Chapter 2: Interacting Systems: A First Look

In this chapter we shall start our study of interacting models that we had introduced in the first chapter. We shall try to discuss some of the techniques used in the analysis of interacting models. One would like to, of course, find exact solutions to interacting problems. Reality, however, bites! There are very few interacting models that succumb to an exact solution. We shall see some in this course. The majority of interacting models however do not yield to the tricks of the theorists. The theorists then become "clever" and try to find approximate solutions to such problems. In many ways the lack of exact solutions is what makes some problems challenging, and even interesting. Our strategy will be to

go "model by model" and learn the tricks of the trade.

One technique of solving problems with interaction is to find a "small parameter" that is involved in the problem. The idea is that if the "small parameter" were zero, we will solve the problem exactly. In a sense we will be doing some kind of perturbation theory that we are familiar in mechanics.

Let us begin.

Interacting Particles Model.

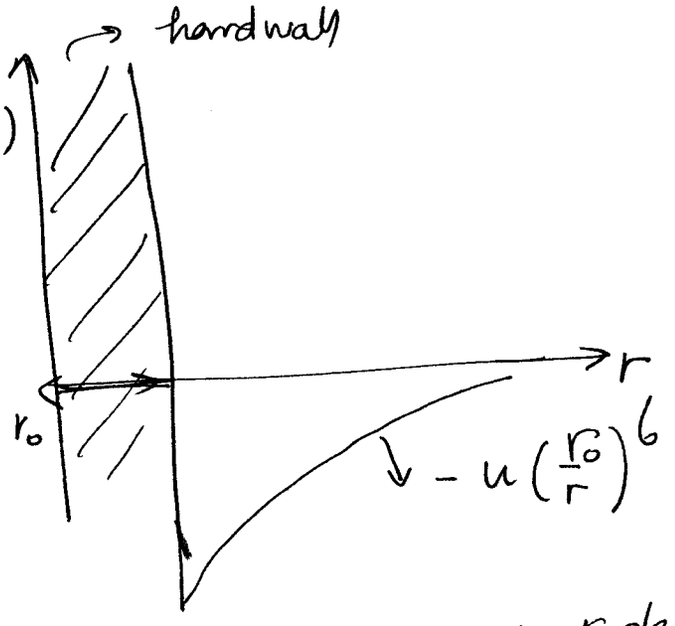
Consider the interacting particles model, with volume V in d-dimension,

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{\langle i,j \rangle} V(\vec{r}_i - \vec{r}_j)$$

We will work in a situation where the average density $n_0 = \frac{N}{V}$

Now, as was discussed, we ~~with exact~~ ~~that n_0~~ is now need to specify the

potential. Let us take it be of the form



$$U(r) = \begin{cases} = \infty & r < r_0 \\ = -u\left(\frac{r_0}{r}\right)^6 & r > r_0 \end{cases}$$

Let us work in the grand ~~canonical~~ & canonical Ensemble.

Here
$$Z = \sum_n e^{n\beta\mu} Z_n$$

where $\beta = 1/T$, μ is the chemical potential and Z_n is the partition function of the n particle system

$$Z_n = \frac{1}{n!\, h^{3N}} \int \prod d\vec{p}_i \cdot d\vec{r}_i \, e^{-\beta\left[\sum_{i=1}^{n} \frac{p_i^2}{2m} + \sum_{<ij>} U(r_{ij})\right]}$$

Now we know from elementary statistical mechanics that

$$\frac{PV}{T} = \ln Z$$

Now ~~sp~~ suppose there are no interactions ($u=0$ and $r_0=0$), then

~~Let us simplify~~ From now on

$$Z_n = \frac{1}{n!}\frac{1}{h^{dn}} V^n \left(\frac{2m}{\beta}\pi\right)^{dn/2}$$

$$= \frac{1}{n!} V^n \left[\frac{m\, 2\pi}{h^2 \beta}\right]^{dn/2}$$

note that $\left[\frac{m}{2\pi\, \hbar^2 \beta}\right]^{1/2} = \frac{1}{\lambda}$

where λ is the thermal de Broglie wave length. We get

$$Z_n^I = \frac{1}{n!}\left(\frac{V}{\lambda^d}\right)^n \qquad \left[\lambda \sim \beta^{1/2} \to 0 \text{ as } T \to \infty\right]$$

$$Z^I = \sum_n \frac{\zeta^n}{n!}\left(\frac{V}{\lambda^d}\right)^n$$

$$= e^{\frac{\zeta V}{\lambda^d}}$$

where ζ is the fugacity.

Note that $\langle N \rangle = \zeta \frac{\partial \ln Z}{\partial \zeta} = \frac{V}{\lambda^d}\zeta$.

We find the nice fact that

$$\boxed{\zeta = n_0 \lambda^d} \quad \text{for Ideal gas}$$

Note that $\zeta \to 0$ as $T \to \infty$ (for fixed n_0).

We now see that

$$\mathcal{Z}^I = l^{n_0 V}$$

$$\Rightarrow \left(\frac{PV}{T}\right)_{Ideal} = n_0 V \Rightarrow \frac{P_{Ideal}}{T} = n_0.$$

(which is a well known elementary result)

Now the key idea is that in the interacting system at high temperature and low density, the fugacity will still be small. Note that if $T \gg u$ (the interaction scale) and $n_0^{-1/3} \gg r_0$, then the effects of the interaction will not be "much" i.e, the fugacity will still be expected to be small. This is the motivation of the ~~virial~~ virial expansion.

$$\frac{P}{T n_0} = \sum_{n=1}^{\infty} a_n (n_0 \lambda^d)^{n-1}$$

a_ns are called the virial coefficients

(Notation vary, so be careful).

The idea is that a_ns are dimensionless numbers that depend on the ratios of the scales in the problem. The effect of the 'interaction' is thus to change the equation of state. We will reach the virial expansion via the low fugacity. For the interact system

$$\frac{PV}{T} = \ln\left[1 + \zeta Z_1 + \zeta^2 Z_2 \cdots\right]$$

$$\simeq \zeta Z_1 + \zeta^2 Z_2 - \frac{1}{2}(\zeta_1 Z_1 + \zeta^2 Z_1)^2$$

$$\simeq \zeta Z_1 + \zeta^2\left[Z_2 - \frac{1}{2} Z_1\right]$$

$$\langle N \rangle = z\zeta \frac{\partial \ln Z}{\partial \zeta} = \zeta Z_1 + 2\zeta^2\left[Z_2 - \frac{1}{2} Z_1^2\right] \cdots$$

We now see that for small fyacts

$$\langle N \rangle \simeq \zeta \frac{V}{\lambda^d} + 2\zeta^2\left[Z_2 \mp \frac{1}{2} Z_1^2\right]$$

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We now have to solve for the fugacity. Noting that ζ is small, we find

$$\zeta = n_0 \lambda^d - 2\underbrace{\left[z_2 - \frac{1}{2} z_1^2\right]}_{Y} (n_0 \lambda^d)^2 + [O(n_0^3)].$$

Note that for the ideal gas

$$z_2 - \frac{1}{2} z_1^2 = 0 \quad \text{(for ideal gas)}$$

and hence $\zeta = n_0 \lambda^d$ (for ideal gas)

The change in the fugacity due to interactions is proportional Y

Now using this expression for the fugacity in the pressure expression, we find

$$\frac{PV}{T} = n_0 \lambda^d z_1 - 2\left[z_2 - \frac{1}{2} z_1^2\right] (n_0 \lambda^d)^2 + (n_0 \lambda^d)^2 \left[z - \frac{1}{2} z_1^2\right]$$

$$= n_0 \lambda^d z_1 - \left[z_2 - \frac{1}{2} z_1^2\right] (n_0 \lambda^d)^2.$$

$$\frac{PV}{T} = n_0 V - \frac{\left(Z_2 - \frac{1}{2} Z_1^2\right)}{Z_1} \frac{n_0^2 V^2}{Z_1}$$

$$= n_0 V \left[1 - \underbrace{\frac{\left(Z_2 - \frac{1}{2} Z_1^2\right)}{Z_1}}_{= a_2} (n_0 \lambda^d) \right]$$

a_1

We have thus obtained

$$\frac{P}{n_0 T} = \left[1 + a_2 (n_0 \lambda^d) \right] \quad (\text{Eq. of State}).$$

a_2 is the virial coefficient, and is entirely determined by two body physics.

Let us now calculate a_2. This involves calculation of Z_2.

$$Z_2 = \frac{1}{2!} \frac{1}{h^{2d}} \int d^d \vec{p}_1 \int d^d \vec{p}_2 \, e^{-\beta \left(\frac{p_1^2}{2m} + \frac{p_2^2}{2m} \right)}$$

$$\times \int d\vec{r}_1 d\vec{r}_2 \, e^{-\beta u(|\vec{r}_1 - \vec{r}_2|)}$$

We see that

$$Z_2 = \frac{1}{2}\,\frac{1}{\lambda^{2d}} \int d\vec{r}_1 d\vec{r}_2\, e^{-\beta u(\vec{r}_1 - \vec{r}_2)}$$

Make the substitution

$$\left.\begin{aligned} \vec{r}_1 &= \vec{R} + \vec{r}/2 \;, & \vec{r}_2 &= \vec{R} - \vec{r}/2 \\ \Rightarrow \quad \vec{R} &= \frac{\vec{r}_1 + \vec{r}_2}{2} \;, & \vec{r} &= \vec{r}_1 - \vec{r}_2 \end{aligned}\right\}$$

$$d\vec{r}_1\, d\vec{r}_2 = d\vec{R}\, d\vec{r}$$

$$\Rightarrow Z_2 = \frac{1}{2}\,\frac{1}{\lambda^{2d}} \int d\vec{R} \int d\vec{r}\, e^{-\beta u(r)}$$

$$= \frac{1}{2}\,\frac{1}{\lambda^{2d}}\, V \underbrace{\int d\vec{r}\, e^{-\beta u(r)}}_{\downarrow}$$

$$u(r) = \begin{cases} \infty & r < r_0 \\ -u\left(\frac{r}{r_0}\right)^6 & r > r_0 \end{cases}$$

$$\Rightarrow C_d \int_{r_0}^{\infty} dr\, r^{d-1} e^{\beta u \left(\frac{r_0}{r}\right)^6} \to \infty \quad \text{(divergent)}$$

(C_d: "Area of surface of sphere")

We thus see that the integral is divergent!

How to tackle this?

Note that we want $Z_2 - \frac{1}{2} Z_1^2$.

But $\frac{1}{2} Z_1^2$ is the ~~partial~~ partition function of two non-interacting particles

$$\frac{1}{2} Z_1^2 = \frac{1}{2}\,\frac{1}{\lambda^{2d}} \int d\vec{R} \int d\vec{r}$$

$$= \frac{1}{2}\,\frac{1}{\lambda^{2d}}\, V \int d\vec{r}$$

So, now we see that

$$Z_2 - \frac{1}{2} Z_1^2 = \frac{1}{2} \frac{1}{\lambda^{2d}} V \underbrace{\int d^d\vec{r} \left[e^{-\beta u(r)} - 1 \right]}$$

$$C_d \left[\int_{r_0}^{\infty} dr\, r^{d-1} \left[e^{\beta u \left[\frac{r_0}{r}\right]^6} - 1 \right] - \int_0^{r_0} dr\, r^{d-1} \right]$$

These integrals can be done analytically (at least by Mathematica)

We now make a physics point that $\beta u \ll 1$. This temperature is much greater ~~that~~ than the sticking energy of atoms.

we get

$$Z_2 - \frac{1}{2} Z_1^2 = \frac{V}{2\lambda^{2d}} C_d \left[\int_{r_0}^{\infty} dr\, r^{d-1}\, \beta u \left[\frac{r_0}{r}\right]^6 - \frac{r_0^d}{d} \right]$$

$$= \frac{V}{2\lambda^{2d}} C_d \left[\beta u \frac{r_0^6}{6-d} \frac{r_0^d}{r_0^6} - \frac{r_0^d}{d} \right]$$

$$= \frac{V}{2\lambda^{2d}} C_d \left[\frac{\beta u}{6-d} - \frac{1}{d} \right] r_0^d .$$

We see that

$$a_2 = -\frac{\left[z_2 - \frac{1}{2}z_1^2\right]}{z_1}$$

$$= -\frac{C_d}{2}\left[\frac{\beta u}{6-d} - \frac{1}{d}\right]\left(\frac{r_0}{\lambda}\right)^d$$

$$= \frac{C_d}{2d}\left(\frac{r_0}{\lambda}\right)^d - \frac{C_d \beta u}{2(6-d)}\left(\frac{r_0}{\lambda}\right)^d$$

Pulling all this back in the eqn. of state we get

$$\frac{P}{T} = n_0\left[1 + \left[\frac{C_d}{2d} - \frac{C_d \beta u}{2(6-d)}\right] n_0 r_0^d\right]$$

$$\frac{P}{T} + \underbrace{\frac{C_d u r_0^d}{2(6-d)}}_{A} \frac{n_0^2}{T} = n_0 + \underbrace{\frac{C_d r_0^d}{2d}}_{B} n_0^2$$

$$\Rightarrow \frac{1}{T}\left(P + A n_0^2\right) = n_0(1 + B n_0)$$

$$\Rightarrow \frac{1}{T}\left(P + A n_0^2\right) \simeq \frac{n_0}{1 - B n_0}$$

$$\Rightarrow P = \frac{n_0 T}{1 - B n_0} - A n_0^2$$

$\rightarrow$ van der Waals !!

We have thus obtained the van der Waals equation of state = (Nobel Prize 1910 or 1911, §1910. Wikipedia says):

We can now interpret the terms

$$B = \frac{c_d r_0^d}{2d}$$ is the excluded volume

$$A = + \frac{c_d r_0^d u}{2(6-d)}$$ is the

reduction in pressure due to attractive interactions. Note that the expansion is valid when $\beta u \ll 1$ and $r_0^d n_0 \ll 1$. This is of to be checked with experimental conditions. to ensure that the theory is acceptable. What does the vdW equation of state tell us? Before we discuss this let us note that this procedure of expanding in a small parameter is quite general and can be developed in diffent contexts.

We note also that a_2 is determined entirely by two-body physics. The idea is that in a dilute system, two particle interactions provide the most important contribution over and above the ideal gas. The virial coefficient a_2 can be calculated using a quantum treatment of the two body problem. This uses scattering theory, and a_2 can be expressed in terms of the scattering phase shift. This is the famous result of Beth and Uhlenbeck. (See Landau-Lifshitz if you are interested. You may benefit from looking at Landau-Lifshitz even if you are not interested!)

Back now to vdW. We can rewrite the eqn. of state as

$$P = \frac{NT}{V - BN} - \frac{AN^2}{V^2}$$

(N - number of particles
V - volume)

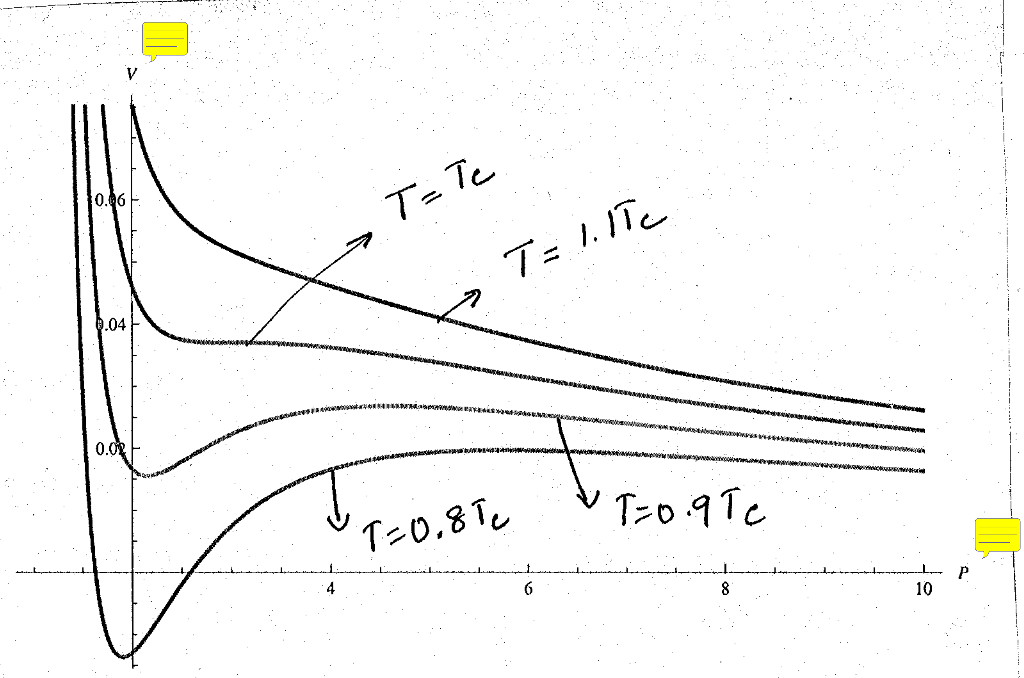


Fig 1

Let us look at how P depends on V at a fixed temperature. Below $T = T_c$, pressure given by the equation of state is not a monotonic function of V. T_c can be obtained by the simultaneous solution of

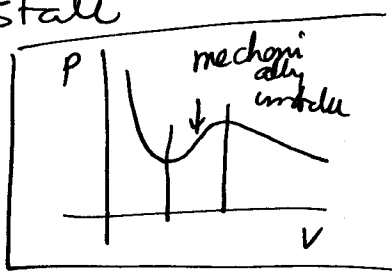
$$P = \frac{T}{v - B} - \frac{A}{v^2}$$

where v is the specific volume $v = \frac{1}{n_0}$.

$$T_c = \frac{8}{27}\frac{A}{B}, \quad v_c = 3B, \quad P_c = \frac{A}{27B^2}$$

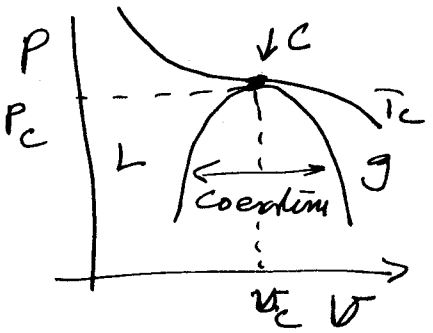
For $T < T_c$, the pressure is not a monotonic function of v. In fact there will be a

regime of v where $\frac{dP}{dv} > 0$, which is not a mechanically stable state



This is a signal that at a fixed temperate, if pressure is decreed, there will be a "sudden" change in the volume at some value.

Back to the point denoted by T_c. The value of v_c and the pressure P_c are all fixed. In fact if our theory is right then we see a beautiful result. The critical point denoted by P_c, v_c at T_c is the point in the phase diagram, ~~Note that~~ where the liquid gas coexistence region "ends".



Now our rats show that

$$\frac{T_c}{P_c v_c} = \frac{8}{3}! \quad \text{or} \quad \frac{P_c v_c}{T_c} = \frac{3}{8} = 0.375$$

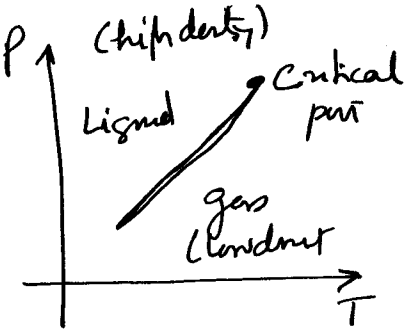
~~Note that~~ The R.H.S is a number, and hence this ratio must be independent of the material.

