Basic Statistical Mechanics

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Lecture - 48
Ising Model and Other Lattice Models Part 5

Welcome back, so we will continue with the Mean Field theory of the Ising model and as I said repeatedly in the Mean Field theory you have the dimension enters to the coordination number gamma and with the by enlarge generally is a good approximation there is no problem with that, so the thing that we have already done is that the decomposition.

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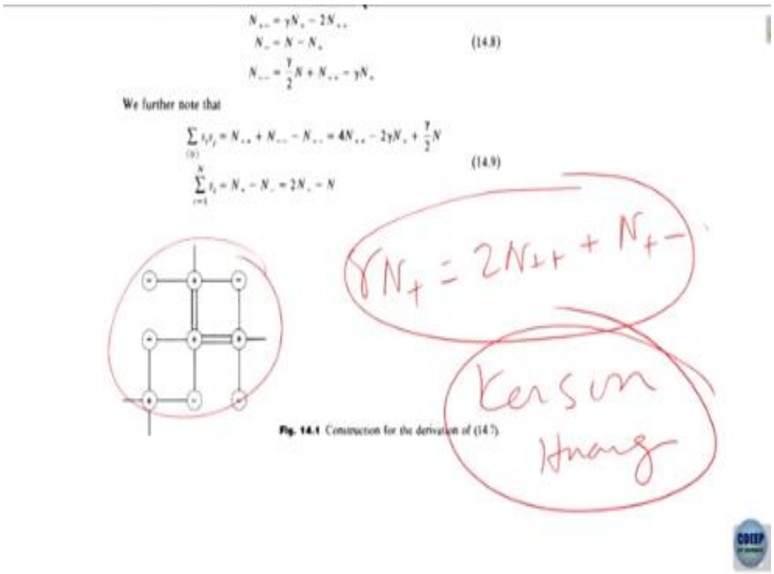

$$N_{+-} = \gamma N_+ - 2N_{++}$$
$$N_- = N - N_+ \qquad (14.8)$$
$$N_{--} = \frac{\gamma}{2}N + N_{++} - \gamma N_+$$

We further note that

$$\sum_{\langle ij \rangle} s_i s_j = N_{++} + N_{--} - N_{+-} = 4N_{++} - 2\gamma N_+ + \frac{\gamma}{2}N$$
$$\sum_{i=1}^{N} s_i = N_+ - N_- = 2N_+ - N \qquad (14.9)$$

$\gamma N_+ = 2N_{++} + N_{+-}$

Kerson Huang

Fig. 14.1 Construction for the derivation of (14.7)

which is this construction of the table, these construction of this thing that you have already done the up-spins is the plus and whenever I draw a line from 1 up spins only from the up spins to all the nearest neighbours, so 2 up spins next to each other then there are 2 lines and that becomes 2 N++, and those kind of a things and for example, this is the condition that we derived that γN+ = 2N++ + N+-, and these are the kind of relations that we just need at length.

So you know these are the things again, so these the book from Kerson Huang at which is the best these from Kerson Huang and this is the best description of Ising model of the Kinetic Mean field theory of Bragg Williams approximation that I am talking here is done this, in this book of Statistical Mechanics.

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$$e^{-\beta A_I(H,T)} = e^{\beta N(\frac{1}{2}\gamma J - H)} \sum_{N_+=0}^{N} e^{-2\beta(\gamma J - H)N_+} \sum_{N_{++}}' g(N_+, N_{++})\, e^{4\beta J N_{++}} \quad (14.11)$$

where $g(N_+, N_{++})$ is the number of configurations that has a given set of values (N_+, N_{++}). The sum $\sum'$ extends over all values of N_{++} consistent with the fact that there are N spins of which N_+ are up. Since $g(N_+, N_{++})$ is a complicated function, the form (14.11) is not a simplification over (14.2) for actual calculations.

14.2 EQUIVALENCE OF THE ISING MODEL TO OTHER MODELS

By a change of names the Ising model can be made to simulate systems other than a ferromagnet. Among these are a lattice gas and a binary alloy.

