh(\beta J \bar{m}) = \bar{m}(1 + 1/N)^{-1} + \mathcal{O}(N^{-2}) \quad (138)$$

- Hubbard-Stratonovich Approach and Steepest Descent:

$$F(y) = \frac{NJ}{2}y^2 - \frac{N}{\beta} \ln \cosh(\beta J y) \quad (139)$$

$$F'(\bar{y}) = 0 \implies \bar{y} = \tanh(\beta J \bar{y}) \quad (140)$$

- Gibbs-Bogoliubov (GB) Inequality:

$$F_{\text{approx.}}(h_0) = -\frac{N}{\beta} \ln \cosh(\beta h_0) + N h_0 \tanh(\beta h_0) - \frac{J}{2}(N-1) \tanh^2(\beta h_0) + F_{\text{approx. } 0}. \quad (141)$$

$$F'_{\text{approx.}}(\bar{h}_0) = 0 \implies \bar{h}_0 = J(1 - 1/N) \tanh(\beta \bar{h}_0) \quad (142)$$

We see then we get consistent equilibrium conditions if we ignore the N^{-1} terms in each equilibrium condition.

7 Key Terms

- **(Gibbs) Free energy:** One should be specific in this definition. For phase transitions, the free energy which is of salient importance is the Gibbs free energy[1] which has as its independent variables, temperature and the order parameter (e.g., volume, magnetization) which is typically extensive. We note the Helmholtz free energy, computed naturally in the canonical ensemble, has as its independent variables temperature and an intensive variable (e.g, pressure, magnetic field)⁴. The Gibbs free energy is the Legendre transform of the Helmholtz free energy⁵.
- **Order parameter:** The physical quantity which is different in two phases of the system and thus can be used as a signal for phase changes.
- **Ehrenfest:** Early 20th century physicist who categorized phase transitions according to their “order”. His definition was as follows: if the n th derivative of the free energy is non-analytic, then the system undergoes a phase transition. Apparently (by wikipedia’s weighty claim) this definition is obsolete. Ehrenfest suffered from depression and at the age of 53 fatally shot his youngest son and killed himself [2].
- **Second order phase transition:** I place this out of order because this seems the phase transition which is easiest to study in statistical mechanics. It is most often represents by a order parameter-temperature phase diagram where the curves for each phase are continuous at the critical point but not-differentiable. Because the order parameter is often the first derivative of the free energy, it’s non-differentiability as a function of T for certain T implies the system it describes has a second order phase transition. Equivalently, it has a *divergent susceptibility and an infinity correlation length*. Examples: ferromagnetic-paramagnetic, superconducting-conducting, superfluid transition.
- **First order phase transition:** By Ehrenfest’s theorem, it is represented by an order parameter-temperature phase diagram which is discontinuous. Wikipedia categorizes such phase transitions as those which involve a latent heat.
- **Critical Exponents:** The exponents which characterize the temperature or field dependent behavior of a number of important thermodynamic quantities when they are near the critical temperature. These

⁴This does not seem to be true for the partition function of the ideal gas

⁵In the QFT analogy, the Helmholtz free energy is to the generating functional for connected correlation functions ($W[J]$) as the Gibbs free energy is to the effective action $\Gamma[\phi_{\text{cl}}]$.

exponents can be roughly calculated in statistical systems using mean field theory, but more sophisticated methods (like the renormalization group) are needed to achieve more accurate calculations.

- **Quantum Phase Transitions:** (Entirely From Wikipedia) “a phase transition between different quantum phases (phases of matter at zero temperature). Contrary to classical phase transitions, quantum phase transitions can only be accessed by varying a physical parameter such as magnetic field or pressure at absolute zero temperature. The transition describes an abrupt change in the ground state of a many-body system due to its quantum fluctuations.”
- **Infinite Order Phase Transitions:** (Entirely From Wikipedia) “Phase transition which is continuous but breaks no symmetries. The most famous example is the Kosterlitz-Thouless transition in the two-dimensional XY model.” The canonical example is the Kosterlitz-Thouless transition.

References

- [1] M. Kardar, *Statistical physics of fields*. Cambridge University Press, 2007.
- [2] G. Farmelo, *The strangest man: The hidden life of Paul Dirac, quantum genius*. Faber & Faber, 2009.
- [3] D. Sherrington and S. Kirkpatrick, “Solvable model of a spin-glass,” *Physical review letters*, vol. 35, no. 26, p. 1792, 1975.
- [4] J. Hubbard, “Calculation of partition functions,” *Physical Review Letters*, vol. 3, no. 2, p. 77, 1959.
- [5] K. Binder and A. P. Young, “Spin glasses: Experimental facts, theoretical concepts, and open questions,” *Reviews of Modern physics*, vol. 58, no. 4, p. 801, 1986.
- [6] K. H. Fischer and J. A. Hertz, *Spin glasses*, vol. 1. Cambridge university press, 1993.