Tables from Atkins (Physical chemistry)

Material	$\frac{P_c V_c}{T_c}$
Ar	0.292
CO_2	0.274
He	0.305
O_2	0.308

These are all quite reasonably close to 0.375. Given the amount of effort that went into the calculations these is quite a successful story.

Actually we can do much more, and we will! Let us calculate the phase digram in the PT-plane. We know that this should look something like this. Our strategy will be the following.



① ~~Fix~~ $T < T_c$

② Find, pressures P_e and P_a which are the extrema of the ~~pressure~~ pressure.

For given P, $P_e < P < P_a$ there are three solutions to v.. $v_e < v_{unstable} < v_g$.

One corresponds to v_g, ~~and~~ the gas, and the other to v_e the liquid. We do not need to

consider $v_{unstable}$.

(3) Now we can calculate the Gibbs free energy g of the liquid and gaseous phases as a function of pressure. They will cross at a particular pressure

$$g_l(P,T) = F(T, v_l) + Pv_l$$

↑ Helmholtz free energy.

$$g_g(P,T) = F(T, v_g) + Pv_g$$

We find the pressure at which the two Gibbs free energies cross.

How to calculate the Helmholtz free energy from the equation of state?

Now $dF(T,v) = -SdT - Pdv$

per particle

at fixed T $F = -\int P dv$

$$F = -\int_{\infty}^{v} dv \left[\frac{T}{v-B} - \frac{A}{v^2} \right]$$

Note that we can regularize this calculation by adding and subtracting the ideal gas contribution.

$$F = -\int_{\infty}^{v} dv \left[\left[\frac{T}{v-B} - \frac{T}{v} \right] - \frac{A}{v^2} \right] + F_{\text{ideal gas}}.$$

$$F(T,v) = \int \left[\frac{T}{v-B} - \frac{T}{v} \right] dv$$

$$= -T \left[\ln [v-B] - \ln v \right]_{\infty}^{v} + \left(-\frac{A}{v} \right)$$

$$= -T \ln \left[\frac{v-B}{v} \right] - \frac{A}{v} + F_{\text{ideal gas}}$$

$$F_{\text{ideal gas}} = \frac{1}{N} \left[-T \ln \left[\frac{1}{N!} \left(\frac{V}{\lambda^d} \right)^N \right] \right]$$

$$= \frac{1}{N} \left[-T \left[(-N \ln N - N) + N \ln \left(\frac{Nv}{\lambda^d} \right) \right] \right]$$

$$= -\frac{T}{N} \left[-N + N \ln \left(\frac{v}{\lambda^d} \right) \right]$$

$$= -T \ln \left(\frac{v}{\lambda^d} \right) \quad \text{(drop 1)}$$

$$\boxed{F(T,v) = T \ln \left(\frac{\lambda^d}{v-B} \right) - \frac{A}{v}}$$

$$G(T,P) = F(T,v) + Pv$$

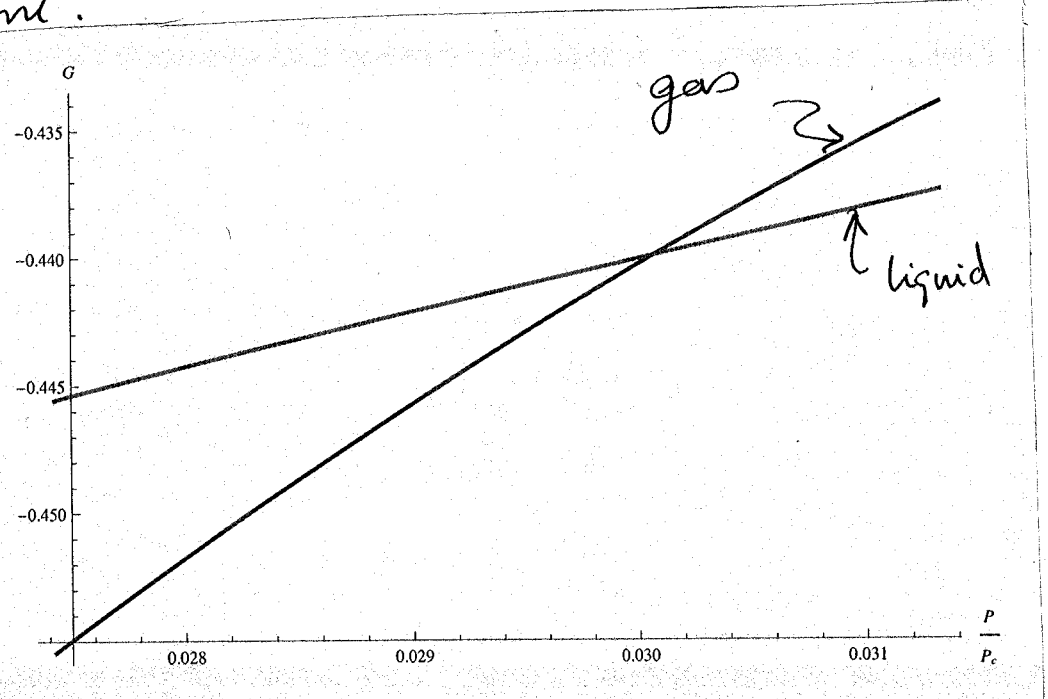
Now we can obtain numerically

$$G(T,P) = T\left[\ln\left[\frac{\lambda^d}{v-b}\right] + \frac{v}{v-b}\right] - \frac{2A}{v}$$

To obtain $G_\ell(T,P)$ put $v = v_\ell$ (which solves the eqn. of state)

and $G_g(T,P)$ put $v = v_g$.

For a given temperature we can plot $G_\ell(T,P)$ and $G_g(T,P)$ as a function of Pressure. We se

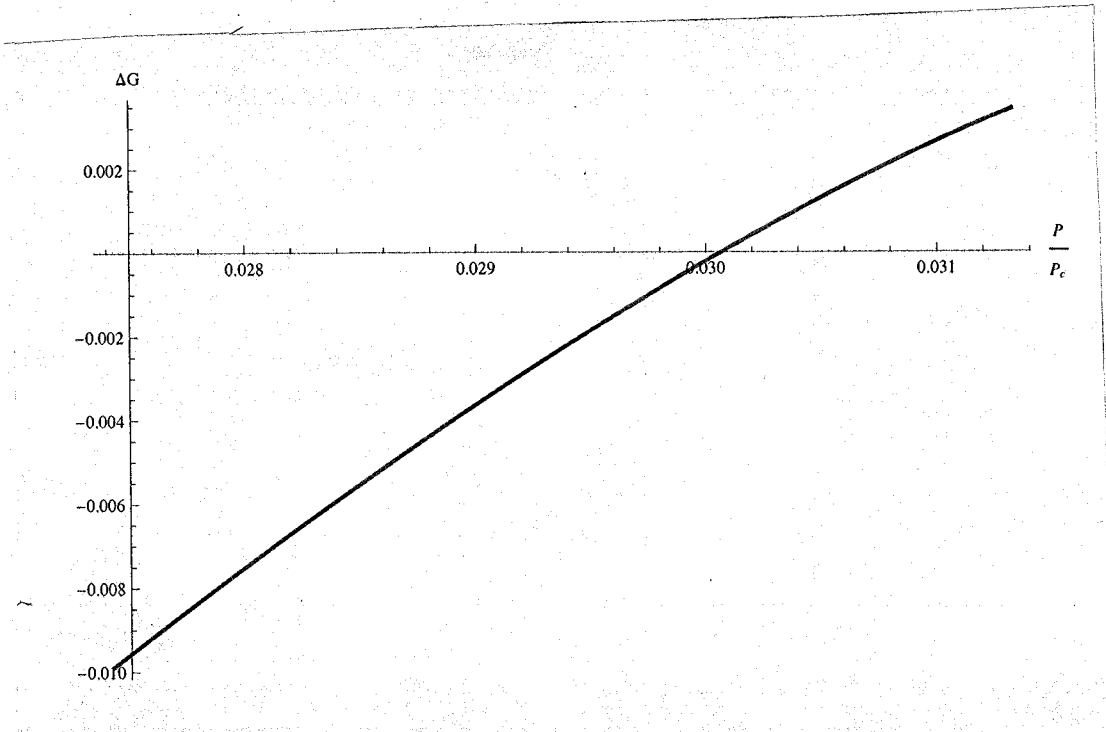


2.

We see that $G_\ell(T, P_F) = G_g(T, P_F)$

where $P_F(T)$ is the ~~[illegible]~~ pressure at the first order transition.

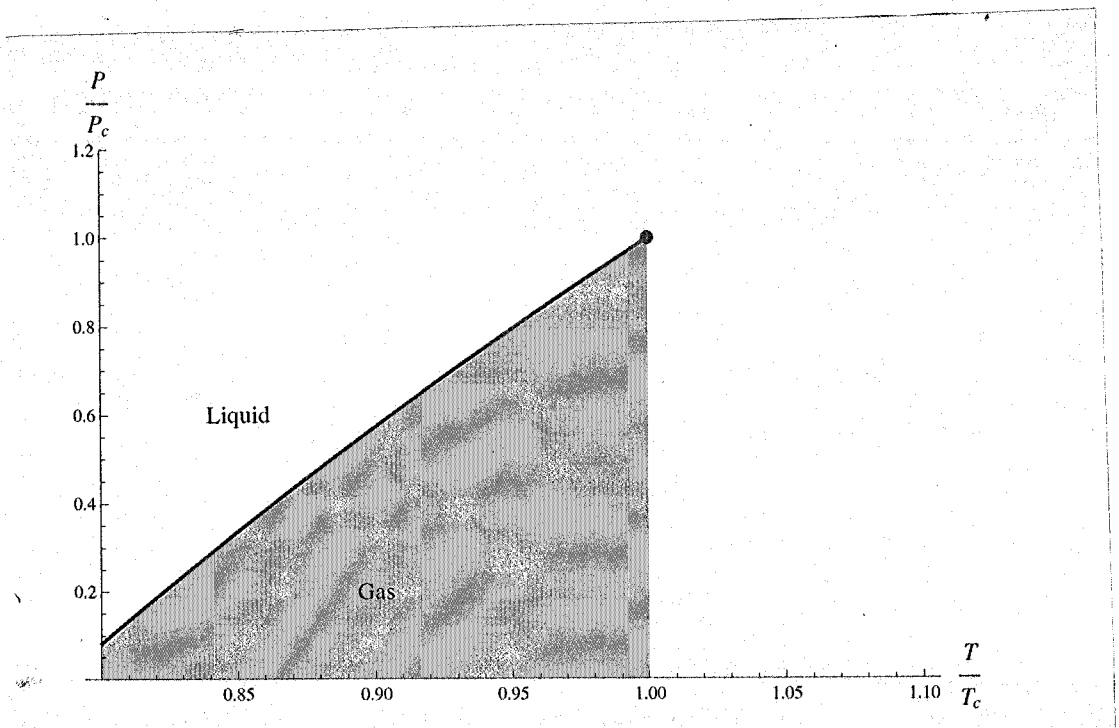
A way to find P_F is to plot $\Delta G = G_g(T,P) - G_\ell(T,P)$



3.

we can obtain P_F by the point where it crosses the zero.

Note that the equality of the Gibbs potential is the familiar equality of the chemical potentials between the two phases. The other conditions are the equality of pressure and temperature which is always met.



This is our calculated phase diagram. We see that there is a first order transition from a liquid to gas if the pressure is reduced. ~~How is our first result of this~~ Note that this first order transition terminates at critical point. We will see the connections to other problems later.

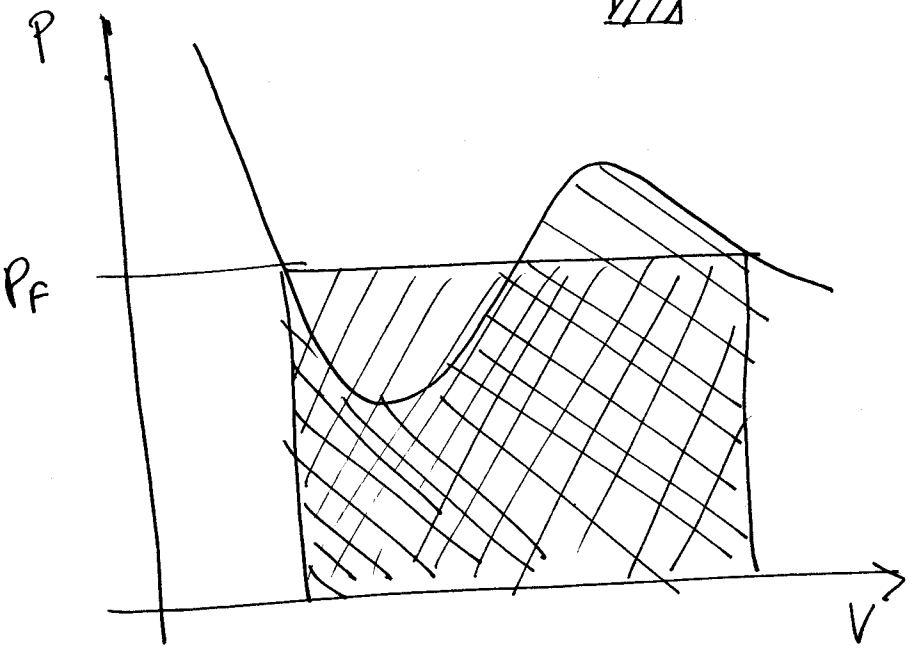
The vdW theory is a land mark in physics, in a sense, it is a key many body problem (classical) that are experimentally consistent ~~[illegible]~~ We will close this discussion by pointing out that the rent derived is consistent with the usual tie line construction

$$G_l(T, P_F) = G_g(T, P_F)$$

$\int_{v_l}^{v_g} P\,dV$

$$\Rightarrow -T\left[\left(\ln\left[\frac{\lambda^d}{v_g - b}\right] + \frac{z}{v_g}\right) - \left(\ln\left[\frac{\lambda^d}{v_l - b}\right] - \frac{z}{v_l}\right)\right]$$

$$+ P_F\left[v_g - v_l\right] = 0$$



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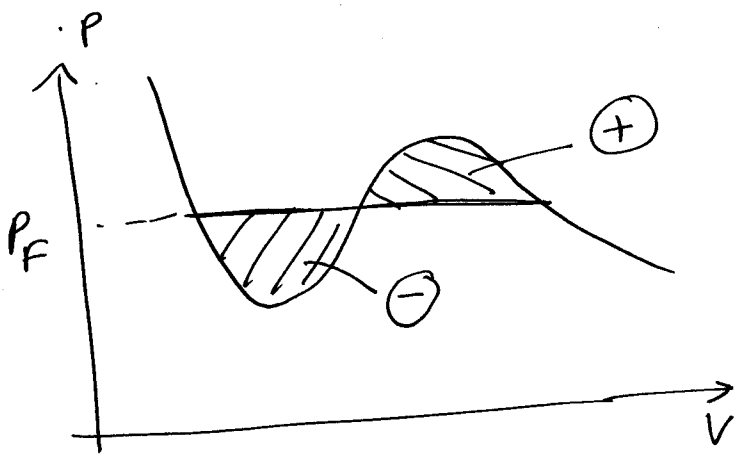


We see that P_F is such that the signed area enclosed with the P_F vanishes. This is the tie line construction!

The Monte Carlo Method

Buoyed by our success in treating the non ideal gas, and discovering the liquid gas transition, we & now continue our study of phases and phase transitions by a study of Ising Model.

Let us write out the Ising model (including a uniform external field h_i)

$$H = -J \sum_{\langle ij \rangle}^{1} s_i \cdot s_j - \sum_{i}^{1} h_i s_i$$

$$x = \{s_i\}$$

$$g(x) = \frac{e^{-\beta \mathcal{H}(x)}}{Z} = P(x)$$

↑ probability.

$$Z = \sum_{x}^{1} e^{-\beta \mathcal{H}(x)}.$$

$$\langle O \rangle = \sum_{x}^{1} P(x)\, O(x).$$

Now if we choose our simulation cell to have N sites, then there will be 2^N x_i's in the

the sum. Consider we take $N = 100^2$ size square in 2D. This means that there will be 2^{20000} spin configration that is approximately $\sim 10^{3}$ which will be impossible to do. For example if it takes 10^{-12} s to add one conbtrn, we will need $10^{\sim} \times 10^{-12}$ s $\simeq 10^{\sim}$ seconds $\Rightarrow 10^{\sim}$ years!!! While we can start the calculation, we may not be around to find out the result since the universe itself may have undergone a phase trasition in this time!

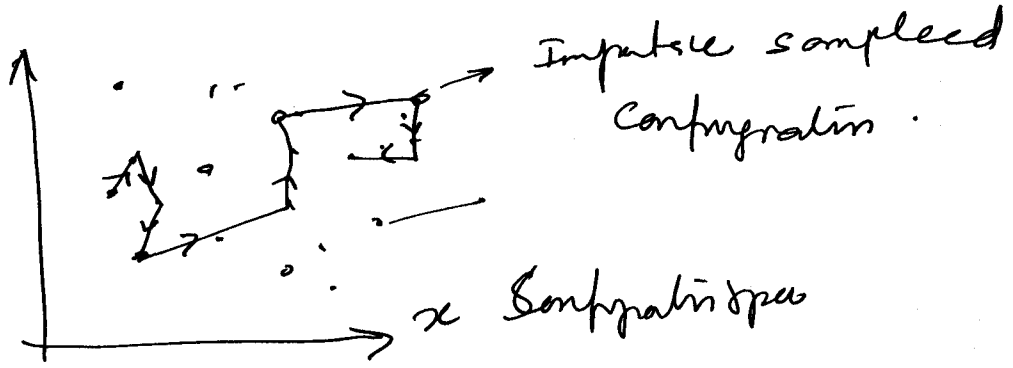
How do we then proceed? The idea is to use the Monte Carlo method - i.e, gamble! Gambling is the solution to our woes! The idea of Monte Carlo method is to sum over only the important configuration that make the most contribution to the sum. The catch however is that we do not quite know $P(x)$, since we do not know Z!

This motivates the need to devise a scheme that will start with a configuration x_1 and "step" to another configuration x_2 comparing $P(x_1)$ and $P(x_2)$... We thus perform a walk in the space of configurations choosing to go from one configuration to another spending "most of our time" in high probability configurations. This is called importance sampling.

Having understood the idea, or problem statement becomes clearer. We need to set up a set of rules or algorithm that walks along in the configuration space performing the importance sample.

When we have obtained such an algorithm, we will produce a sequence of configurations (i.e, the importance sampled configurations) as a function of the "step" or "time".

In other words our algorithm ~~ensures~~ endows us with a dynamics - the key question is how to create this algorithm.



~~We core ideas~~

This mathematical frame work most useful for this purpose is the theory of Markov chains.

To discuss this let us set the notation Let us label the configuration $x_1 \ldots x_{2^N}$ and call $P(x_m)$ as $P(m)$. Now $\sum_n P_n = \sum_m P_m$.

The key concept is that of Markov transition matrix $W(n,m) = W(n \leftarrow m)$. This defines the probability of moving from configuration m to n in a "step".

If we now take $W(n,m)$ to be independent of "time" or the "step", then the probability of $m \to n$ in a step is independent of how the system got to m. This is a stochastic process which is called a Markov chain.

Now $\sum_n W(n,m) = 1$. and $W(n,m) \geq 0$.

Now we ask the question. Suppose the W matrix is given, and we know the probability distribution of the configuration $P(n,t)$, ~~we can ask~~ at step t.