Lattice Gas

A lattice gas is a collection of atoms whose positions can take on only discrete values. These discrete values form a lattice of given geometry with γ nearest neighbors to each lattice site. Each lattice site can be occupied by at most one atom. Figure 14.2 illustrates a configuration of a two-dimensional lattice gas in which the atoms are represented by solid circles and the empty lattice sites by open circles. We neglect the kinetic energy of an atom and assume that only nearest neighbors interact, and the interaction energy for a pair of nearest neighbors is assumed to be a constant $-\epsilon_0$. Thus the potential energy of the system is equivalent to that of a gas in which the atoms are located only on lattice sites and interact through a two-body potential $v(|\mathbf{r}_i - \mathbf{r}_j|)$ with

$$v(r) = \begin{cases} \infty & (r = 0) \\ -\epsilon_0 & (r = \text{nearest-neighbor distance}) \\ 0 & (\text{otherwise}) \end{cases} \quad (14.12)$$

So then, one important thing in this process going through that, so this was the kind of things that we have been discussing all this time that the writing down the Hamiltonian in terms of this what exactly I was telling before I do the mean field approximation, then this is the partition function this is fairly Universal notation we find everywhere in the world the same every book we would have this notation.

So that is an equivalence that means this between devising more elemental theories are fairly well documented and we will articulate it. Because these are kind of, so important that we have to be more or less in addition; now I just told you that this before I go to the next step there is to show the importance of Ising model that, this is applied to so many different things one of them is the lattice gas.

In the lattice gas you say okay, I will at lattice where I have if there is a gas molecule then there is if there, so I want in it gas where a lot of empty spaces and I want to model that by saying okay if there is a particle then there is a black and there is no particle that is empty. So that simple thing essentially is again N+ when there is a N+ goes over to your occupied, N- is gas particles but there is nothing there and the two next to each other is N+-, if 2 occupied next to the N++. So you can now map the Ising model into lattice gas and you can do wonderful stuff.

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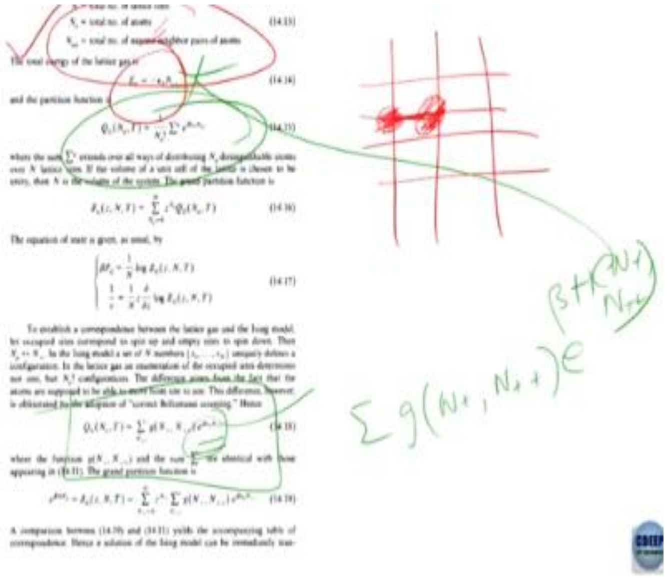

So then again that as we said here total number of lattice sites, then these total number of atoms are occupied so in this lattice, when they are occupied they are occupied that is N++ when they are empty that is N-, and total number of nearest neighbour pairs is N++. So exactly that thing, when you map that you can now get the and so if you say, when they are next to each other there is an attraction and that attraction is epsilon.

Then that gives you that, so it is like two parallel spins a ferromagnetic interaction and then I can write the partition function I can write the partition function like that. And then, I can now get the exactly decompose into this, only difference is that the beta H term here is given by this term, but again I have to evaluate the same thing : $\sum g(N_{+,}N_{++})e^{\beta H(N_+ + N_{++})}$ that is this thing, so I have done.

So one thing, number of ways of distributing atoms, N+ atoms into the N, N number of lattice sites, now something extremely important comes out of that then if my number of atoms occupied atoms my black dots or my here white dots, if that is equal to N+ then I know N+ and -N- gives me the magnetization and what does N+ gives me here? N+ gives me density, so then I immediately have a wonderful Isomorphism, which is goes a very long way that magnetization is equivalent to density.

That exactly correct turned out to be, that is the way we can transform one equation state or magnetic system into equation state for the gas liquid system, it is a far-reaching consequence. So now we now just discussed that how lattice gas model can be mapped into Ising model, we may discuss one more interesting thing.