Then $P(n,t+1) = \sum_m W(n,m) P(m,t)$.

$$\Rightarrow P(n,t+1) - P(n,t) = \left[\sum_m W(n,m) P(m,t)\right] - P(n,t)\Big].$$

This is called the Master equation

Now let us assume that $P(n,t)$ is a steady distribution. We thus see that

$$\sum_m W(n,m) P(m) = P(n).$$

Thus W matrix ~~needs~~ must be such that $P(n)\left[= \frac{e^{-\beta E(n)}}{Z}\right)$ is the right eigenvector with eigenvalue 1. Thus our goal is to find a transition matrix W with non negative entries and $\sum_n W(n,m) = 1$.

~~Without 2 right eigenvectors~~ which has $P(n)$ as the right eigenvector with eigenvalue of 1! This looks pretty ~~hopeless~~ hopeless! W is of the order $2^N \times 2^N$!! In fact it is not clear that such a W exists and even if it does, it is certainly not clear that it is unique!

So how do we proceed!

Actually the theory of Markov chains allows us to beat this problem!

We need some concepts to use a key theorem of Markov chains.

1. Visit probability:- $V(n,m;t)$. This is the probability that the system reaches ~~state~~ n at time t for the first time given that the system was in configuration m at time $t=0$.

2. The total visit probability

$$V(n,m) = \sum_t V(n,m;t)$$

3. If $V(n,m) \neq 0$ $\forall m,n$, any state can be reached from any other state.

Such a markov chain is said to be irreducible. → This is a key idea.

The next idea is that of recurrence. A state is called ~~positive recurrent~~ recurrent if $V(m,m) = 1$. The mean recurrance time $t_m = \sum_t^1 t\, V(m,m,t)$. If $t_m < 0$ the state m is called positive recurrent.

If all the states are positive recurrent, the chain is called ergodic.

The third idea:- ~~of~~ A chain is called aperiodic if no state repeats in a periodic manner.

Now we have a theorem of Markov chains:

An ergodic aperiodic irreducible Markov chain has a unique stationary probability distribution.

The key point is that of irreducibility - ie, every state must be reachable from every other state. Aperiodicity and ergodicity are easier in our case since the space of configurations is finite even if large.

Now we knew that we need to chose one irreducible chain.

One way to chose this is in such a way that

$$W(n,m)\,P(m) = W(m,n)\,P(n).$$

This is called the <u>detailed balance</u> condition. This makes $P(n)$ a right eigenvector of W is an automatic fashion.

The next step is to write

$$W(n,m) = A(n,m)\;S(n,m)$$

($A(n,m)$: Acceptance; $S(n,m)$: Suggestion)

Let us assume that we have decided up on the $S(n,m)$. Now detailed balance gives

$$\Rightarrow \frac{A(n,m)}{A(m,n)} = \frac{S(m,n)\,P(n)}{S(n,m)\,P(m)} = \frac{S(m,n)\,e^{-\beta E(n)}}{S(n,m)\,e^{-\beta E(m)}}$$

$$= h(n,m).$$

Now take

$$A(n,m) = F(h(n,m))$$ where F is a function.

Thus the condition above can be satisfied if $F(y) = y\,F(1/y)$

The famous Metropolis algorithm is

$$F(y) = \min(1, y)$$

$$= \min\left[1, \frac{S(m,n)\, e^{-\beta E(n)}}{S(n,m)\, e^{-\beta E(m)}}\right]$$

Our algorithm is complete if we specify $S(n,m)$.

The popular choice of the suggestion matrix is based on single spin flip. At any step pick a site (i_s) at random and flip the spin on the site. This makes $S(n,m) = \frac{1}{N}$ (n is the state m with the spin at site i_s flipped.) Note $S(n,m) = 1/N$!

Thus the acceptance matrix becomes

$$F(y) = \min\left\{1, e^{-\beta \Delta E}\right\}$$

$$\Delta E = E(n) - E(m)$$

[redacted]

We now have a complete specification of the W matrix. By construction $P(n)$ is the right eigenvector with eigenvalue 1.

This will now produce a sequence of states n, and the expectation value of any operator is

$$\langle O \rangle = \frac{1}{N_{mc}} \sum_{n=1}^{N_{MC}} O(n)$$

(note that the $P(n)$ term is not there) where N_{mc} is the number of Monte Carlo steps taken.

We can see that our chain is irreducible, one can reach any spin configuration from any other spin configuration. While we do not have a proof that it is aperiodic, we note that aperiodicity is quite natural.

Here is the full algorithm

→ start with a random configuration.

Do $i = 1, N_{mc}$

Do $j = 1, N$

- Pick a site at random
- calculate ΔE of this state

If $[\Delta E \leq 0]$

Accept the spin flipped state

Else calculate

$y = e^{-\beta \Delta E}$

generate a random number $r \in [0,1]$

If $r < y$ accept the state,

else do not.

See next page

Monte Carlo Algorithm

(1) Start with a random configuration

(2) Do $i = 1$, NMC sweeps

Do $j = 1$, N

- Pick a site i_s at random

→ Calculate ΔE for flipping the spin at the site i_s.

→ If ($\Delta E < 0$) then

Accept the new configuration

Else

Calculate $y = e^{-\beta \Delta E}$

Pick a random number $r \in (0,1)$

If ($r < y$) then

Accept new configuration

End if

End if.

End Do

Update observables

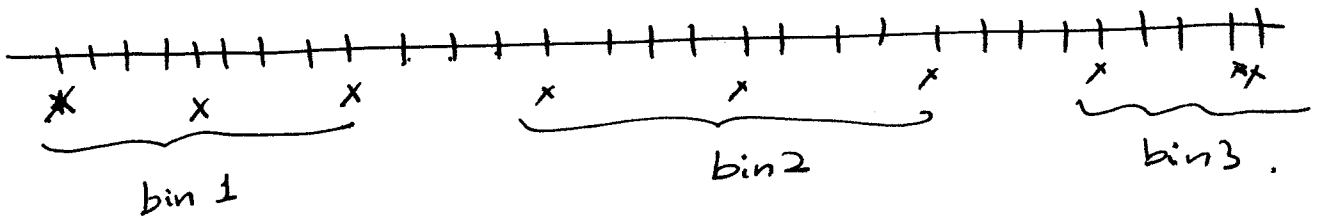
End Do.

Note that we have organized the calculation in terms of Monte Carlo sweeps. A sweep consists of N Monte Carlo steps.

Finally We need to note a couple of more things.

① Sampling should not be done on every monte carlo sweep. This is to avoid correlated sampling.

② Error estimation is crucial in Monte Carlo simulations. There are many sources of error, such as sampling error, systematic errors etc. We will not have the time to discuss this in detail in this course. Here is what is usually done



1 → monte carlo sweep

2 → sampling steps.

3 → Bins.

$$O_{mean} = \frac{1}{N_{samples}} \sum_i^{} O(sample)$$

$$O_{SD} = \frac{1}{N_{bin}} \left(\sum_{bins}^{} \left[O_{mean}^{bin} \right]^2 \right) - O_{mean}^2$$

$$\text{Standard Error} = \frac{\sqrt{O_{SD}}}{\sqrt{N_{bins}}}.$$

Analysis of the Ising Model.

For the next few hours we will focus our attention on the ising model on the d-hypercubic lattice. As we now know, we need only the ferromagnetic version.

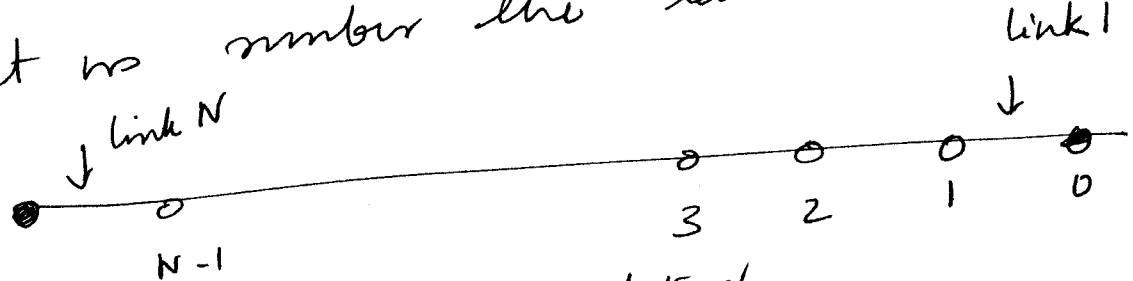
We will first start with $d=1$.

$d=1$. Question: Given ~~the~~ chain $d=1$, and the Ising model

$$H = -J \sum_i S_{i+1} S_i$$

with periodic boundary conditions

Let us number the lattice as



$N = 0$ (periodic boundary condition)

Note that we are numbering to the left: (Nothing holy about numbering to the right).

We ask the following question: Can the Ising model in $d=1$ spontaneously order?

Let us start with something that we know for sure. The ground state is either the state with all spins +1 or -1 → this is two fold degenerate. Magnetization = ±1.

We ask what is the excitation of the system? The physical idea of this question is the following:- we know that

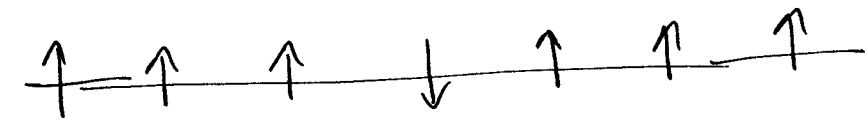
$$M = \sum_x^{-1} \rho(x)\, \mu(x).$$ In the ground state

$M = +1$ (for all spins up).

If we find out the nature of the lowest excitation, then we can check if they "destroy" the magnetization or not. We can see how much the magnetization is "affected" by such excitations and come to some conclusions. Note that this is quite a general idea and we will use this in multiple contexts.

Back to our question, what is the excitation above the ferromagnetic ground state? A key point about the excitation that we ask is, if it is gapped or gapless!

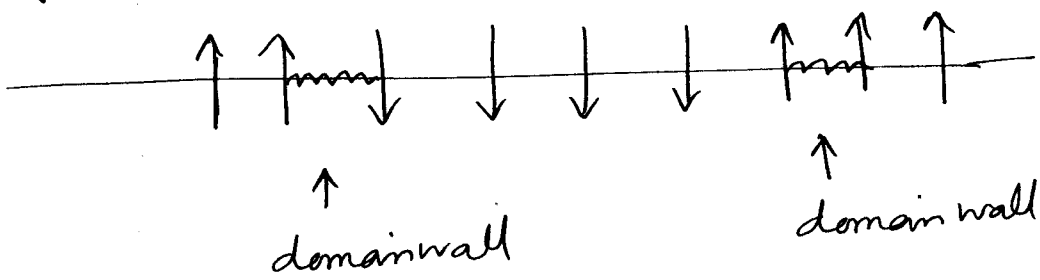
A gapped excitation is one that requires a finite amount of energy even in the thermodynamic limit. If the energy of an excitation can be made as small as we please (particularly by choosing larger system sizes) then the system has gapless excitations. What is the excitation with the smallest energy in the Ising model. Well it is a single spin flip! For example a state



Such as the one shown here. Note that this state costs energy 2J, even in the thermodynamic limit! Thus the excitation is gapped!

Now, we ask what is the degeneracy of this excitation. You might be tempted to say the spin can be flipped at any one site, and hence it must be N! But that is not quite true!

This is because, we can have a spin configuration such as



which still costs energy $2J$! Now the degeneracy of such excitation $= {}^{N}C_{2} = \frac{N(N-1)}{2}$ which is the number of ways of choosing two links. Note that if such excitations proliferate, then they will destroy the magnetization, but we are counting on the fact that the system is gapped! But we should really check this.... let us calculate the free energy of one such excitation (made of 2 domain walls).

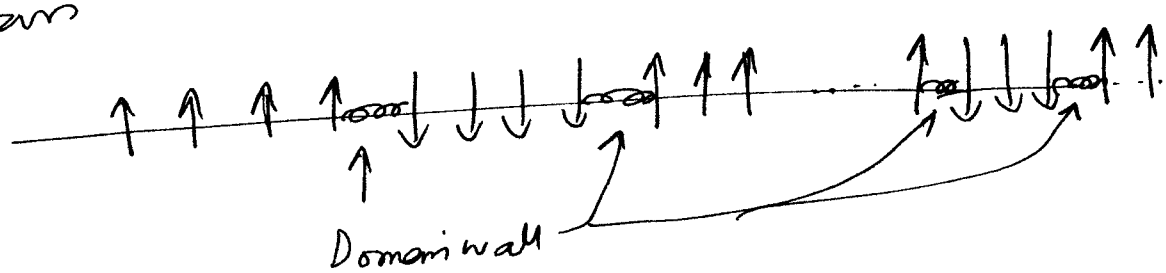
$$F = U - TS. = 2J - T \ln \frac{N(N-1)}{2}$$

$$\lim_{N \to \infty} = 2J - 2T \ln N.$$

$$= 2(J - T \ln N)!$$

We see that in the limit of $N \to \infty$ ~~at fixed $T > 0$~~ at fixed $T > 0$ (greater than zero), there

excitations are spontaneous! There is a lot of entropy gain by having such excitations, and the system will choose to proliferate them. ~~Note that~~ If this argument can be made more precise by noting the two such excitons

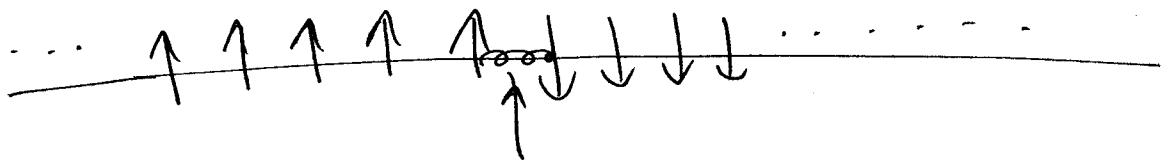


The free energy is

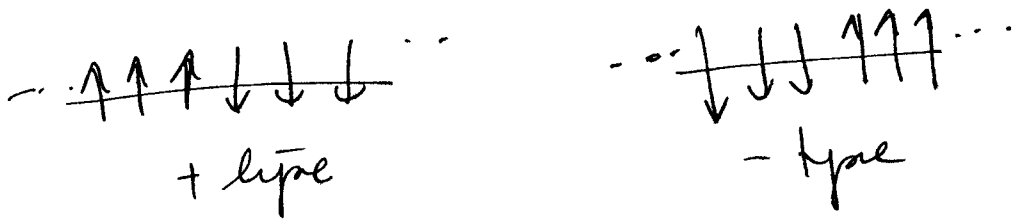
$$F \sim 4J - 4\bar{T}\ln N!$$

and thus the energy cost goes linearly in the number of excitons, while the entropy gain also goes linearly, but with a coefficient that depends on the system size. We thus see that these excitons will proliferate and hence the $T=0$ ferro state will be destroyed. Note that the last argument follows from the fact that the excitations There is one other subtle point to be noted. We started with Ising, that the excitons are single spin flips. But in the thermodynamic

limit $N \to \infty$, the lowest energy excitation is a domain wall



which has energy J. and a degeneracy of N (since periodic boundary conditions). Thus we see that every spin flip can be thought of as a combination of two kinds domain walls. that are an adjacent kinds. Note two additional parts: The bonds. Note two additional parts: The domain wall is an "emergent" excitation in the sense that we need the full spin configuration to check for the presence of domain walls. → it is "many body". Note also that there are two types of domain walls the + type and - type



+ type

- type

A creature living in the 1D Ising ferromagnet will describe the world as having + type and - type particles! They attract each other!

This looks awfully like what we see in electrostatics! Could it be that the electric charge is some kind of an excitation of some "fundamental" field? Intriguing indeed, but let us come back to planet earth!!

The exact solution: Actually it turns out that we can obtain the exact free energy of the Ising model.

Note that

$$Z = \sum_{\{s_i\}} e^{+\frac{J}{T}\sum_i s_{i+1}s_i}$$

~~Note the~~ Now the partition function is determined only by the link variable

λ_i (lambda, l-for link) $\lambda_i = s_{i+1}s_i = \pm 1$ ← allowed values

We have $\prod_{i=1}^{N} \lambda_i = 1$

which is a constraint on the link variable.

Now If λ_i's are specified, then ~~does~~ determines two spin configurations

$$s_i = \left(\prod_{j=1}^{i} \lambda_j\right) s_0$$

So can be ± 1 so, this means that each of $\{\lambda_i\}$ [(N-1) independent] defines two independent spin configuration. [Note $2^N = 2^{N-1} \cdot 2$]

We thus get

$$Z = 2 \sum_{\{\lambda_i\}}^{1} e^{\frac{J}{T}\sum_i^1 \lambda_i}$$

Let us choose open instead of the periodic boundary condition, then there are N-1 independ λ_i s. We get

$$Z = 2\left[2\cosh\frac{J}{T}\right]^{N-1}$$

Thus the free energy density is

$$\frac{F}{N} = -\frac{1}{N}\ln 2 - T \ln\cosh\left(\frac{J}{T}\right).$$

Note that this is an analytic function of temperature and hence there is no finite T phase transition in the 1D ising model. There is, however, a phase transion at $T=0$(!) due to the non-analyticity.

This exactly corroborates with what we found by physical arguments. At $T=0$, there is symmetry breaking, but it is restored as at any finite temperature however small! (The stated result is true in the thermodynamic limit)

We will now explore further into the state of the Ising model in 1d at finite temperature. Suppose we ask what is the spin correlation $\langle S_{i+n} S_i \rangle$, we will find it quite difficult to calculate using the link variables λ_i. Instead, we will use a beautiful trick invented by Kramers and Wannier called the transfer matrix method.

To see what this is, we also introduce a uniform magnetic field h. utility

$$H = -J \sum_i S_{i+1} S_i - h \sum_i S_i$$

The last term is rewritten as

$$H = -J \sum_i S_{i+1} S_i - \frac{h}{2} \sum_i (S_{i+1} + S_i)$$

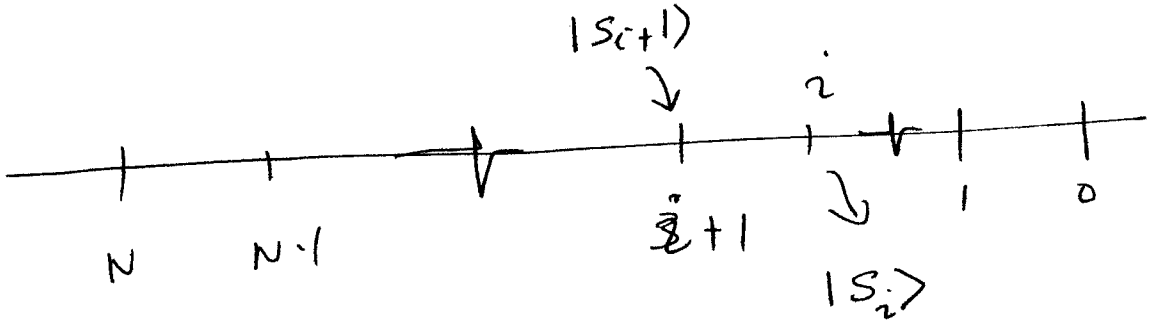
Now

$$Z = \sum_{\{S_i\}} e^{\sum_i \left[\frac{J}{T}(S_{i+1}S_i) - \frac{h}{2}(S_{i+1}+S_i)\right]}$$

$$= \sum_{\{S_i\}} \prod_i \left[e^{\frac{J}{T}(S_{i+1}S_i) - \frac{h}{2T}(S_{i+1}+S_i)} \right]$$

$$\prod_i (i)$$

↳ elements of a matrix



Now introduce two states $|S_i\rangle$ at each site.