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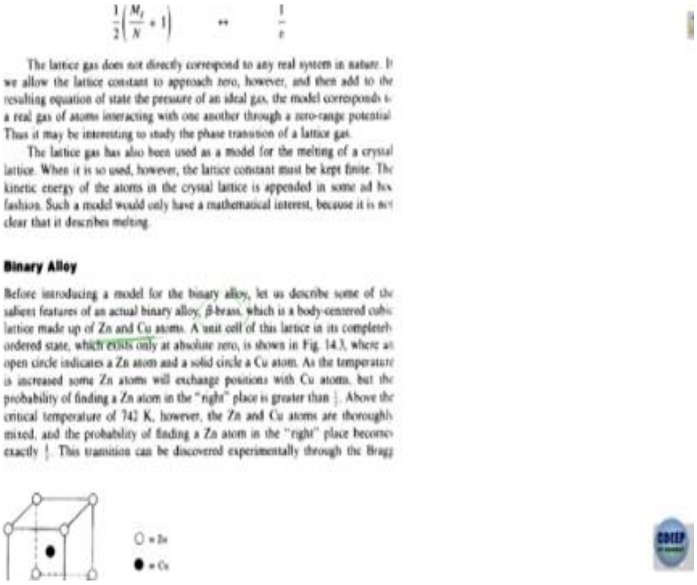

$$\frac{1}{2}\left(\frac{M_I}{N}+1\right) \quad \leftrightarrow \quad \frac{1}{v}$$

The lattice gas does not directly correspond to any real system in nature. If we allow the lattice constant to approach zero, however, and then add to the resulting equation of state the pressure of an ideal gas, the model corresponds to a real gas of atoms interacting with one another through a zero-range potential. Thus it may be interesting to study the phase transition of a lattice gas.

The lattice gas has also been used as a model for the melting of a crystal lattice. When it is so used, however, the lattice constant must be kept finite. The kinetic energy of the atoms in the crystal lattice is appended in some ad hoc fashion. Such a model would only have a mathematical interest, because it is not clear that it describes melting.

Binary Alloy

Before introducing a model for the binary alloy, let us describe some of the salient features of an actual binary alloy, β-brass, which is a body-centered cubic lattice made up of Zn and Cu atoms. A unit cell of this lattice in its completely ordered state, which exists only at absolute zero, is shown in Fig. 14.3, where an open circle indicates a Zn atom and a solid circle a Cu atom. As the temperature is increased some Zn atoms will exchange positions with Cu atoms, but the probability of finding a Zn atom in the "right" place is greater than $\frac{1}{2}$. Above the critical temperature of 742 K, however, the Zn and Cu atoms are thoroughly mixed, and the probability of finding a Zn atom in the "right" place becomes exactly $\frac{1}{2}$. This transition can be discovered experimentally through the Bragg

And that is, these are all from Kerson Haung, now the binary alloy is brass, β-brass, beta brass and that is zinc and copper, and then I am now occupied my lattice sites are occupied either by zinc atom, I can now consider disorder transition that takes place at 742 Kelvin in this case, that you can immediately see that my up spin could be copper, my down spins are zinc or other way around and I can again write down a Hamiltonian.

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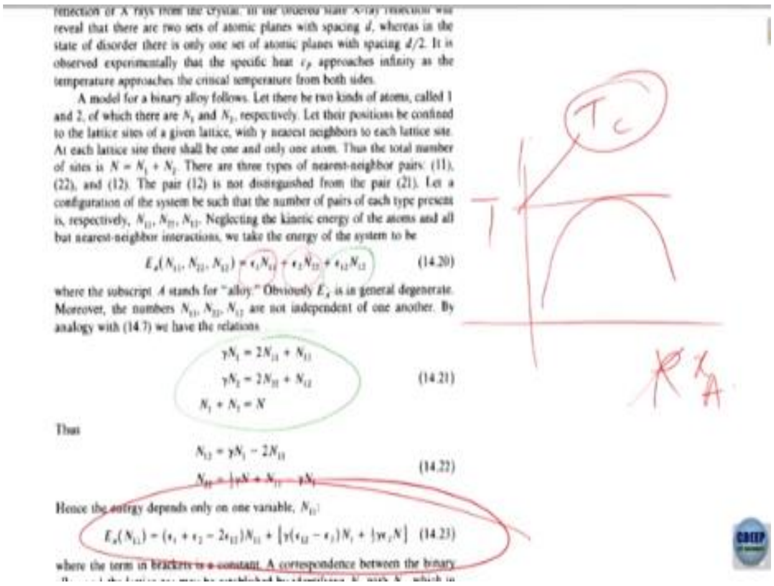

reflection of X rays from the crystal. In the ordered state X-ray reflection will reveal that there are two sets of atomic planes with spacing d, whereas in the state of disorder there is only one set of atomic planes with spacing $d/2$. It is observed experimentally that the specific heat c_P approaches infinity as the temperature approaches the critical temperature from both sides.

A model for a binary alloy follows. Let there be two kinds of atoms, called 1 and 2, of which there are N_1 and N_2, respectively. Let their positions be confined to the lattice sites of a given lattice, with γ nearest neighbors to each lattice site. At each lattice site there shall be one and only one atom. Thus the total number of sites is $N = N_1 + N_2$. There are three types of nearest-neighbor pairs: (11), (22), and (12). The pair (12) is not distinguished from the pair (21). Let a configuration of the system be such that the number of pairs of each type present is, respectively, N_{11}, N_{22}, N_{12}. Neglecting the kinetic energy of the atoms and all but nearest-neighbor interactions, we take the energy of the system to be

$$E_A(N_{11}, N_{22}, N_{12}) = \epsilon_1 N_{11} + \epsilon_2 N_{22} + \epsilon_{12} N_{12} \tag{14.20}$$

where the subscript A stands for "alloy." Obviously E_A is in general degenerate. Moreover, the numbers N_{11}, N_{22}, N_{12} are not independent of one another. By analogy with (14.7) we have the relations

$$\begin{aligned} \gamma N_1 &= 2N_{11} + N_{12} \\ \gamma N_2 &= 2N_{22} + N_{12} \\ N_1 + N_2 &= N \end{aligned} \tag{14.21}$$

Thus

$$\begin{aligned} N_{12} &= \gamma N_1 - 2N_{11} \\ N_{22} &= \tfrac{1}{2}\gamma N + N_{11} - \gamma N_1 \end{aligned} \tag{14.22}$$

Hence the energy depends only on one variable, N_{11}:

$$E_A(N_{11}) = (\epsilon_1 + \epsilon_2 - 2\epsilon_{12})N_{11} + \left[\gamma(\epsilon_{12} - \epsilon_2)N_1 + \tfrac{1}{2}\gamma\epsilon_2 N\right] \tag{14.23}$$

where the term in brackets is a constant. A correspondence between the binary

So sure enough I write down a Hamiltonian exactly same way, I now say okay, my copper-copper is energy interaction at the epsilon1, my copper and zinc - zinc, this is thing and if I want copper-zinc then like that, so this kind of binary mixture we have talking binary alloy that like, copper and copper like each other and zinc and zinc like each other low temperature of course here there is a more long-range interactions because of the metalicity and all those things.

But at a level high temperature when you are talking order disorder transition those things but we have to say copper and copper like each other and zinc and zinc like each other very much like a binary mixture that we do and we will talk a little bit about that later. So now I exactly have the same conservation rules that mean I start with the 5 here these three numbers N11, N22 and N 12.

And then I have the conditions just I have done before exactly same, that up spin-up spin now copper and copper down spin-down spin, zinc and zinc and copper and zinc and 12 and copper + zinc is total number of lattice sites N, and then I eliminate and I now get my energy our Hamiltonian, I get Hamiltonian in terms of their N++,N+-, I get in N1, N1 that means N1 is number of lattice sites occupied by copper or zinc whatever.

And N11, copper and copper are nearest neighbours, so these thing they are exactly same what I have reduce to exactly same that my Ising model. So now I showed two cases gas liquid transition and binary alloy which are completely isomorphic and that in one shot it explain beautiful many things, for example if I do binary mixture I give it just one example before I pass on against density then this is what gas liquid transition and this is the critical temperature T_C.

Now, if I now do that with a mole fraction x of one species is exactly same graph, this is exactly same when I plot magnetization against temperature, because I already told you density is like magnetization. So in one shot in one formulation you are getting three very fastly different phenomena which is the magnetization, gas liquid transition and order-disorder transition and phase separation in binary alloys.

This is just amazing, that is why one takes the Ising model so seriously both in static equilibrium properties and this and our language of its transition is completely dependent on Ising model, this is the most important system in this statistical mechanics, okay?

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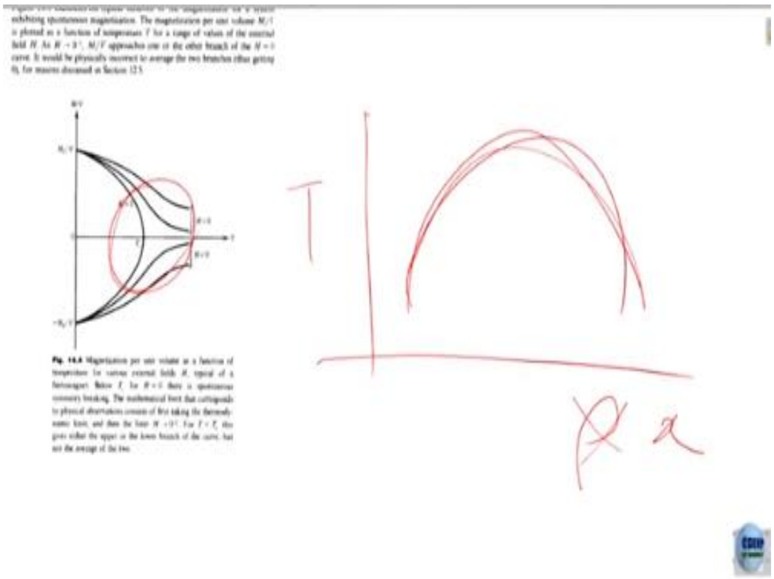