$|S_i\rangle \begin{cases} |\uparrow\rangle_i \\ |\downarrow\rangle_i \end{cases}$

The terms or $\Pi(i)$ are

$$\langle S_{i+1} | \mathbf{T}(i) | S_{i+1} \rangle$$

$$\Pi(i) = e^{\frac{J}{T}(\sigma^z_{i+1}\sigma^z_i) - \frac{h}{2T}(\sigma^z_{i+1}+\sigma^z_i)}$$

We then see that

$$Z = \sum_{\{S_i\}} \langle S_{i+1} | T(i) | S_i \rangle.$$

Which when written out explicitly gives

$$Z = \sum_{\{S_i\}} \langle S_0 | T(N-1) | S_{N-1} \rangle \langle S_{N-1} | T(N-2) | S_{N-2} \rangle \ldots \langle S_{i+1} | T(i) | S_i \rangle \ldots \langle S_1 | T(0) | S_0 \rangle$$

Thus summing over the spin configuration, noting that all $T(i)$s are the same gives,

$$Z = \sum_{S_0} \langle S_0 | T^N | S_0 \rangle = \text{trace} T^N !$$

$$\tilde{J} = \frac{J}{T}$$

Now
$$T = \begin{bmatrix} e^{\tilde{J}+\tilde{h}} & e^{-\tilde{J}} \\ e^{-\tilde{J}} & e^{\tilde{J}-\tilde{h}} \end{bmatrix} \qquad h = \frac{h}{T}$$

How do we calculate the trace of T^N?

Well we note that T is a real symmetric matrix. So it can be diagonalized

$$T \; U = U V$$

U orthogonal matrix

V diagonal matrix of Eigenvalues.

We can easily find U and V.

First let us find V

$$V = \begin{pmatrix} v_1 & \\ & v_2 \end{pmatrix} \qquad v_{1,2} = e^{\tilde{J}} \cosh(\tilde{h}) \pm \sqrt{e^{2\tilde{J}} \sinh^2 \tilde{h} + e^{-2\tilde{J}}}$$

Note $v_{1,2} > v_2$

and $$U = \begin{bmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix}$$

where $\tan\theta = e^{-2\tilde{J}} / \sinh\tilde{h}$

Rough work (Ignore)

$B_z = e^{\tilde{J}} \sinh\tilde{h}$

$B_x = e^{-\tilde{J}}$

$\tan\theta = e^{2\tilde{J}} / \sinh\tilde{h}$

Thus $$Z = \mathrm{Tr}\, T^N$$

$$= v_1^N + v_2^N$$

$$= v_1^N \left(1 + \left(\frac{v_2}{v_1}\right)^N\right)$$

Since $v_2 < v_1$ in the thermodynamic limit we get

$$Z = \left[e^{\tilde{J}} \cosh(\tilde{h}) + \sqrt{e^{2\tilde{J}} \sinh^2 \tilde{h} + e^{-2\tilde{J}}} \right]^N$$

When $\tilde{h} = 0$

$$Z = \left[2 \cosh \tilde{J} \right]^N$$

$$\Rightarrow F = -NkT \ln\left(2 \cosh\frac{J}{T}\right)$$

You might say what is new here! Well this trick allows us to calculate many things for example

$$\langle S_i \rangle = \sum_{\{S_i\}} T(i+1) \cdots$$

$$= \frac{1}{Z} \sum_{\{S_i\}} e^{\tilde{J}(S_N S_{N-1}) + \frac{\tilde{h}}{2}(S_N + S_{N-1})} \cdots e^{\tilde{J}(S_{i+1} S_i) + \frac{\tilde{h}}{2}(S_{i+1} + S_i)} S_i$$

$$= \frac{1}{Z} \mathrm{tr}\left[T(N-1) \cdots T(i+1)\, T(i)\, \sigma_z\, T(i-1) \cdots \right]$$

$$= \frac{1}{Z} \mathrm{tr}\left[T^{N-i}\, \sigma_z\, T^{i} \right] = \mathrm{tr}\left[\sigma_z T^N \right].$$

Similarly

$$\langle S_{i+n} S_i \rangle = \frac{1}{Z} \mathrm{tr}\left[T^{N-(i+n)}\, \sigma_z\, T^{n}\, \sigma_z\, T^{i} \right]$$

$$= \frac{1}{Z} \mathrm{tr}\left[\sigma_z T^n \sigma_z T^{N-n} \right].$$

Now

$$\mathrm{tr}\left[\sigma_z T^N \right] = \mathrm{tr}\left[U^{\dagger} \sigma_z U V^N \right]$$

$$= \mathrm{tr}\left[\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \begin{pmatrix} z_1^N & 0 \\ 0 & z_2^N \end{pmatrix} \right]$$

$$\mathrm{tr}\begin{bmatrix} \cos\theta\, v_1^N & + \sin\theta\, v_2^N \\ \sin\theta\, v_1^N & - \cos\theta\, v_2^N \end{bmatrix}$$

$$\langle S_i \rangle = \frac{1}{Z} \cos\theta \left(v_1^N - v_2^N \right)$$

$$N \to \infty \Rightarrow \quad \cos\theta = \cos\left[\tan^{-1}\left[e^{2\tilde{J}} / \sinh\tilde{h} \right] \right]$$

Now

$$\langle S_{i+n} S_i \rangle = \frac{1}{Z} \mathrm{tr}\left[\begin{bmatrix} \cos\theta\, v_1^n & \sin\theta \\ \sin\theta\, v_1^n & -\cos\theta\, v_2^n \end{bmatrix} \begin{bmatrix} \cos\theta\, v_1^{N-n} & + \sin\theta\, v_1^{N-n} \\ \sin\theta\, v_1^{N-n} & -\cos\theta\, v_2^{N-n} \end{bmatrix} \right]$$

$$= \frac{1}{Z} \mathrm{tr}\begin{bmatrix} \cos^2\theta\, v_1^N + \sin^2\theta \left(\frac{v_2}{v_1}\right)^n v_1^N & \text{Shift} \\ \text{Shift} & \sin^2\theta\, v_2^{N-n} v_1^n + \cos^2\theta\, v_2^N \end{bmatrix}$$

↳ Subleading.

$$\lim_{N\to\infty} \langle S_{i+n} S_i \rangle = \cos^2\theta + \sin^2\theta \left(\frac{v_2}{v_1}\right)^n$$

$$\text{Now } \langle \delta S_{i+1} \delta S_i \rangle = \langle S_{i+n} S_i \rangle - \langle S_{i+n} \rangle \langle S_i \rangle$$

$$= \sin^2\theta \left(\frac{v_2}{v_1}\right)^n .$$

Let we put $\tilde{h} = 0$, we get

$\theta = \frac{\pi}{2}$, and $\frac{v_2}{v_1} = \tanh \tilde{J}$

$\Rightarrow \langle \delta S_{i+n} \delta S_i \rangle = e^{-n/\xi} \Rightarrow \xi = \left[\ln \left[\frac{v_1}{v_2}\right]\right]^{-1}$

ξ is the correlation length defined as

$$\xi = \left[\ln \frac{1}{\tanh \tilde{J}}\right]^{-1}$$

When $T \to 0$ $\tilde{J} \to \infty$ and $\xi \to \infty$.

The approach to $T=0$, and the rentlig broken symmetry phase are signalled by a divergent correlation length.

What happen in the opposite limit, i.e. when $T \to \infty$? When $\tanh \tilde{J} \simeq$

For large $\tilde{J}$ $\tanh \tilde{J} \simeq 1 - e^{-2\tilde{J}}$

$\Rightarrow \frac{1}{\tanh \tilde{J}} = 1 + e^{-2\tilde{J}}$

$\Rightarrow \ln \left[1 + e^{-2\tilde{J}}\right] \simeq e^{-2\tilde{J}}$

$\Rightarrow \xi \sim e^{2J/T}$.

Ising model on a square lattice

We will now expand into the second dimension, i.e, move to d=2, and consider a nice square lattice.

Key question is regarding the phase diagram in the T-h plane which we have been chasing. As usual the strategy will be to start with a point we know, i.e, the T=0 and h=0 point where we know that the state is the grand state where all the spins are pointing up:

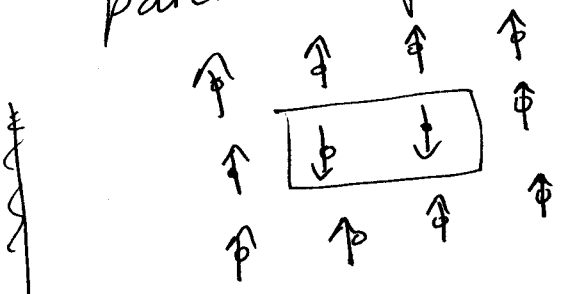
$$H = -J \sum_{\langle ij \rangle} s_i s_j$$

(Ferromagnetic state M=1)

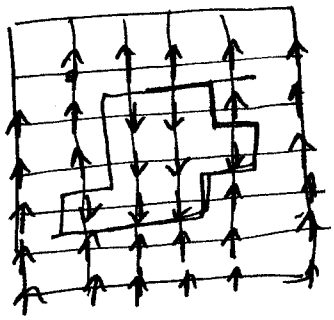
Now we ask what are the excitations of the system, and do they reduce M?

Now it is easy to see that the excitations are "patches" of down spins

For example,



We will now find a way to characterize these excitons. Generically, these domain ~~can~~ of ↓ spins ~~the~~ can be characterized by its boundary, the domain wall. The length of the domain wall is the number of broken bonds, and is characterized by a number ℓ.



(The figure shows a configration with $\ell = 14$)

The smalest value of $\ell = 4$ which breaks four bonds. Now given ℓ, the energy of the configuration is completely specified. this (relative to the ground state) is.

$$E(\ell) = 2J\ell.$$

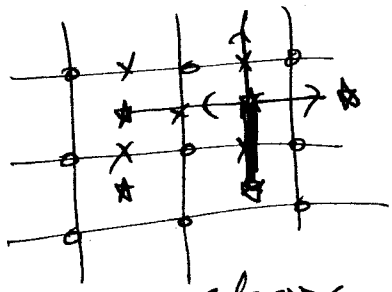
Now two points are to be observed.

1. If I have a domain of length ℓ, then the number of spins flipped is proportial to the area A of the domain. But the area is bonded by the perimeter $A \leq \frac{\ell^2}{4}$

Thus a domain with perimeter ℓ can ~~be~~ reduce the magnetization at most by $\ell^2/4$; $\Delta M \leq \frac{\ell^2}{4}$

How many ways are there for a domain of perimeter ℓ to form. $\Rightarrow \Omega(\ell)$

Well, we need to pick ℓ bonds that are connected

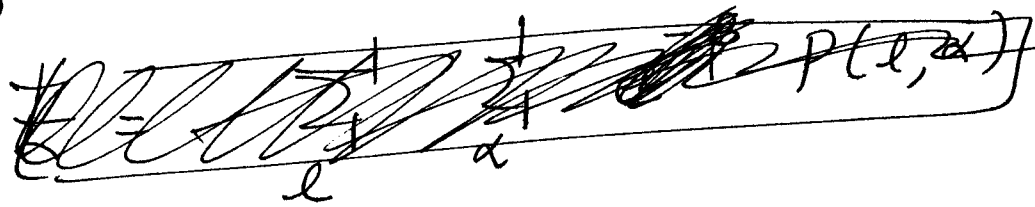


The first bond can be chosen in $2N$ ways. How do we choose the next $\ell-1$? A bond connects the ★s in the picture. For one ★ there are three possible ways of choosing the next star. This gives

$$\Omega(\ell) \leq 2N\, 3^{\ell-1}$$

Why is there a "$\leq$"? This is because we have to ensure that the loop returns back where it started. Thus the number of possibilities are bounded by $\Omega(\ell)$. But this is not a problem for us in that we are <u>overcounting</u> the number of ways in which the order can be destroyed - and if the magnetization still survives, then we can be sure that we are okay! This is also an example of estimates and bounds that are frequently used in statmech (& hard problems)

Alright! So, we now write



Now we have

$$Z = \sum_{\ell}^{1} \sum_{\alpha}^{1} e^{-\beta 2 J \ell} > 1$$

where α runs over all configurations in $\Omega(\ell)$

Now, the expected value of number of down spins is $\langle N_\downarrow \rangle$

$$\langle N_\downarrow \rangle \leq \sum_{\ell}^{1} \sum_{\alpha}^{1} \frac{\ell^2}{4} P(\ell,\alpha)$$

where $P(\ell,\alpha) = \dfrac{e^{-\beta 2 J \ell}}{Z} \leq e^{-2\beta J \ell}$

$$\langle N_\downarrow \rangle \leq \sum_{\ell}^{1} \sum_{\alpha}^{1} \frac{\ell^2}{4} e^{-\frac{2J}{T}\ell}$$

$$\leq \sum_{\ell}^{1} \frac{\ell^2}{4} \Omega(\ell)\, e^{-\frac{2J}{T}\ell}$$

$$\leq \sum_{\ell}^{1} \frac{\ell^2}{4} e^{-\left(\frac{2J}{T} - \ln 3\right)\ell}$$

$$\langle N_\downarrow \rangle \leq \sum_{\ell=4,6\ldots}^{N} \ell^2 e^{-\xi \ell}$$

define $\xi = \dfrac{2J}{T} - \ln 3$

$$\langle N_\downarrow \rangle \leq \frac{N}{6} e^{-4\xi} \sum_{m=0,\ldots}^{1} (2m+4)^2 e^{-2\xi m}$$

$$\leq \frac{N}{6} e^{-4\xi} \sum_{1}^{1} (4m^2 + 16m + 16) e^{-2\xi m}$$

$$\leq \frac{N}{6} e^{-4\xi} \left[4 \left| \frac{1 - 3e^{2\xi} + 4e^{4\xi}}{(e^{2\xi} - 1)^3} \right| \right]$$

$$\xi = \frac{2J}{T} - \ln 3, \quad \text{as} \quad T \to 0,$$

The above goes to

$$\langle N_\downarrow \rangle \leq \frac{2N}{3} \times 4 e^{-6\left(\frac{2J}{T} - \ln 3\right)}$$

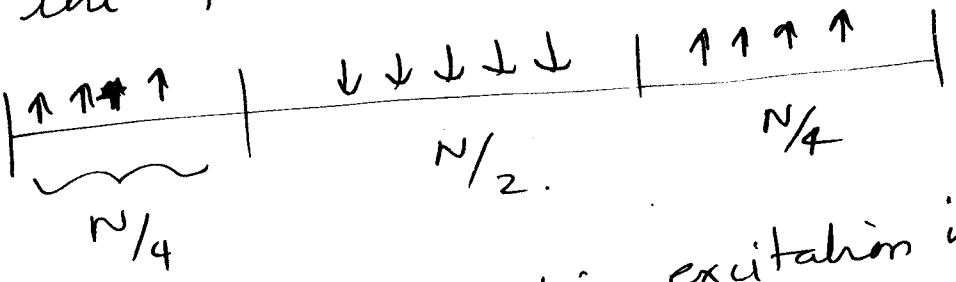
$$\Delta M = \frac{\langle N_\downarrow \rangle}{N} \leq 8 \times 3^5 \times e^{-\frac{12J}{T}} << 1/2$$

Thus ΔM ~~can be made~~ $T << J$ is indeed small. The argument due to Peierls now shows that in 2-d the Ising model should have an ~~phase~~ ordered phase at low ($T << J$) temperatures. This implies a possible phase transition, since one can argue similarly that a $T >> J$, there is no order.

So what changed when we went from

$d=1 \rightarrow d=2$.

Consider the following excitons that produce zero total magnetism



The energy cost of this excitation is $2J$ and does not scale with the size of the system! There is a large entropy associated with these excitations and they proliferate to destroy the order.

The story changes in 2d., the energy of the excitation also scales with system size (i.e. for excitons that have total spin 0), $E \sim J\sqrt{N/2}$,

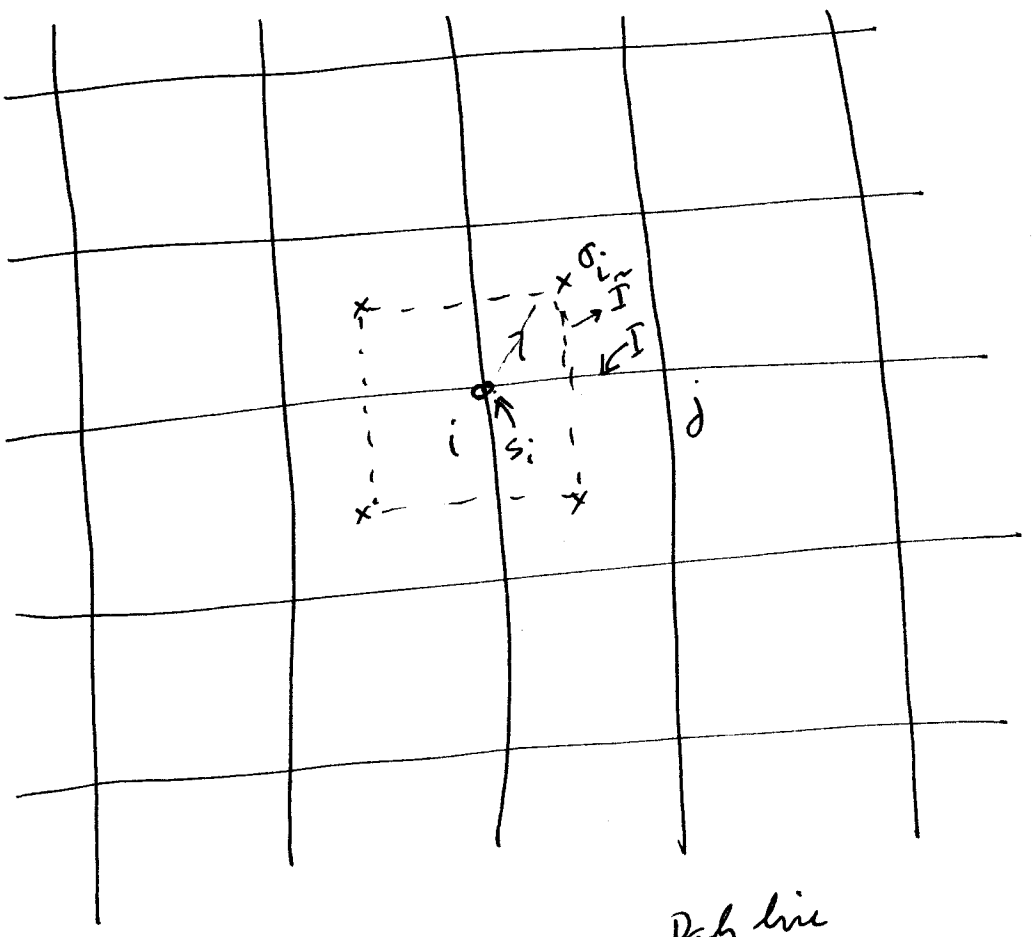
while the entropy goes as N^2

Now we see that the exponential energy penalty kills such excitations and this is what gives an order at low temperatures!