Let us continue and these are saying this is the magnetic transition that is happening magnetization against temperature, this is same as I can instead of that I can plot it rho versus T and exactly same thing, so this is the classic critical point when a magnetic system, so order-disorder transition, mole fraction all these things are the same.

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This is one of the most huge, huge successes of the Ising model.

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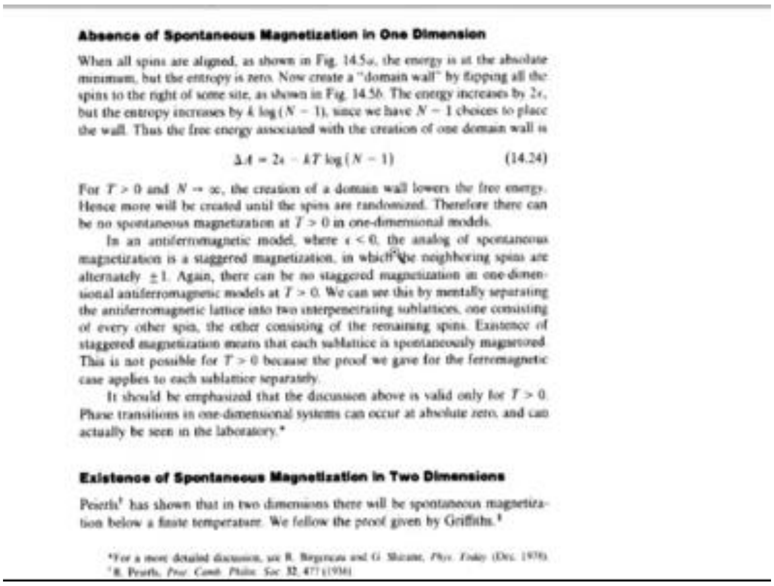

Absence of Spontaneous Magnetization in One Dimension

When all spins are aligned, as shown in Fig. 14.5*a*, the energy is at the absolute minimum, but the entropy is zero. Now create a "domain wall" by flipping all the spins to the right of some site, as shown in Fig. 14.5*b*. The energy increases by 2ϵ, but the entropy increases by $k \log(N - 1)$, since we have $N - 1$ choices to place the wall. Thus the free energy associated with the creation of one domain wall is

$$\Delta A = 2\epsilon - kT \log(N - 1) \tag{14.24}$$

For $T > 0$ and $N \to \infty$, the creation of a domain wall lowers the free energy. Hence more will be created until the spins are randomized. Therefore there can be no spontaneous magnetization at $T > 0$ in one-dimensional models.

In an antiferromagnetic model, where $\epsilon < 0$, the analog of spontaneous magnetization is a staggered magnetization, in which the neighboring spins are alternately ± 1. Again, there can be no staggered magnetization in one-dimensional antiferromagnetic models at $T > 0$. We can see this by mentally separating the antiferromagnetic lattice into two interpenetrating sublattices, one consisting of every other spin, the other consisting of the remaining spins. Existence of staggered magnetization means that each sublattice is spontaneously magnetized. This is not possible for $T > 0$ because the proof we gave for the ferromagnetic case applies to each sublattice separately.

It should be emphasized that the discussion above is valid only for $T > 0$. Phase transitions in one-dimensional systems can occur at absolute zero, and can actually be seen in the laboratory.*

Existence of Spontaneous Magnetization in Two Dimensions

Peierls† has shown that in two dimensions there will be spontaneous magnetization below a finite temperature. We follow the proof given by Griffiths.‡

*For a more detailed discussion, see R. Birgeneau and G. Shirane, *Phys. Today* (Dec. 1978).

†R. Peierls, *Proc. Camb. Philos. Soc.* 32, 477 (1936).

So, now we go ahead and we complete our task of the mean field theory and that will be now little bit .

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So the way we do now is this is order disorder transition. That done. I do not need to do that but what instead; I will do what I was continuing with, okay?

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14.4 THE BRAGG-WILLIAMS APPROXIMATION

L, α

So now the mean field theory is same, the way I am the level I am doing is Bragg Williams approximation and this is thing and I need to make it little bit fatter now, so this is I introduced long range order parameter and short range order parameter L Sigma N+ 1 and we said the same thing and now.

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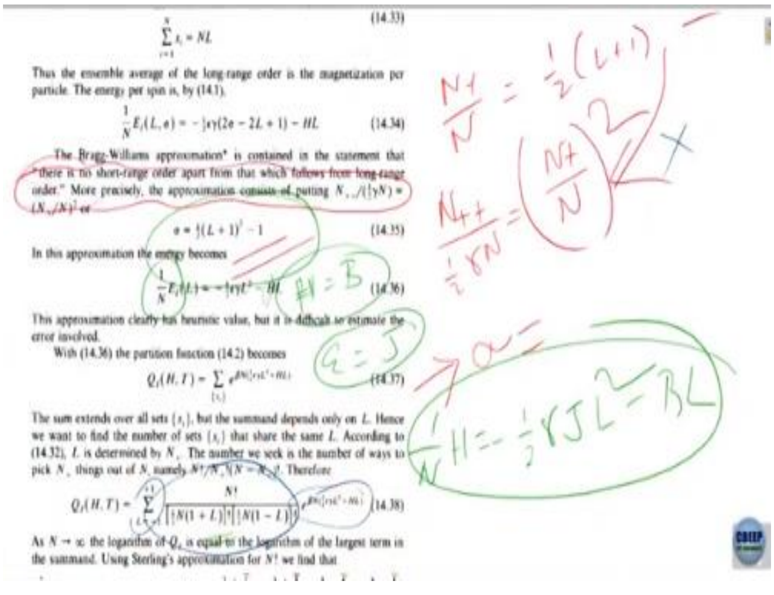

$$\sum_{i=1}^{N} s_i = NL \qquad (14.33)$$

Thus the ensemble average of the long-range order is the magnetization per particle. The energy per spin is, by (14.1),

$$\frac{1}{N}E_I(L,\sigma) = -\tfrac{1}{2}\epsilon\gamma(2\sigma - 2L + 1) - HL \qquad (14.34)$$

The Bragg-Williams approximation* is contained in the statement that "there is no short-range order apart from that which follows from long-range order." More precisely, the approximation consists of putting $N_{++}/(\frac{1}{2}\gamma N) = (N_+/N)^2$ or

$$\sigma = \tfrac{1}{2}(L+1)^2 - 1 \qquad (14.35)$$

In this approximation the energy becomes

$$\frac{1}{N}E_I(L) = -\tfrac{1}{2}\epsilon\gamma L^2 - HL \qquad (14.36)$$

This approximation clearly has heuristic value, but it is difficult to estimate the error involved.

With (14.36) the partition function (14.2) becomes

$$Q_I(H,T) = \sum_{\{s_i\}} e^{\beta N(\frac{1}{2}\epsilon\gamma L^2 + HL)} \qquad (14.37)$$

The sum extends over all sets $\{s_i\}$, but the summand depends only on L. Hence we want to find the number of sets $\{s_i\}$ that share the same L. According to (14.32), L is determined by N_+. The number we seek is the number of ways to pick N_+ things out of N, namely $N!/N_+!(N-N_+)!$. Therefore

$$Q_I(H,T) = \sum_{L=-1}^{+1} \frac{N!}{[\frac{1}{2}N(1+L)]!\,[\frac{1}{2}N(1-L)]!} e^{\beta N(\frac{1}{2}\epsilon\gamma L^2 + HL)} \qquad (14.38)$$

As $N \to \infty$ the logarithm of Q_I is equal to the logarithm of the largest term in the summand. Using Sterling's approximation for $N!$ we find that

$$\frac{N_+}{N} = \frac{1}{2}(L+1)$$

$$\frac{N_{++}}{\frac{1}{2}\gamma N} = \left(\frac{N_+}{N}\right)^2$$

$H = B$

$\epsilon = J$

$\rightarrow \sigma =$

$$\frac{1}{N}H = -\frac{1}{2}\gamma J L^2 - BL$$

I make the approximation that short range order parameter is given by long range order parameter. So the approximation is contained in the statement that there is no longer short range order apart from the long range order. That means approximation statement that, no short range order other than long range order, and once I do that I do this then I get, when I make $\frac{N_{++}}{\gamma N/2} = \left(\frac{N_+}{N}\right)^2$ that translates into σ.