We can do even better, if we follow Kramers & Wannier

After Peierls showed that order is possible in the 2d Ising model (square lattice), Kramers and Wannier followed up with a beautiful result — the calculation of the T_c — without actually calculating it! This work introduced a key idea — the idea of duality and dual models. Let us walk through the derivation of Kramers and Wannier's

$$H = -J \sum_{\langle ij \rangle}^{1} S_i S_j$$



Solid line - lattice, ---- Dash line dual lattice

From here onward J stands for $\bar{J}/T$.

$$Z = \sum_{\{S_i\}} e^{\bar{J}\sum_{\langle ij\rangle} S_i S_j} = \sum_{\{S_i\}} \prod_{\langle ij\rangle} e^{J S_i S_j}$$

Now we notice that

$$e^{J S_i S_j} = \cosh J + S_i S_j \sinh J.$$

Let us introduce the link variable λ_I (I denotes the bonds B, going from 1, 2N)

Now what we do is we define a new variable

~~$\alpha_I \quad \frac{1}{2}(1-\lambda_I) = \begin{cases} 0 & \lambda_I = 1 \\ 1 & \lambda_I = 0 \end{cases}$~~

~~Here we consider~~

~~$e^{J\lambda_I} = \cosh J + (S_i S_j) \sinh J$~~

α_I which goes from on 0, 1 (annoli variable related to ~~$\frac{1}{2}(1-\lambda_I)$~~ and write

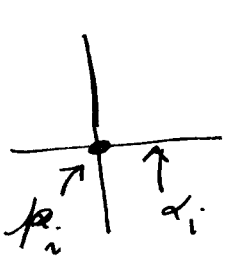
$$e^{J S_i S_j} = \sum_{\alpha_I=0}^{1} f_{\alpha_I} (S_i S_j)^{\alpha_I}$$

$$f_0 = \cosh J$$

$$f_1 = \sinh J.$$

$$Z = \sum_{\{S_i\}} \prod_{\substack{\langle ij\rangle \\ \equiv I_j}} \sum_{\alpha_I}^{1} f_{\alpha_I} (S_i S_j)^{\alpha_I}$$

$$Z = \sum_{\{\alpha_I\}}' \left(\prod_I f_{\alpha_I} \right) \sum_{\{s_i\}}' \prod_I (s_i s_j)^{\alpha_I}$$



$$\sum_{\{\alpha_i\}}' \prod_I f_{\alpha_I} \qquad \sum_{\{s_i\}}' \prod_i (s_i)^{p_i}$$

where $p_i = \sum_{I/i}' \alpha_I$ $\quad I/i$ means the i is an end of the bond I.

Note that there are ~~N, α_i vars~~ $2N$ α_I variables.

We can now perform the sum over s_i

$$\sum_{\{\alpha_I\}}' \left(\prod_I f_{\alpha_I} \right) \prod_i \left(1 + (-1)^{p_i} \right)$$

which is zero if any p_i is odd!

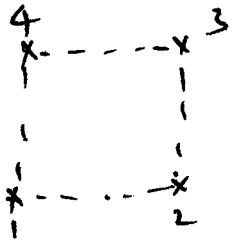
So all the α_I are not indepnd $\sum_{I/i}' \alpha_I$ must be divisible by 2. $\forall i$. This gives N Contradtn. hence there are only n Indepnd αs.

Thus

$$Z = 2^N \sum_{\{\alpha_I\}}' \prod_I f_{\alpha_I}$$

where $\sum_{I/i}' \alpha_I$ must be even $\forall i$

Now how do we implement this constraint? Here is a brilliant observation. Look at the figure on page 54. Define a dual lattice by the crosses shown, and put ising spin variable σ_i on these sites: Now make



the following observation. If 1, 2, 3, 4 are sites on the plaquette,

$$\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_4\sigma_1 \text{ is divisible}$$

by 4! We can check this very easily.

Now define the link variables μ_I associated with the dual lattice $\mu_I = \sigma_i\sigma_j$

~~Note~~ Now define

$$\alpha_I = \frac{1}{2}(1-\mu_I)$$

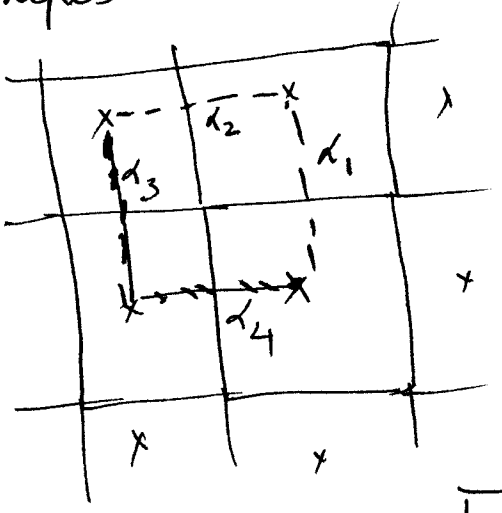
Note that α_I now satisfies the constraint

$$\gamma_i = \sum_I \alpha_I \text{ is}$$

$$= 2 - \frac{1}{2}\sum_I \mu_I.$$

$\sum_I \mu_I$ is divisible by 4

$\Rightarrow \gamma_i$ is divisible by 2!



Now,

$$Z = 2^N \sum_{\{\alpha_I\}} \prod f_{\alpha_I} \qquad \sum_i \alpha_i = \text{even}$$

$$= 2^N \sum_{\{\mu_I\}} \left(\prod f_{\alpha_I} \right)$$

↑ expression in terms of μ_I

↑ no constraint! (but 2N variables)

$$f_{\alpha_I} = (1-\alpha_I)\cosh J + \alpha_I \sinh J$$

$$= \frac{1}{2}(\mu_I + 1)\cosh J + \frac{1}{2}(1-\mu_I)\sinh J$$

$$= \frac{1}{2}\left(e^J + e^{-J}\mu_I\right)$$

Now we can define a new quantity J^* such that

$$f_{\alpha_I} = e^J\left(1 + \tanh J^* \mu_I\right)$$

$$e^{-2J} = \tanh J^*$$

$$e^J = \frac{1}{\sqrt{\tanh J^*}}$$

$$f_{\alpha_I} = \frac{1}{2\cosh J^* \sqrt{\tanh J^*}} \left(\cosh J^* + \mu_I \sinh J^*\right)$$

$$= \frac{1}{\sqrt{2\sinh(2J^*)}} \left(\cosh J^* + \mu_I \sinh J^*\right)$$

$$\Rightarrow Z = \frac{2^N}{\left(\sqrt{2\sinh 2J^*}\right)^{2N}} \sum_{\{\mu_I\}} \prod_I \left(\cosh J^* + \mu_I \sinh J^*\right)$$

But note that $\{\mu_I\} \Rightarrow$ half the sum of $\{\sigma_i\}$ dual!

$$\Rightarrow Z = 2^N \frac{1}{2} \frac{1}{(\sinh 2J^*)^N} \sum_{\{\sigma_i\}} \prod_{\langle ij \rangle} \left(\cosh J^* + \sigma_i \sigma_j \sinh J^*\right)$$

$$= \frac{1}{2} \frac{1}{(\sinh 2J^*)^N} \sum_{\{\sigma_i\}} \prod_{\langle ij \rangle} e^{J^* \sigma_i \sigma_j} !$$

which is an Ising model with coupling J^* ! ! ! !

To see the physics put T back.
What we see is that [Change in NOTATION)

$$e^{-2J/T} = \tanh\left(\frac{J}{T^*}\right)$$

Correct

Thus the ising model on one lattice is DUAL to the Ising model on the dual lattice

Note as $T \to \infty$, $T^* \to 0$ and and vice versa! Now at T_c, $T = T^* = T_c$!! At T_c the model is self dual.

$$e^{-2J/T_c} = \frac{1 - e^{-2J/T_c}}{1 + e^{-2J/T_c}}$$

$$\Rightarrow \quad (1 + e^{-2J/k_c})(1 + e^{-2J/k_c}) = 1 - e^{-2J/k_c}$$

$$* \quad x^2 + 2x - 1 = 0 \Rightarrow x = \frac{-2 \pm \sqrt{4+4}}{2}$$

$$\sqrt{8} - 2$$

$$\Rightarrow J/T_c = -\frac{1}{2} \ln\left[\frac{\sqrt{2}-1}{1}\right]$$

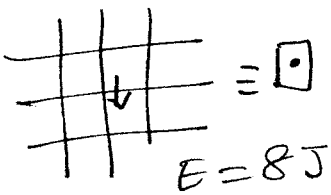
$$= \frac{1}{2} \ln\left(\frac{1}{\sqrt{2}-1}\right) = \frac{1}{2} \ln\left(\frac{\sqrt{2}+1}{2}\right)$$

Having seen the duality argument which predicts a phase transition for the 2-d Ising model, we now use the opportunity to understand this idea, even while learning some calculational technique. This is called "series expansion." Virial expansion is also a type of series expansion which we have already seen. The idea of any series expansion is to start from a state that we know an exact solution for, and identify a "small parameter". One then expands the partition function (or something related) in a series in the "small parameter." While the techniques and ideas that we will develop have wide applicability, we will focus on the 2-d square lattice Ising model.

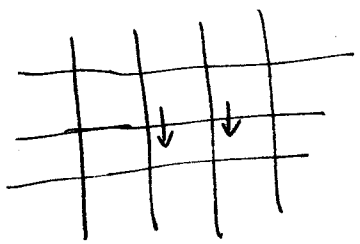
Low temperature expansion:

We know that the ground state at $T=0$, is the fully polarized state of all up (or down) spin. As we have seen before, the excitations are spin flips.

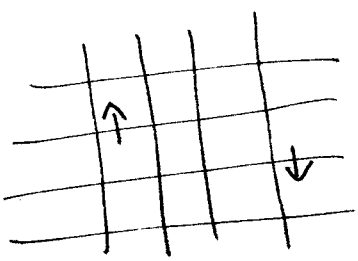
The ground state energy can be taken to be zero. With respect to this, the first excited state is a single spin flip with energy $8J$ (since it breaks 4 bonds). This state is N fold degenerate. (N)



What is the next excited state; this will, of course, have two spin flips. But there are two types of configurations possible with two spin flips one is where the spins are adjacent while the other is when the ~~spins are~~ sits are unconnected



or



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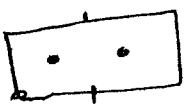


≡

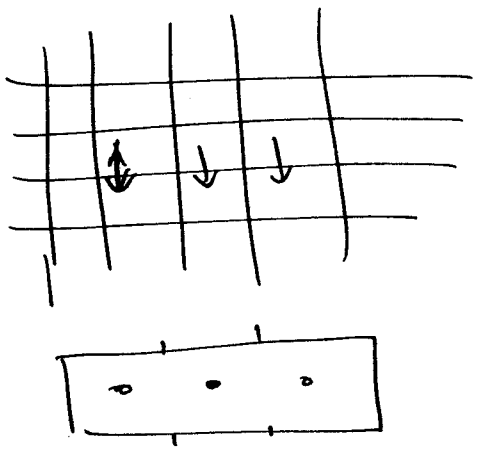
$E_{2nn} = 12J$

$Degen = 2N$

$E_{nnn} = 16J$

$Degen = \frac{N(N-5)}{2}$

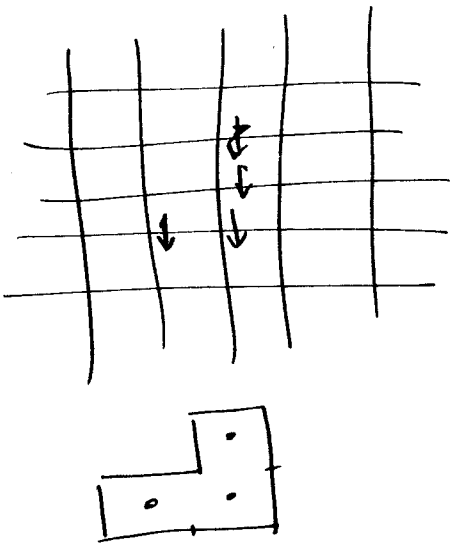
What about the next excited state? Well there will be three spin flips. And there will be three types of configs.



~~2N~~

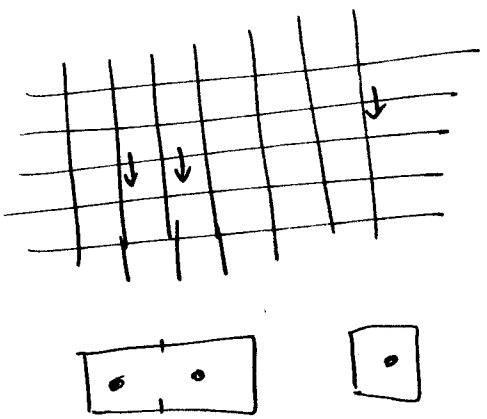
Energy 16 J

Degen = 2N



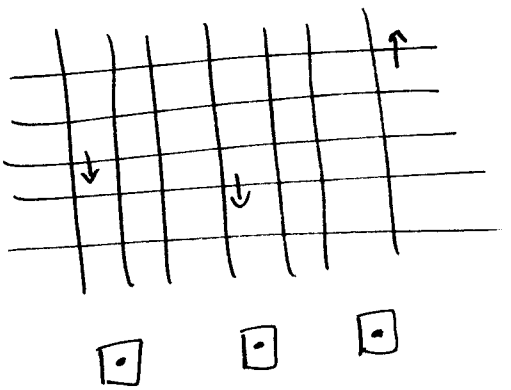
Energy 16 J

Degen = 4N.



E = 20 J

D = 2N × (N-8)



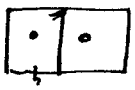
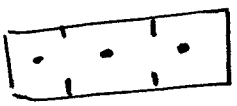
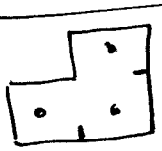
E = 24 J

$$D = \frac{N[4(N-17) + (N-13)(N-14)}{6}$$

~~Let us collect all this into a table~~

One can go on with this. The key observation is that for energy N_f spin flips there are "connected" and "disconnected" configurations. Connected configurations are "lower order" make up the disconnected configurations of the higher order. Let us tabulate our findings

connected or Disconnected

N_f	Config	Type	Energy	Degen
1		C	8J	N
2		C	12J	2N
		D	$2\times 8J = 16J$	$\frac{N(N-5)}{2}$
3		C	16J	2N
		C	16J	4N
		D	20J	$2N(N-8)$
		D	24J	$\frac{N(4(N-11)+(N-13)(N-8))}{6}$

Note that all connected diagrams always have degeneracy proportional to N. This is crucial to We now have all that we need to expand the partition function.

$Z = \sum_k$

$$Z = 1 + N \times \square + (2N) \begin{array}{|c|c|}\hline \cdot & \cdot \\ \hline \cdot \\ \cline{1-1} \end{array} + \frac{N(N-5)}{2} (\square\square)$$

$$+ 2N \left(\begin{array}{|c|c|c|}\hline \cdot & \cdot & \cdot \\ \hline \cdot \\ \cline{1-1} \end{array} \right) + \cdots .$$

Well what have we achieved? Nothing much! Let us look at the free energy

(Note that $\square \equiv e^{\text{energy of diagram}}$)

$$-\beta F = \ln Z$$

$$-\beta F = \ln \left(1 + N \times \square \cdots \right)$$

Use $\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} \cdots$

Now

$$-\beta F = \left(N \times \square + 2N \left(\begin{array}{|c|c|}\hline \cdot & \cdot \\ \hline \cdot \\ \cline{1-1} \end{array} \right) + \frac{N(N-5)}{2} (\square\square) \right)$$

$$+ \frac{1}{2} \left(N \times \square + 2N \left(\begin{array}{|c|c|}\hline \cdot & \cdot \\ \hline \cdot \\ \cline{1-1} \end{array} \right) + \cdots \right)^2$$

Note that there is something funny here. If we keep only terms to order x, we are in trouble! Reason is that $\frac{F}{N}$, i.e. free energy per site, and should be independent of N!

But all is not lost! Some thing remarkable happens.

Conder the ~~lorem~~ term $-\frac{1}{2}\left[N \times \boxed{\cdot} + \dots\right]^2$

This gives $-\frac{N^2}{2}\left(\boxed{\cdot} \times \boxed{\cdot}\right)$. Note that this term cancels the ~~disconn~~ N^2 in the disconnected terms $\frac{1}{2}$ at order x^1.

This is actually a quite general result, and is related to something called the linked cluster theorem. ~~It~~ In essence the higer powers of N are precisely cancelled by higer order ~~term~~ disconnected terms.

$$-\beta f = N\boxed{\cdot} - \frac{5N}{2}\left(\boxed{\cdot}\,\boxed{\cdot}\right) + 2N\left(\boxed{\cdot\!\!-\!\!\cdot}\right) \dots$$

The main messge so fare are

(1) There is a systematic way to obtain free energy expansions in term of digrams representy excitations.

(2). We have seen an idea that connected digrams are the key — linked cluster theorm

(3) Although we have not yet seen this these techniques can be used to estimate critical exponents.

High Temperature expansion

Let us now move to high temperature i.e $T \gg J$. What should be our exact solution here, and what should be our small parameter! One might be quite naturally tempted to use J/T as the small parameter. But it turns out that one can do something much smarter.

$$Z = \sum_{\{S_i\}} e^{\frac{J}{T}\sum_{\langle ij\rangle} S_i S_j}$$

$$= \left[\cosh \frac{J}{T}\right]^{2N} \sum_{\{S_i\}} \prod_{\langle ij\rangle} (1 + t\, S_i S_j).$$

$$t = \tanh\left(\frac{J}{T}\right) = \tanh \tilde{J}.$$

We will use t as the small parameter.

Now $$Z = \left[\cosh \tilde{J}\right]^{2N} \sum_{\{S_i\}} \prod_{I} (1 + t\, \lambda_I)$$

λ_I is the bond variable.

This expression naturally allows for a series expansion in powers of t

$$Z = [\cosh \tilde{J}]^{2N} \left(\sum_{\{S_i\}} \left(\sum_m t^m \mathcal{S}_m \right) \right)$$

where $$\mathcal{S}_m = \sum_{I_1 \neq I_2 \neq \cdots I_m} \mu_{I_1} \mu_{I_2} \mu_{I_3} \cdots \mu_{I_m}.$$

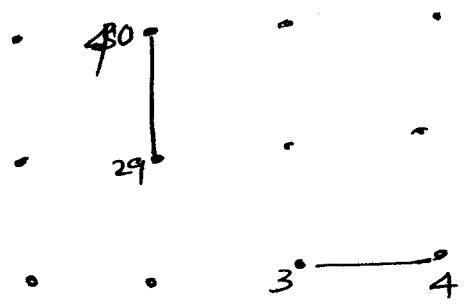
We can re arrange this as

$$Z = [\cosh \tilde{J}]^{2N} \left[\sum_m t^m \left(\sum_{\{S_i\}} \mathcal{S}_m \right) \right].$$

Now Consider $$\sum_{\{S_i\}} \sum_{I_1 \neq I_2 \neq I_m} \mu_{I_1} \cdots \mu_{I_m}$$

The key point is that each term of $\mathcal{S}_m$ has m bonds all of which are different. Such a term can be represented diagrammatically by drawing a solid line corresponding to the bond I_2

Consider a term that multiples t^2



Note the term is $S_{29} S_{40} S_3 S_4$.

Now when we sum over the spin carrying this term vanishes. Thus we see that there is no t^2 term!

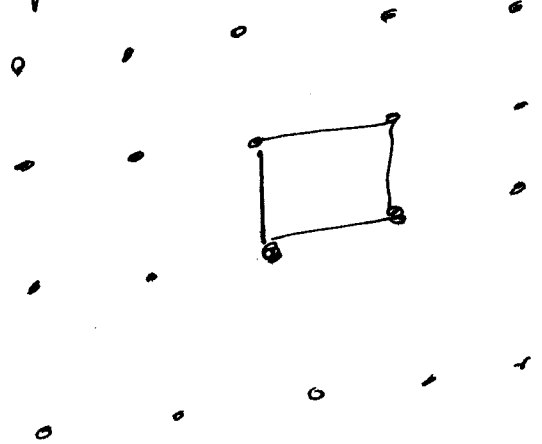
In fact there is no t^3 term aswell!

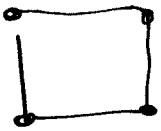
The first non trivial term is t^4.