Because this is nothing but it L remember the L+ you know $\frac{N_+}{N}=\frac{1}{2}\left(L+1\right)$ when I use that into here I get see this condition. Let us see when I use this into that, then I get this condition $\sigma\approx\frac{1}{2}\left(L+1\right)^2-1$, now that essentially means that I have the Hamiltonian now completely in Kerson Huang *H* is my B so my Hamiltonian is then one over N, what is energy one over H $\frac{H}{N}=-\frac{1}{2}J\gamma L^2-BL$.

So just making a note that; H is my B and this gamma by gamma but this epsilon is my J. This notation I am using a little bit more model like we use J for Ising model not epsilon as Kerson Haung as used, and we do like to use Hamiltonian H but not E as I use Hamiltonian for H that deprives me of H for magnetic field so I used to B, but B equal to H nu. So this there is no room for any confusion here, once I do that then I right now I am in a completely free domain now.

I know how to go I know the how many ways I can get N+ up spins in N and that of course is N factorial by N + factorial, N-N factorial, so that is I have written here and N+ is half N 1 + L the other is N 1 - L, so I can write N factorial by N + factorial, N - factorial then that is the whaler or in factorial 2 N+ so that is the way I have written here. That is I have written here this is the number of ways to distribute.

And for a given configuration with L because I started with N + and N + + that was the exact then, I made the approximation mean field approximation and as a result of mean field approximation I have on the N+ then I go back I already have L and Sigma and when I eliminate N++, I eliminate Sigma, I have only L, but it has a consistent way in a consistent way so I have the Hamiltonian and then I know how to so I put the Hamiltonian here and do and behold I have fully.

Now I can evaluate that, so in the large particle limit N going to infinity I can take the logarithm to get the free energy and then I make the approximation I make the Stirling's approximation just what we done in Mayer's theory, we have done in the canonical partition function, again and again we have picked up the maximum term.

So of the sum I pick up the maximum term, yeah so I be see hope that one, I take the log whatever given and then I maximize it with respect to L and maximizing with respect to L is same as maximizing with is to L +, right? So remember if you know already have not noticed note that L is nothing but they may be essentially the magnetization of the system.

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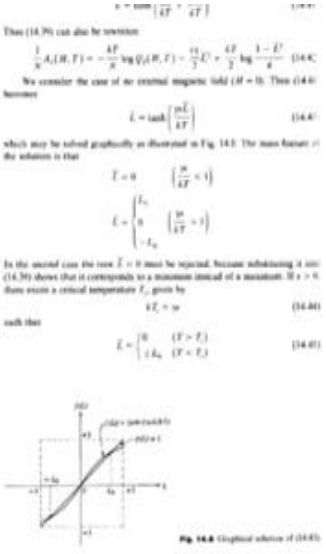

And so things that well and good so, then we can go and once we do that then the thing that happens is that I get an equation which is the following that, Okay?

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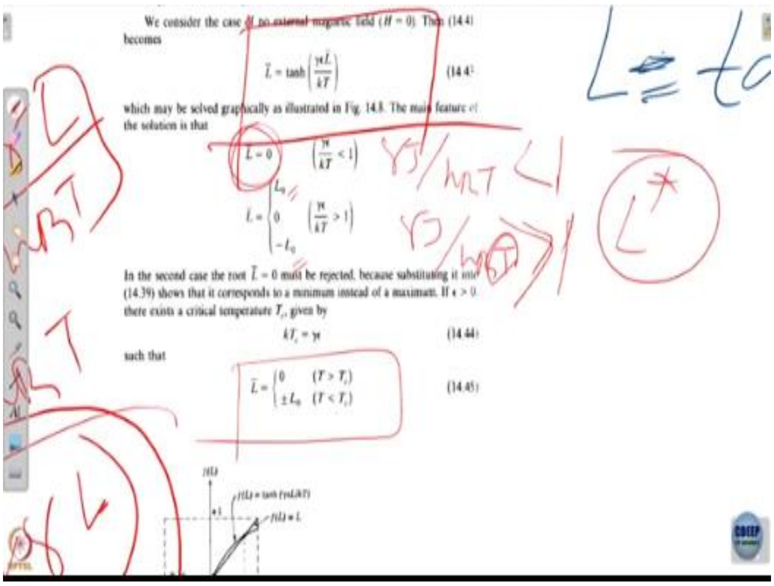