Now for t^4 term there will several types of digram for $\mu_{I_1} \mu_{I_2} \mu_{I_3} \mu_{I_4}$.

The key thing is the only closed loops will produce non zero answers.

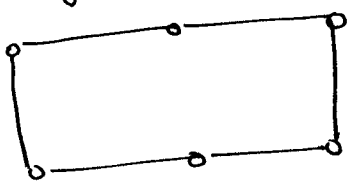
For example



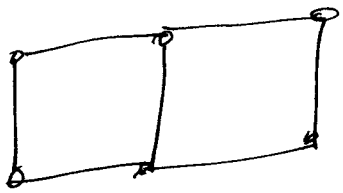
Now $\sum_{\{S_i\}}^{1}$  $= 2^N$.

Note that there are N such contrib-
utions
What happens at order t^5 → Nothing!
there is no contribution

At t^6 we get

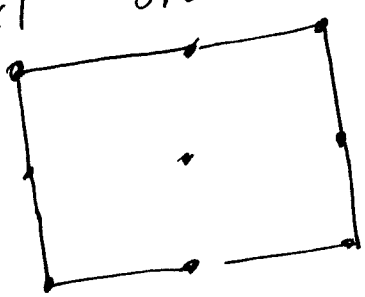
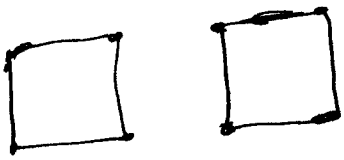


which again gives a factor of 2^N, and
there a 2N such terms.

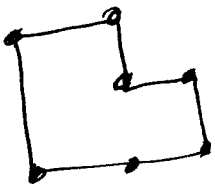
How about t^7, a diagram corresponding
to this is  $\leftrightarrow t^7$

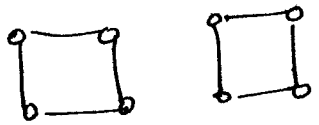
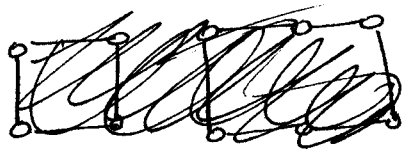
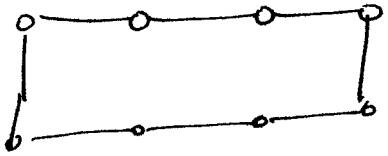
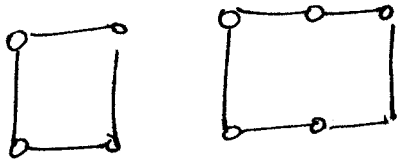
but a little thought will convince you that
this will give 0!

The next order is t^8, we have

 or 

↓ Disconnected

→ connected ↓ ↓ $N(N-5)$
N · or  $\frac{}{2}$

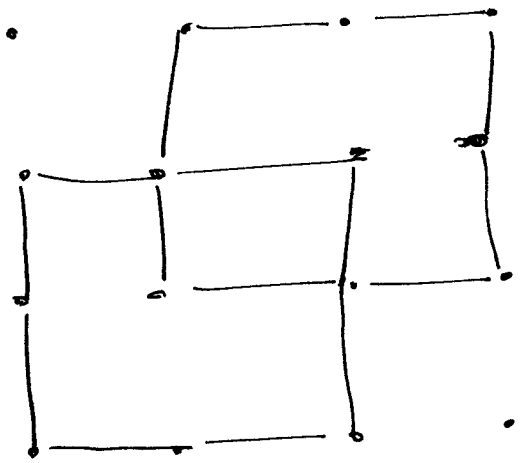
order	diagram	Type	Combinatoric factor
t^8		D &	$\frac{N(N-5)}{2}$
t^8	 	C	$2N$
t^{10}		D	$2N(N-8)$

$\therefore$ and so on.

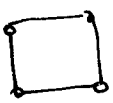
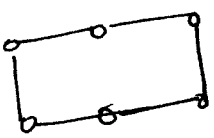
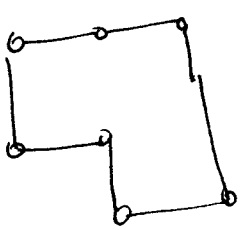
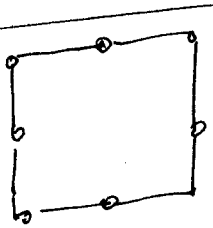
$$Z = (\cosh \tilde{J})^{2N} 2^N \Big[1 + N\Big(\square\Big) + 2N\Big(\square\!\square\Big) + 4N\Big(\square\!\square\Big) + N\Big(\square\!\square\Big) + \frac{N(N-5)}{2}\Big(\square\ \square\Big) + 2N\Big(\square\!\square\Big) + 2N(N-8)\Big(\square\ \square\Big) \cdots \Big]$$

This is the high temperature expansion. The free energy will again be correctly extensive by linked cluster theorem [72]

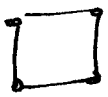
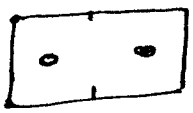
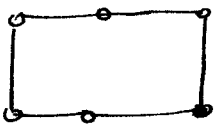
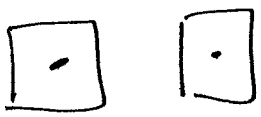
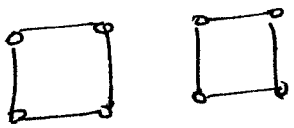
At higher orders we can get things like this



This is an allowed digram of order t^{16}.
But this is a disconnected digram as it is the product of connected ones at order t^8
Let us tabulate

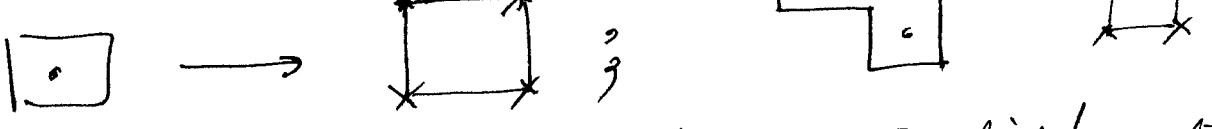
order	digram	Type	Combinatoric factor
t^4		C	N
t^6		C	2N
t^8		C	4N
		C	N

We now compare the the low and high temperate expansion, we suddenly see a beautiful correspondence

Low T	High T	Combinatoric factor
		N
		2N
		$\frac{N(N-5)}{2}$

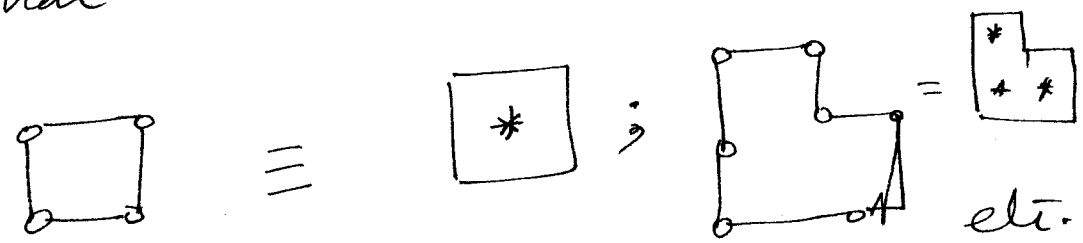
and soon!

We see that there is a 1-to-1 correspondence between the low and high temperate series! where $e^{-2\tilde{J}}$ corresponds to $\tanh \tilde{J}$! Now comes the key realization → the two temperate graphs can be put on the dual lattice



and this then <u>locks into</u> the high temperate

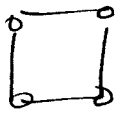
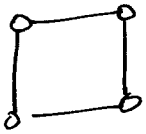
expansion of some other model.
If we define $\tanh \tilde{J}^* = e^{-2\tilde{J}}$
then the mapping is complete!
~~We can show that~~ We now also see that
one can view the high temperature
expansion as the low temperature of
the dual model!



This gives the relation

$$e^{-2\tilde{J}^*} = \tanh \tilde{J}$$

which is completely consistent with the
relationship found by mapping the low
temperature expansion to the high T of
the dual.
What this discussion allows us is to
understand duality in a "physical way".
Consider the high T expansion of the
original model. This is written in
terms of spin flips $\boxdot$. These can

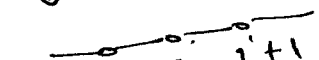
be viewed as "point defects" of the ordered phase. Proliferation (by thermal excitation) of these point defects is what destroys the order. Now look at the high temperature expansion. Terms like  are things that contribute to ordering! In other words the high T expansion looks at terms that are favoring the spins to order. Now here is the key connection a diagram like  which looks at "ordering" tendency of at high temperature is equivalent to  which is the defect of the dual! In other words "ordering in" the model is the defect of the dual model!" → to state this idea crudely but vividly! In fact this idea is a key one, and has been used in many other contexts. We hope to be able to see more examples of this as we go along in this course.

The Quantum Ising Model or The Transverse Field Ising Model (QIM/TFIM)

So far we have focused on phase transitions that are driven by external parameters such as Temperature. We will now see that phase transitions occur even at zero temperature. Such phase transitions are called quantum phase transitions since they are driven by quantum mechanics. We look at a concrete example for such a phase transition in some detail. We will see some remarkable facts, particularly related to the connections between quantum and classical problems.

The quantum problem we are interested in is called the quantum Ising model or the transverse field Ising model (TFIM). We will focus

on the 1-d chain (although the TFIM can be defined on any lattice). The Hilbert space of the system is spanned by $\prod_i |\alpha\rangle_i$ ← site label, $\alpha = \uparrow$ or $\downarrow$.



The Hamiltonian

$$H_{TFIM} = \underbrace{-J \sum_i^1 \sigma_{i+1}^z \sigma_i^z}_{H_J} \underbrace{- h \sum_i^1 \sigma_i^x}_{H_h}$$

where σ_i^z and σ_i^x are the usual symmetries, Note apart from the usual symmetries, the Hamiltonian has an Z_2 symmetry associated with spin rotation about the x axis.

$$U_x = e^{-i\frac{\pi}{2}\sum_i^1 \sigma_i^x} = \prod_i (-i)[\sigma^x]_i$$

It is customary to set $h = gJ$, the transverse magnetic field in dimensionless unit is g

$$H_{TFIM} = J\left[-\sum_i^1 \sigma_{i+1}^z \sigma_i^z - g\sum_i \sigma_i^x\right].$$

The question we ask is what is the ground state $|g\rangle$ of the system as a

function of g starting from $g=0$.
Let us consider two special cases.

① $\underline{g=0}$

Here the ground state is either $|g\rangle =$
$|F\rangle = |\uparrow\uparrow\uparrow\ldots\uparrow\rangle$ or $|\bar{F}\rangle |\downarrow\downarrow\downarrow\ldots\downarrow\rangle$
The ground state $\underline{\text{breaks}}$ Z_2 symmetry!

$$U_x |F\rangle = |\bar{F}\rangle$$
↳ upto a phase.

We can define an operator which measures an order parameter as

$$M \quad \frac{1}{N}\sum_i \sigma_i^z$$

and $M = \langle M \rangle = \langle F|M|F\rangle = 1$.

clearly indicating the broken symmetry.

In this limit $(J=0, h>0)$

② $\underline{g=\infty}$.

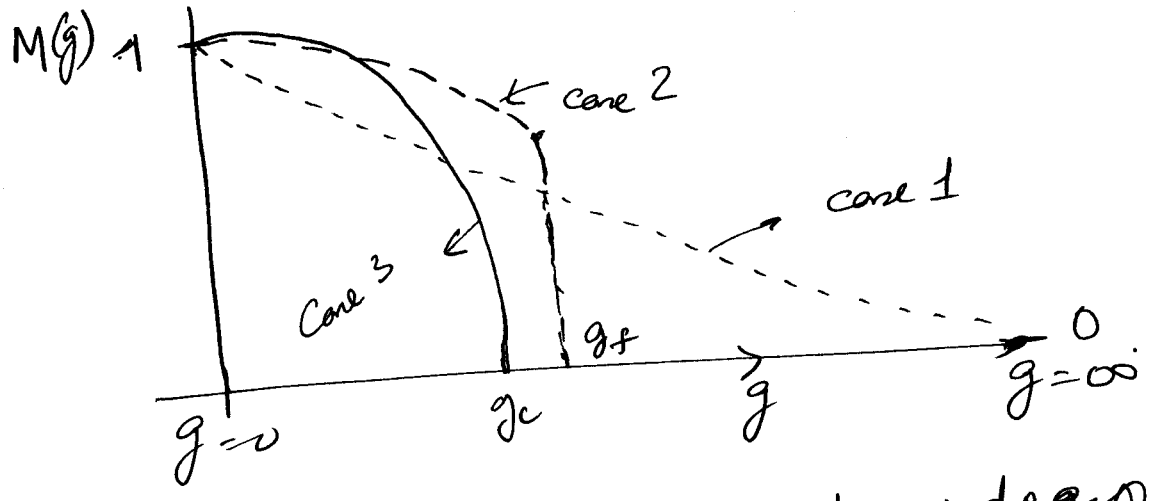
The ground state is

$$|g\rangle = |R\rangle = \prod_i \left(\frac{1}{\sqrt{2}}(|\uparrow\rangle_i + |\downarrow\rangle_i)\right)$$
$$= |\rightarrow\rightarrow\rightarrow\ldots\rightarrow\rangle.$$

$U_x |R\rangle = \underset{\text{phase}}{\uparrow} |R\rangle$ and hence $|R\rangle$ is Z_2 invariant!

and $\langle R|M|R\rangle = 0$.

We see that if we plot M as a function of g, $M(g) = \langle g|M|g\rangle$ where $|g\rangle$ is the ground state for g, then we know the answer at two points namely $g=0$, and $g=\infty$



Now we ask the question how does M(g) vary with g. There are three possibilities

Case 1: Smooth variation from $g=0$ to $g=\infty$. Nothing interesting happens.

Case 2: There is a sudden jump in M(g) at some g_f. This state to the ~~left~~ $g < g_f$ is Z_2 symmetry broken, while for $g > g_f$, there is Z_2 symmetry. If this is what happens,

this would be an example of a first order quantum phase transition

Case 3: $M(g)$ falls smoothly (continuously) and attains the value 0 at $g = g_c$. For $g > g_c$, $M = 0$ and ~~symmetric~~ state is Z_2 symmetric. This is an example of a continuous quantum phase transition, sometimes simply referred to as "quantum phase transition" and occurs at $g = g_c$.

Case 3 would be the most interesting case where we have a continuous change from a state of one symmetry to another by tuning the parameter in the Hamiltonian. In other words, this phase transition (as stated) is being brought about by quantum dynamics (Note $[H_J, H_h] = 0$)! This "entropy" has no role in this as this happens at $T = 0$.

Our goal is to find out which of these cases is realized in the TFIM.

How do we proceed? One way is what we did in the classical Ising model. ~~Stat~~ start with the known solution and walk "near" it to see what the state is for small excursions about the known solution.

Let us work at $g = \infty$.

Here the grand state is

$$|R\rangle = |\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rangle.$$

The fist excitied state is sp

$$|i\rangle = |\rightarrow\rightarrow\underset{i}{\leftarrow}\rightarrow\rightarrow\cdots\rangle$$

and is n fold degenerate

the energy of the state is $2h$ (compared to the grand state).

The seeond exciteed state is

$$|i,j\rangle = |\rightarrow\underset{i}{\leftarrow}\rightarrow\cdots\underset{j}{\leftarrow}\rightarrow\rangle.$$

with 2 $spinflips and this has energy $4h$.

We can tabulate these things:

(Spectrum at $g=\infty$)

N_c # of spinflips	Label	Picture	Relative Energy	Degeneracy
0	$\|g\rangle = \|R\rangle$	$\|\rightarrow\rightarrow\rightarrow\rightarrow\rightarrow\rangle$	0	1
1	$\|i\rangle$	$\|\rightarrow\rightarrow \underset{i}{\leftarrow} \rightarrow \rightarrow\rangle$	$2h$	N
2	$\|i,j\rangle$	$\|\rightarrow\rightarrow \underset{i}{\leftarrow} \cdots \underset{j}{\leftarrow} \rightarrow\rangle$	$4h$	$\frac{N(N-1)}{2}$
3	$\|i,j,k\rangle$	$\|\rightarrow\rightarrow \underset{i}{\leftarrow} \cdots \underset{j}{\leftarrow} \cdots \underset{k}{\leftarrow} \rightarrow\rightarrow\rangle$	$6h$	$\frac{N(N-1)(N-2)}{3\cdot 2\cdot 1}$
⋮		⋮		

Now suppose $J \neq 0$ $\frac{J}{h} \ll 1$.

Then H_J term can be treated perturbatively.

$$H = \underbrace{H_h}_{\text{"main piece"}} + \underbrace{H_J}_{\text{perturbation}}$$

$$H_J = -J \sum_i^{'} \sigma_{i+1}^z \sigma_i^z$$

Now define $\tilde{\sigma}_i^+$ and $\tilde{\sigma}_i^-$ which are spin raising and lowering operators in the x-polarized basis

$$\sigma_i^z = \tilde{\sigma}_i^+ + \tilde{\sigma}_i^-$$

$$\Rightarrow H_J = -J \sum_i^1 (\tilde{\sigma}_{i+1}^+ + \tilde{\sigma}_{i+1}^-)(\tilde{\sigma}_i^+ + \tilde{\sigma}_i^-)$$

We can rewrite this as

$$H_J = \overbrace{-J \sum_i^1 \tilde{\sigma}_{i+1}^+ \tilde{\sigma}_i^+}^{H_J^+} \overbrace{-J \sum_i^1 \tilde{\sigma}_{i+1}^- \tilde{\sigma}_i^-}^{H_J^-} \underbrace{-J \sum_i^1 (\tilde{\sigma}_{i+1}^+ \tilde{\sigma}_i^- + \tilde{\sigma}_{i+1}^- \tilde{\sigma}_i^+)}_{H_J^f}$$

Note that H_J^+ connects the N_s sector of the Hilbert space with N_s+2 sector. Similarly H_J^- connects N_s sector with the N_s-2 sector. Now H_J^f does not take the state out of the N_s sector, it only flips neighbors spins.

We thus see that the ground state energy eigenvalue is

$$E_g = \underbrace{E_{g=\infty}}_{=-Nh} + \sum_{\langle i,j\rangle}^{1} \frac{\langle R|H_J^-|i,j\rangle\langle i,j|H^+|R\rangle}{-4h}$$

$$= -Nh - N\frac{J^2}{4h} + \cdots$$

Although there are $\frac{N(N-1)}{2}$, $|i,j\rangle$ states only $|i,i+1\rangle$ states contribute and hence we see

$$E_g = -NJg\left[1 + \frac{1}{4g^2} + \cdots\right]$$

The state

$$|g\rangle = |R\rangle \sum_i^1 \frac{J^2}{4h}\,|i,i+1\rangle.$$

↑ unnormalized.

Now $\langle g|M|g\rangle = 0$!

and thus we see that for large g ($g>0$, but $<\infty$),

. $M=0$, which means that case 1 is excluded!

What about the excitation gap when $g < \infty$? To see this we need to calculate the change in the energy of the excited states. In leading order, H_J mixes $|i\rangle$ with other states

Now $\langle i|H|j\rangle = 2h\delta_{ij} - J(\delta_{j,i+1} + \delta_{j,i-1})$

This is a hopping Hamiltonian and the energy eigenvalues are

$k \in (-\pi, \pi)$

$$\mathcal{E}(k) = 2h - 2J\cos k$$

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_i' e^{ik\cdot x_i} |i\rangle$$

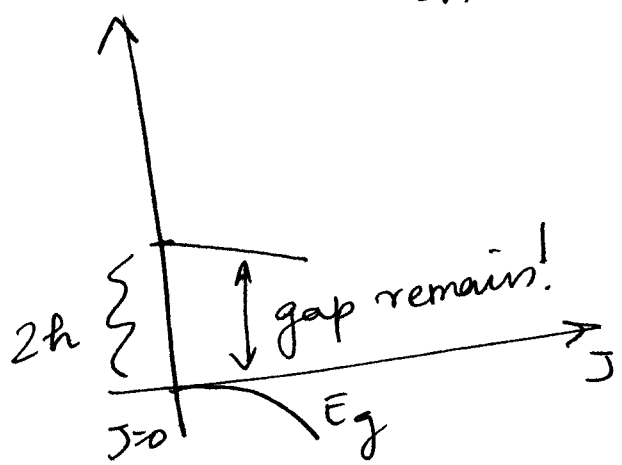
So the energy of the lowest Excited state to is $2h - 2J$ (Relative to the $|R\rangle$ state at $g=\infty$)

$=$

We see that the excited state has a gap. → system remains gapped for $g < \infty$!

$$\frac{\mathcal{E}_g}{g} = 2\left(1 - \frac{1}{g}\right)$$

We are therefore quite sure that the state for $g < 0$ is "not like" the $|R\rangle$ state with minor modifications.



Now let us look at the other end! i.e, near $g = 0$. Here J is finite and $h \gg 0$ with $\frac{h}{J} = g \ll 1$.

Now the ground state $|g=0\rangle = |F\rangle$ with energy $-hNJ$.

What about the first excited state?

The first excited state is

is a domain wall! The state is
$|\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle$ (i, i+1) an has energy
with reppect to $|F\rangle$ which is $2J$.

What is the second excited state?
This is a single spin a finit domain
spin flip, (a single spin flip is a
speial case of this)

$|\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\ldots\rangle$ (i ≠ j)

We can now make a table, where the
excitats are labelled by number of domain
walls. N_d

N_d	Label	Picture	Relative energies	Degeneracy
0	$\|g\rangle = \|F\rangle$	$\|\uparrow\uparrow\uparrow\uparrow\ldots\uparrow\rangle$	0	-
1	$\|i\rangle$	$\|\downarrow\downarrow\downarrow\downarrow\downarrow\uparrow\ldots\uparrow\rangle$ (i, i+1)	$2J$	N
2	$\|i\ j\rangle$	$\|\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle$ (i, j)	$4J$	$\frac{N(N-1)}{2}$
3	$\|i, j\ k\rangle$	$\|\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\rangle$ (i, j, *)	$6J$	$\frac{N(N-1)(N-2)}{3.2.1.}$

Now we consider a small $\# h$,

$$H = -J\sum_i^1 \sigma_{i+1}^z \sigma_i^z - h\sum_i^1 \sigma_i^x$$

$$\underbrace{-h\sum_i^1 (\sigma_i^+ + \sigma_i^-)}_{H_h}.$$

We now see that H_h connects N_d with N_d+2 and N_d-2. since a spin flip can create two domain walls or kill two domain walls.

We Immediately have

$$|g\rangle \quad E_g = -NJ + \sum_i^1 \frac{\langle R|H_h|i,i+1\rangle\langle i,i+1|H_h|R\rangle}{-4J}.$$

$$\Rightarrow E_g = -NJ - \frac{Nh^2}{4J} \quad (!!)$$

↳ why this exclamation?

$$|g\rangle = |R\rangle + \sum_i \frac{h}{4J}|i,i+1\rangle.$$

↑ unnormalized

Now $M(g) = \dfrac{\langle g|M|g\rangle}{\langle g|g\rangle}$.

$$\langle g|g\rangle = \left(1 + \frac{N\frac{h^2}{16J^2}}{}\right)$$

$$\langle g|M|g\rangle = \frac{1}{N}\left[\frac{\langle R|M|R\rangle + \frac{1}{4}\sigma \frac{h^2}{16J^2}\langle i,i+1|M|i+1,i\rangle}{\left(1+\frac{N h^2}{16J^2}\right)}\right]$$

$$= \frac{1}{N}\left[\frac{N + N(N-4)\frac{h^2}{16J^2}}{\left(1+\frac{N h^2}{16J^2}\right)}\right]$$

$$M = \left(1+(N-4)\frac{h^2}{16J^2}\right)\left(1-\frac{N h^2}{16J^2}\right)$$

$$= \left(1 + (N-4)\frac{h^2}{16J^2} - N\frac{h^2}{16J^2}\right)$$

$$= \left(1 - \frac{1}{4}\frac{h^2}{J^2}\right) = \left(1-\frac{g^2}{4}\right)!$$

(Note how the linked cluster theorem secretly operates to kill the power of N)!

We now see that there is finite magnetic for a finite g.

What about the excitation gap?
To see this, consider the manifold with one domain wall. Here the ~~Energy~~

$$\langle i|H|j\rangle = 2J\delta_{ij} - h(\delta_{j,i+1} + \delta_{j,i-1}).$$

which again gives a dispersion

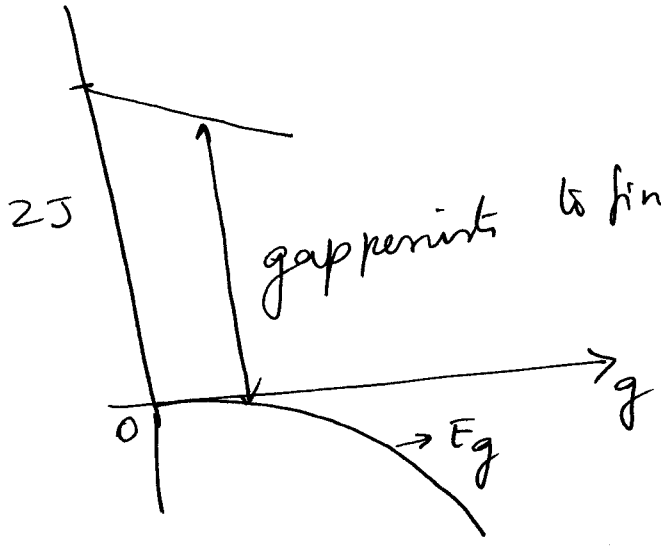
$$\varepsilon(k) = 2J - 2h\cos k!$$

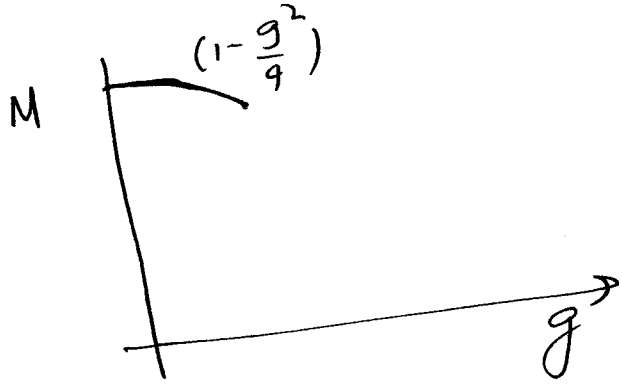
Thus the smallest value of $\varepsilon(k)$ (Relative to the $|F\rangle$ state) is

$$\Delta\varepsilon = 2J - 2h.$$

is Energy gap.

Thus we see that





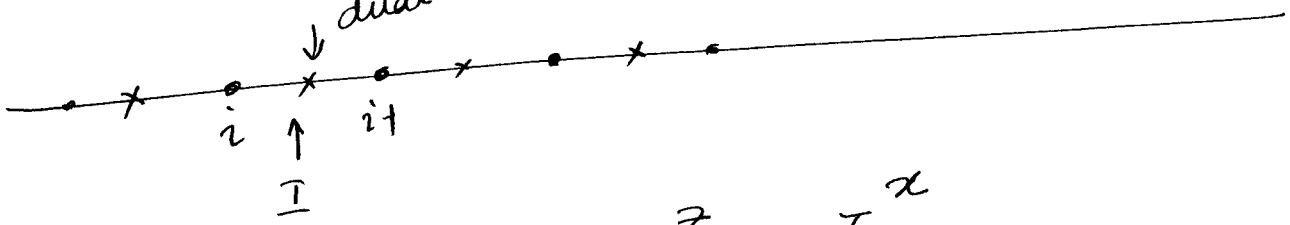
Based on this analysis we are now absolutely certain that the scenario is either case 2 or case 3!

Actually we have learnt much more, if we look at our results carefully. A comparison of the spectrum near $g=0$ and $g=\infty$ shows that there is a 1-1 mapping between the excitations. The ground states energies also look very similar!

	Near $g \approx 0$	Near $g \approx \infty$
ground state Energy	$-N\left(J + \frac{h^2}{4J}\right)$	$-N\left(h + \frac{J^2}{4h}\right)$
Excitation	$2J - 2h\cos k$	$2h - 2J\cos k$

It strongly suggest that there is some kind of $J \leftrightarrow h$ duality or $g \leftrightarrow \frac{1}{g}$ duality!!

Duality of the TFIM.



$$\sigma^z_{i+1}\,\sigma^z_i = \tau^x_I .$$

Define

and

$$\prod_{j\le i} \sigma^x_i = \tau^z_I$$

Note that the operator algebra is fully satisfied.

$$(\tau^x_I)^2 = \pm 1 \quad ; \quad (\tau^z_I)^2 = \pm 1$$

$$\tau^x_I\,\tau^z_I + \tau^z_I\,\tau^x_I$$

$$= \prod_{j<i} \sigma^x_i \left[\underbrace{\sigma^z_i\,\sigma^x_i + \sigma^x_i\,\sigma^z_i}_{=0} \right] \sigma^z_{i+1}$$

$$= 0!$$

So the algebra is fully satisfied.

$$= \left(\prod_{j\le i} \sigma^x \right) \left[\sigma^z \right] = 0$$

Now consider this

$$H = -J \sum_i \sigma^x_{i+1} \sigma^z_i - h \sum_i \sigma^x_{i+1}$$

note a small trick.

Now $\sigma^z_{i+1} \sigma^z_i = \tau^x_I$

and $\sigma^x_{i+1} = \tau^z_{I+1} \tau^z_I \begin{pmatrix} 1 & 1 \\ 0 & 6 \end{pmatrix}$

Thus $H = -J \sum_i \tau^x_I - h \sum_i \tau^z_{I+1} \tau^z_I$

Then $H = -Jg \left[\sum_I \tau^z_{I+1} \tau^z_I + \frac{1}{g} \sum_I \tau^x_I \right]$.

We see that the dual of the ~~THIM~~ TFIM is also a ~~THIM~~. TFIM!

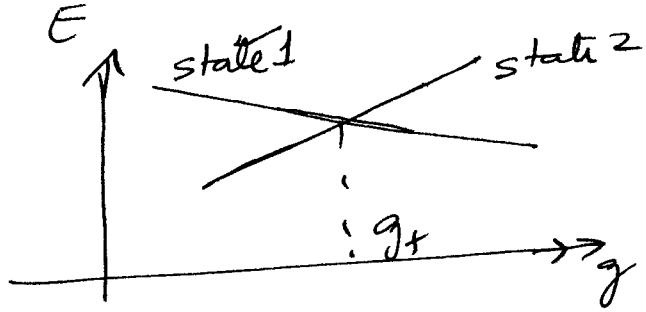
The duality relation can be expressed as $H[\sigma, g] = g H[\tau, 1/g]$

Thus the long speroom of σ maps to the high g spectrum of τ and vice versa. We see that the model

is <u>self dual</u> when $g = 1$. We expect this to be the critical point. It is precisely the same spot as in the classical 2D, Ising model.

We know that something happens at $g_{cr} = 1$, but is it a first order (case 2) or second order (continuous, case 3) transition. What are the signatures of a 1st order vs. continuous transition:

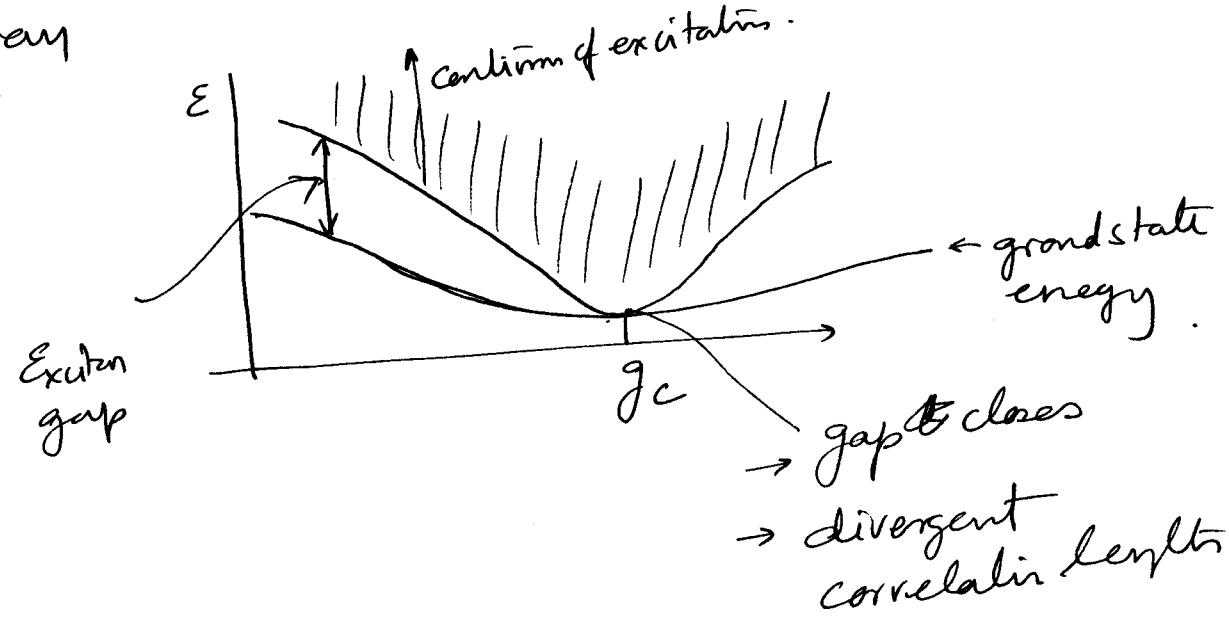
A first order transition is usually a "level crossing"



there is a cross and this produces the sudden change of phase since the symmetry of state 1 and state 2 are (usually) different. (This is similar to a finite T first order phase transition)

Even just to the left/right of g_c correlation lengths are finite.

A continuous transition occurs in quite a different way



Here there is an exciton gap when the system is not at the critical point. We now have to decide if which of these pictures one applicable to our case. What is quite remarkable is that there is an exact solution of this problem for any g! We will actually now work out this solution.

The basic idea of the exact solution is to identify that the domain wall excitation is actually a "particle"! It turns out that if the theory is written in terms of this particle then. First we begin with a rotational change which does not change the physics.

$$H = -J \sum_i^{'} \sigma_{i+1}^{x} \sigma_i^{x} - h \sum_i^{'} \sigma_i^{z}$$

Now make the following observation

$$\sigma_i^{+} \sigma_i^{-} + \sigma_i^{-} \sigma_i^{+} = 1 \; !$$

Thus one might be tempted

Make $\sigma_i^{+} \stackrel{?}{=} c_i^{+}$ and $\sigma_i^{-} \stackrel{?}{=} c_i$

But this will not satisfy

$$c_i^{+} c_j^{+} + c_j^{+} c_i^{+} = 0 \quad \text{and}$$

other relations.

Now note that $c_i^{+} c_i \stackrel{?}{=} \sigma_i^{+} \sigma_i^{-}$

$$= \frac{1}{4}\left((\sigma_i^{x} + i\sigma_i^{y})(\sigma_i^{x} - i\sigma_i^{y}) \right)$$

$$= \frac{1}{4}\left[1 + -i\left(\sigma_i^x \sigma_i^y - \sigma_i^y \sigma_i^x\right) + 1 \right]$$

$$\frac{1}{2}(\sigma_i^z + 1)$$

=

Now defin

$$c_i^+ \equiv \left(\prod_{i<j}(-\sigma_j^z)\right)\sigma_i^+$$

$$c_i = \left(\prod_{i<j}(-\sigma_j^z)\right)\sigma_i^-$$

$$c_i^+ c_i \equiv \sigma_i^+ \sigma_i^- = \frac{1}{2}(\sigma_i^z + 1).$$

$$c_i^+ c_\ell^+ + c_\ell^+ c_i^+ \qquad i<\ell$$

$$= \left(\prod_{i<j<\ell}(-\sigma_j^z)\right)\left(\sigma_i^+ \sigma_i^z \sigma_\ell^+ + \sigma_\ell^+ \sigma_i^z \sigma_i^+\right)$$

$$= \left(\prod_{i<j<\ell}-\sigma_j^z\right)\underbrace{-\left(\sigma_i^+ \sigma_i^z + \sigma_i^z \sigma_i^+\right)}_{=0}\sigma_\ell^+$$

Hence this is correct! condition is satisfied.

We further need,

$$c_i^\dagger c_\ell + c_\ell c_i^\dagger \overset{?}{=} \delta_{i\ell} \qquad i \le \ell.$$

$$= \left(\prod_{i<j<\ell}(-\sigma_j^z)\right)\left(-\sigma_i^+ \sigma_i^z \sigma_\ell^- - \sigma_\ell^- \sigma_i^z \sigma_i^+\right).$$

If $\ell \neq i$ then it is 0.

else $\left(\sigma_i^+ \sigma_i^- + \sigma_i^- \sigma_i^+\right)$

will not be present

All conditions are satisfied; $c_i^\dagger$ are fermionic.

Now Let us express the σ operators in terms of fermions.

Note that

$$c_i^\dagger c_i = \frac{1}{2}(1+\sigma_i^z)$$

$$\Rightarrow \quad \sigma_i^z = (2 c_i^\dagger c_i - 1)$$

$$\prod_{j<i} -\sigma_j^z = \prod_{j<i}(-(2 c_i^\dagger c_i - 1))$$

$$= \prod_{j<i}(1 - 2 c_i^\dagger c_i)$$

Now $(1-2c_i^\dagger c_i) = e^{-i\pi c_i^\dagger c_i}$

$\Rightarrow \prod_{j<i}(-\sigma_j^z) = e^{-i\pi \sum_{j<i} c_j^\dagger c_j}$

Thus we see that

$\sigma_i^+ = \left(e^{-i\pi \sum_{j<i} c_j^\dagger c_j}\right) c_i^\dagger$

$\sigma_i^- = \left(e^{i\pi \sum_{j<i} c_j^\dagger c_j}\right) c_i$

$\sigma_i^z = 2c_i^\dagger c_i - 1.$

Now $\sigma_{i+1}^x \sigma_{xi}^x = (\sigma_{i+1}^+ + \sigma_{i+1}^-)(\sigma_i^+ + \sigma_i^-)$

$= \sigma_{i+1}^+ \sigma_{i+1}^+$

$= (\sigma_{i+1}^+ + \sigma_{i+1}^-)(\sigma_i^+ + \sigma_i^-)$

$= \sigma_{i+1}^+ \sigma_i^+ + \sigma_{i+1}^+ \sigma_i^- + \sigma_{i+1}^- \sigma_i^+ + \sigma_{i+1}^- \sigma_i^-$

or $(\sigma_{i+1}^+ + \sigma_{i+1}^-)\sigma_i^+ \rightarrow$ 1 term

$= e^{-i\pi c_i^\dagger c_i} (c_{i+1}^\dagger + c_{i+1}) c_i^\dagger$

$= (c_{i+1}^\dagger + c_{i+1})(-c_i^\dagger)$

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2nd term

$$(\sigma^+_{i+1} + \sigma^-_{i+1})\,\sigma^-_i$$

$$= (c^+_{i+1} + c_{i+1})\,c_i$$

We therefore have

$$H = -J \sum_1^1 (c^+_{i+1} + c_{i+1})(-c^+_i + c_i) - h \sum_1^1 (2c^+_i c_i - 1)$$

If we ~~use~~ drop a constant, we get (in unit of J)

$$H = \sum_1^1 (c^+_{i+1} + c_{i+1})(c^+_i - c_i) - 2g \sum_i^1 c^+_i c_i$$

$$= -\sum_1^1 (c^+_{i+1} c_i + c^+_i c_{i+1}) - 2g \sum_i^1 c^+_i c_i + \sum_i^1 c^+_{i+1} c^+_i + c_i c_{i+1}$$

If we go over to k space, then

$$\mathcal{H} = -\sum_k^1 2(g + \cos k)\, c^+_k c_k - i \sin k\, c^+_k c^+_{-k} + i \sin k\, c_{-k} c_k$$

k in [~~0~~ $[-\pi, \pi]$.

If we focus on $[0, \pi]$, we can write

$$\mathcal{H} = -\sum_{k>0}' 2(g+\cos k)(c_k^\dagger c_{+k}^\dagger + c_{-k}^\dagger c_{-k}) - 2i \sum_{k}' \sin k \,(c_k^\dagger c_{-k}^\dagger - c_k c_{-k})$$

$$\mathcal{H} = \sum_{k>0}' (c_k^\dagger \; c_{-k}) \begin{bmatrix} 2(g+\cos k) & -2i\sin k \\ 2i\sin k & -2(g+\cos k) \end{bmatrix} \begin{bmatrix} c_k \\ c_{-k}^\dagger \end{bmatrix}$$

+ Constants

We will not get into the details of this. This Hamiltonian has a spectrum whose lowest ~~states~~ excited states form a band (Energy relative to ground state)

$$E(k, g) = 2\sqrt{(g+\cos k)^2 + \sin^2 k}$$

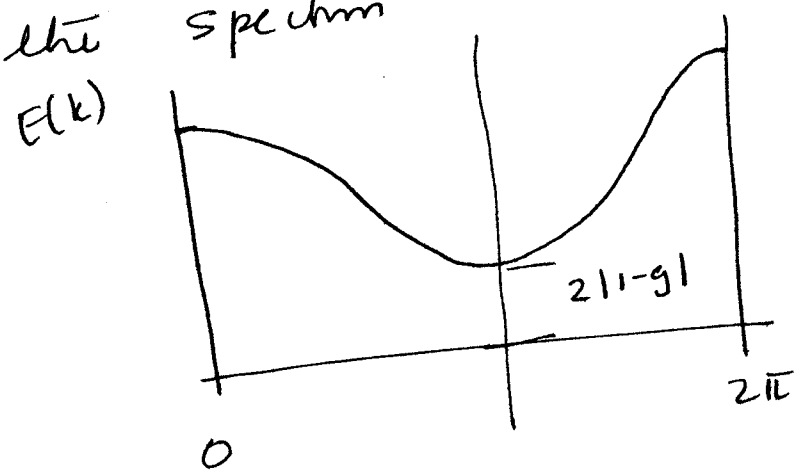
$$= 2\sqrt{1 + 2g\cos k + g^2}$$

We now can obtain Excitation gap which is the smallest value of $E(k, g)$.

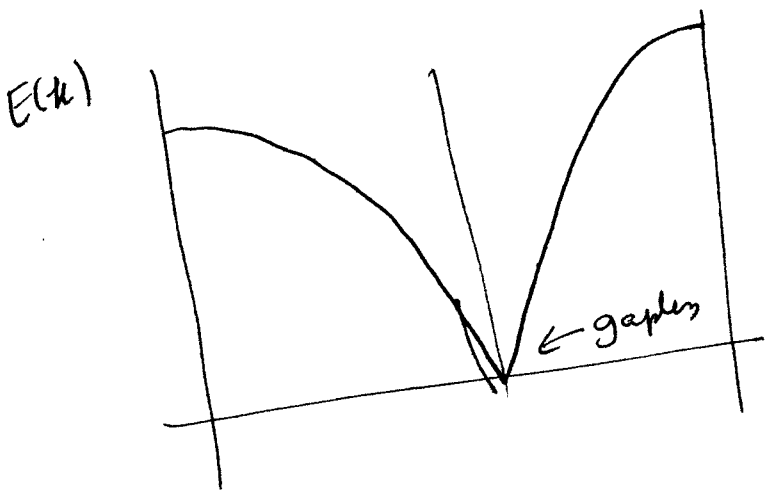
$\rightarrow$ gap $\Delta(g) = 2\sqrt{(1-g)^2} = 2|1-g|$!

The result certainly agrees with our perturbative calculation for $g \ll 1$ and $g \gg 1$. → nice! But we find something quite amazing: the gap closes at $g = 1$. i.e., $g = 1$ is a gapless state!

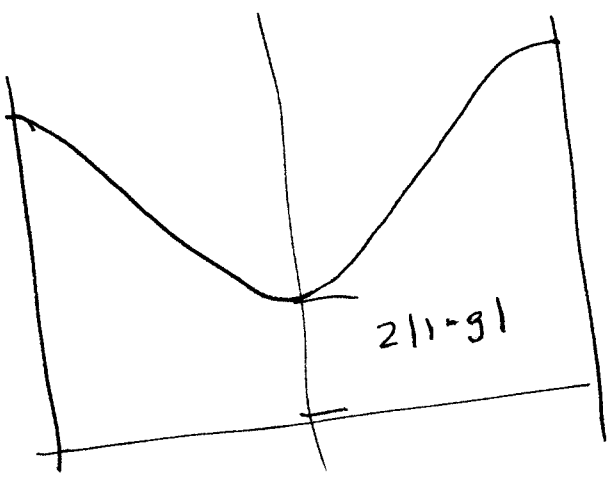
Here is the spectrum



$g < 1$



$g = 1$



$g > 1$.

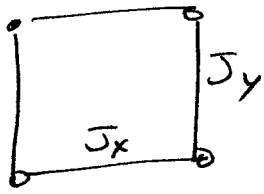
Thus the structure of the spectrum is that of Case 3! We have a continuous or quantum phase transition. At $g = g_c = 1$. The system is gapless. One can go on to show that this implies a divergent correlation length, further cementing the fact that we are looking at a continuous phase transition.

There is a completely different perspective on this. For $g < 1$ or $g > 1$ there are "emergent particles" (whose dispersion we have found), but the particles are massive! (mass of particle $\equiv$ gap of excitation!) The critical point corresponds to massless fermionic particles!

Quite remarkably, this quantum phase transition of the 1d TFIM is actually the same as the phase transition at finite temperature of the square lattice Ising model.

We shall now try to understand this connection. ~~Before that~~ we need to arm ourselves with some background to see this connection.

The first thing we need to note is a generalization of the square lattice Ising model to the anisotropic Ising model



with J_x along the x bonds and J_y along the y-bond. We can show (and you will) that the dual of the anisotropic Ising model is also the anisotropic Ising model. The T_c of this system is obtained by

$$\sinh\left(2\frac{J_x}{T_c}\right)\sinh\left(2\frac{J_y}{T_c}\right) = 1.$$

(This follows from the duality analysis)

It turns out that the nature of the transition (we will understand later precisely what this means) is identical to the isotropic case.

The second point is that regards quantum systems. Consider a quantum system with Hamiltonian H_Q in contact with a heat bath at T_Q (This T_Q is introduced so that we don't confuse with T, the temperature of an classical system). $\beta_Q = 1/T_Q$.

Now at any finite temperature, the partition function is

$$Z = \operatorname{tr} e^{-\beta_Q H_Q} = \sum_{\alpha}^{1} \langle \alpha | e^{-\beta_Q H_Q} | \alpha \rangle$$

$|\alpha\rangle$ is a complete set of states.

Now $$e^{-\beta_Q H_Q} = \prod_{n=1}^{N} e^{-\Delta\tau H_Q(n)}$$

where $$\Delta\tau = \frac{\beta_Q}{N}$$

$$= Z = \sum_{\alpha_n}^{1} \prod_{n=0}^{N} \langle \alpha_{n+1} | e^{-\Delta\tau H_Q(n)} | \alpha_n \rangle.$$

$$|\alpha_0\rangle = |\alpha_N\rangle = \sum_{\alpha_n}^{1} \prod_{n=0}^{N-1} \langle \alpha_{n+1} | \Pi(n) | \alpha_n \rangle$$

Transfer matrices!

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We see that $e^{-\Delta\tau H(n)}$ can be interpreted as a transfer matrix.

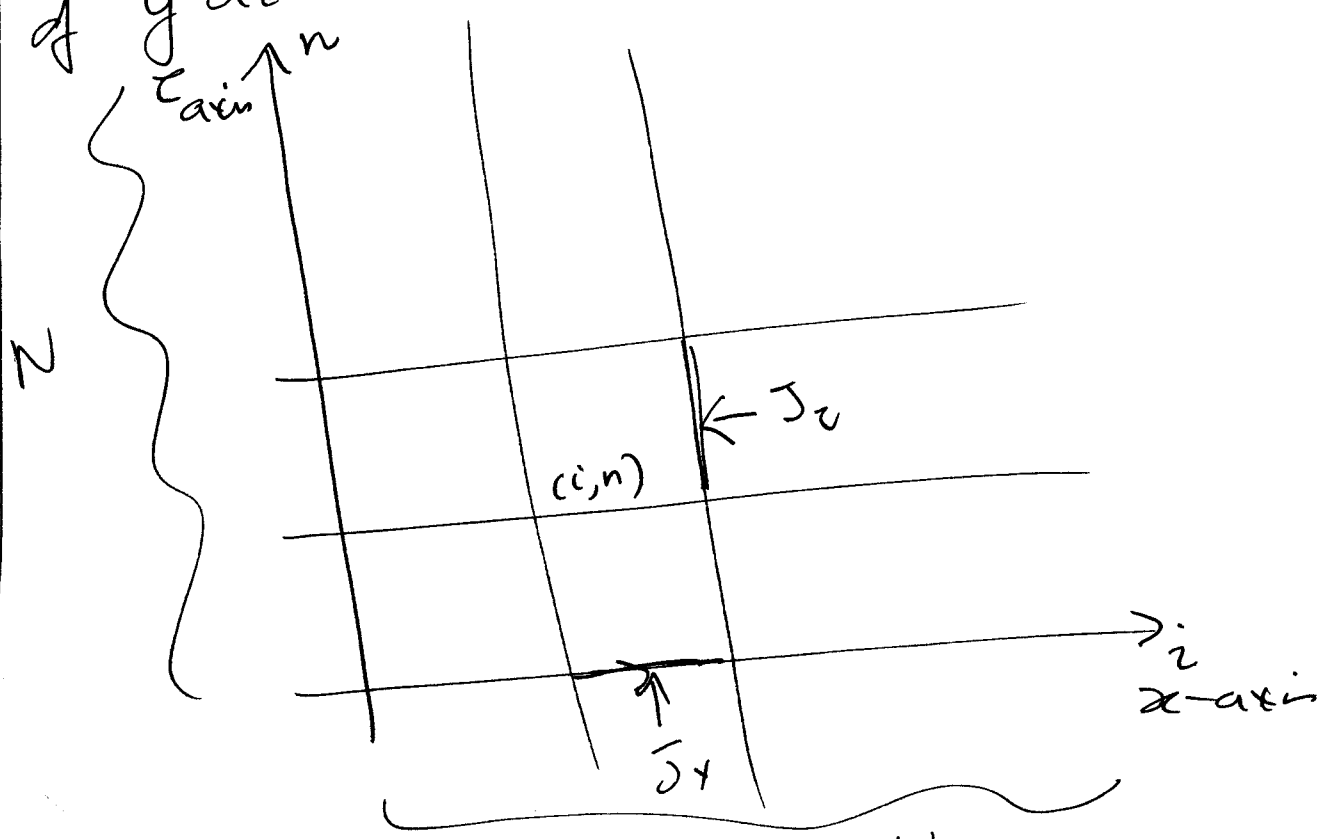
Now what happens at $T_Q \to \infty$.

Then if we let $\Delta\tau \to 0$ and then $N \to \infty$ such that $\Delta\tau N \to \infty$!

Then

$$Z_{T_Q=0} = \sum_{\alpha_n} \prod_{n=0}^{\infty} \langle \alpha_{n+1} | \mathbb{I}(n) | \alpha_n \rangle.$$

Let us now work with an anisotropic classical ~~Hei~~ Ising model. Instead of y axis we will call it the τ axis



$$H = -J_x \sum_n \sum_i \underbrace{\left(S(i,n)\, S(i,n) + S(i+1,n+1)\, S(i,n+1) \right)}_{\Phi(n)}$$

$$\underbrace{-J_c \sum_n \sum_i S(i,n+1)\, S(i,n)}$$

$$+ J_c \sum_n \sum_i \underbrace{\left(S(i,n+1) - S(i,n) \right)^2}_{F(n)}$$

Now

$$Z = \sum_{\{S\}} \prod_n e^{-\frac{J_c}{} F(n) + J_x \Phi(n)}$$

$$= \sum_{\{S\}} \prod_n \langle S_{n+1} | \, T(n) \, | S_n \rangle$$

We have interpreted these terms as matrix elements of a $2^N \times 2^N$ transfer matrix : $|S_n\rangle$ is the set of 2^N states on the n^{th} τ-row.

Now we make the question

Can we write $T(n) = e^{-\Delta\tau H_Q}$

and if so, what is $\Delta\tau$ and what is H_Q?

This requires some guess work and cleverness. Fortunately there have been others who had the inspiration! We will steal their ideas!

Now for a given $|S_n\rangle$, we can write $|S_{n+1}\rangle$ states via spin flips.

- for ~~each~~ one

$|S_n^{(0)}\rangle = |S_n\rangle$ 1 state

$|S_n^{(1)}\rangle =$ one spin flip on $|S_n\rangle$ N states

⋮

and so on.

Now

$$\langle S_n^0 | T(n) | S_n^{\bullet} \rangle = \langle S_n | e^{-\Delta\tau H_Q} | S_n \rangle$$

$$= e^{\tilde{J}_x \Phi(n)}$$

$$\langle S_n^{(1)} | T(n) | S_n \rangle = \langle S_n^{(1)} | e^{-\Delta\tau H_Q} | S_n \rangle$$

$$\cong -\Delta\tau \langle S_n^{(1)} | H_Q | S_n \rangle$$

$$\cong e^{-2\tilde{J}_\tau} e^{\tilde{J}_x \Phi(n)}$$

$$\langle S_n^{(m)} | T(n) | S_n \rangle = \langle S_n^{(m)} | e^{-\Delta\tau H_Q} | S_n \rangle$$

(m flips)

$$= e^{-2m\tilde{J}_\tau} e^{-\Delta\tau \Phi(n)}$$

We now can see that, we can identify a $\Delta\tau$ in the following way

$\Delta\tau \sim J_x$ and $\Delta\tau \sim e^{-2\tilde{J}_\tau}$.

. We can choose $\Delta\tau = e^{-2\tilde{J}_\tau}$

and $\Delta\tau \cdot J_x = \lambda \Delta\tau$.

Thus we see that the term

$Q(n)$ corresponds to.

$$-\lambda \sum_i^1 \sigma_z(i+1, n)\, \sigma_z(i, n)$$

What about the other term

$$H|\varphi^{(1)}\rangle = \tilde{H}(n) - \lambda \sum_i^1 \sigma_z(i+1)\, \sigma_z(i, n)$$

Question is what is $\tilde{H}(n)$?

Note that $\langle s_n^{(1)}| e^{-\Delta\tau H_Q} |s_n\rangle \overset{\lim \Delta\tau \to 0}{\cong}$ (Using trotter decomposition)

$$\langle s_n^{(1)}| e^{-\Delta\tau \tilde{H}(n)} |s_n\rangle\, e^{-\Delta\tau(-\lambda Q(n))}$$

Use $e^{-\Delta\tau(\tilde{H} - \lambda \sum_i^1 \sigma^z \sigma^z)} \simeq e^{-\Delta\tau \tilde{H}}\, e^{-\Delta\tau(-\lambda \sum_i^1 \sigma^z \sigma^z)}$

$$= e^{-\Delta\tau(-\lambda Q(n))}$$

$$= \Delta\tau\, e^{-\Delta\tau(-\lambda Q(n))}$$

$$\langle s_n^{(m)} | e^{-\Delta\tau \tilde{H}(n)} | s_n \rangle$$

$$= (\Delta\tau)^m e^{-\Delta\tau(-\lambda Q(n)}$$

We see that as $\Delta\tau \to 0$ this contribution goes to zero, ~~the~~ only the leading contribution $\langle s_n^{(1)} | e^{-\Delta\tau \tilde{H}(n)} | s_n \rangle$ survives.

We see that choosing $\tilde{H}(n) = -\sum_i \sigma_x(i,n)$ does the job of correctly picking up the matrix element.

Thus

$$\langle s_{n+1} | T(n) | s_n \rangle = \langle s_{n+1} | e^{-\Delta\tau H_Q(n)} | s_n \rangle.$$

Thus

$$Z = \sum_{\{s\}} \prod_{n=\phi}^{N} \langle s_{n+1} | e^{-\Delta\tau H_Q(n)} | s_n \rangle$$

$\Delta\tau \to 0$ $N \to \infty$.

But this is the $T_Q = 0$ problem of H_Q!

$$H_Q = -\sum_i \sigma_x(i) - \lambda \sum_i \sigma^z(i+1)\sigma_i^z$$

which is the TFIM! Thus the

b)

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Zero temperature TFIM physics is same as that of the anisotropic Ising model. To see this note

$$\Delta\tau = e^{-2\tilde{J}_z}$$

and $$\lambda\Delta\tau = \tilde{J}_x$$

as $\Delta\tau \to 0$ $\tilde{J}_z \to \infty$ and $\tilde{J}_x \to 0$

which is an extremely anisotropic model. One can give arguments that the critical properties of such anisotropic system is identical to the original isotropic model. Thus the exact solution of TFIM can is also an exact solution of the classical Ising model.

One can see that based on duality we have

$$\sinh 2\tilde{J}_x^c \sinh 2\tilde{J}_z^c = 1.$$

Note that in the lim $\tilde{J}_z \to \infty$ $\tilde{J}_x \to 0$

$$\sinh 2\tilde{J}_x^c \to 2\tilde{J}_x^c$$

$$\sinh 2\tilde{J}_z^c \to \frac{1}{2} e^{2\tilde{J}_z^c}$$

Thus $$e^{-2\tilde{J}_z^c} = \tilde{J}_x^c.$$

Pulling this in

$$\Delta\tau = e^{-2\tilde{J}_\tau^c} = \tilde{J}_x^c$$

$$\Rightarrow \lambda \tilde{J}_x^c = \tilde{J}_k^c \Rightarrow \lambda = 1.$$

Thus T_c of the clerical system corresponds to $\lambda = 1$.

This analysis not only provides a solution of a 2-d clerical Ising model, but also provides a crucial connection-

A d-dimension Quantum ground state problem is equivalent to a (d+1) dimensional ~~q~~ clerical ~~gases~~ stat mech problem. Later, or may be in another course, we will see that this statement ~~can't~~ has to be made more precise (actually $d \equiv d+z$ where z is called the dynamical critical exponent!

This brings us to the end of ~~chapter 6~~ this chapter. We will now move on to other (more approximate) approaches.