We consider the case of no external magnetic field ($H = 0$). Then (14.41) becomes

$$\bar{L} = \tanh\left(\frac{\gamma\epsilon\bar{L}}{kT}\right) \quad (14.42)$$

which may be solved graphically as illustrated in Fig. 14.8. The main feature of the solution is that

$$\bar{L} = 0 \qquad \left(\frac{\gamma\epsilon}{kT} < 1\right)$$

$$\bar{L} = \begin{cases} L_0 \\ 0 \\ -L_0 \end{cases} \qquad \left(\frac{\gamma\epsilon}{kT} > 1\right)$$

In the second case the root $\bar{L} = 0$ must be rejected, because substituting it into (14.39) shows that it corresponds to a minimum instead of a maximum. If $\epsilon > 0$, there exists a critical temperature T_c, given by

$$kT_c = \gamma\epsilon \quad (14.44)$$

such that

$$\bar{L} = \begin{cases} 0 & (T > T_c) \\ \pm L_0 & (T < T_c) \end{cases} \quad (14.45)$$

I get an equation by doing that which is let me write down because it is not very visible here, L equal to tan hyperbolic, $L = \tanh\left(\frac{B}{k_B T} + \frac{\gamma JL}{k_B T}\right)$ so this is called a implicit solution or a transcendental equation, where I have a L on the left hand side I have L on the right hand side and given a B, I have to solve that the numerically. Now B is 0 the external magnetic field is zero, I have this beautiful solution which is this one, that means $L = \tanh\left(\frac{\gamma JL}{k_B T}\right)$.

In many places dimension K is introduced which is J by KBT then $L = \tanh(K\gamma L)$, low and behold these has a beautiful phase transition scenario that when we show and this is given here these phase transitions scenario is described beautifully here. That when this has only solution of this equation is, that is at when temperature is high so gamma J by KBT is less than 1 then all even less than 1 only solution is L average, which is the maximum term actually.

I prefer it L* but that L average that only solution is the magnetisation zero, so this is the random system number of spins, up spins is same as number of down spins. However, a solution appears when you go to lower temperature, so when you go to lower temperature, that means $\left(\frac{\gamma J}{k_B T} > 1\right)$ temperature is small, so this becomes greater than 1 then a solution appears.

Actually two solutions appears one of them are up spins and as for down spins, and you get the one can show that this root that 0 must be it corresponds to a minimum, not to a maximum so you can neglect, reject that term. So then the solution reduces to the following things that L, these two solutions to T greater than T_C you have no magnetization disorder system below T_C it can be either + or - it has to be true, you cannot;

In the absence of magnetic field they are both are equally likely there is no way to choose one of the other, the way the solution is made by doing a graphical method which is meant which is shown here. You the graphical solution is done in the following way that you plot L and tan hyperbolic L and then you when they become equal to 1 then that is the solution, and the graph goes like this, crosses here at 1 and crosses here at 1.

So, these are the two solutions that you get and it is a, let me see if I can get it a little bit up there should be something here a cursor.

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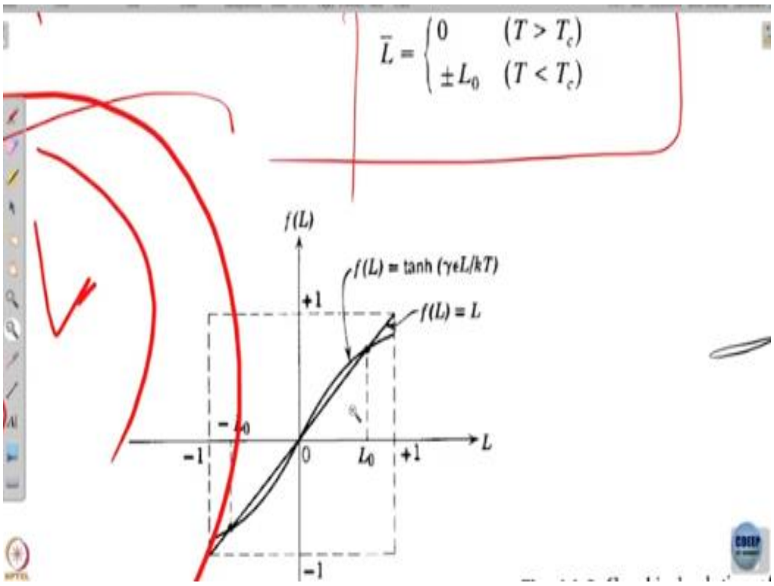

$$\bar{L} = \begin{cases} 0 & (T > T_c) \\ \pm L_0 & (T < T_c) \end{cases}$$

So this is the, this line is the going selecting you when that become equal to tan hyperbolic and L, so this is the L versus L, this line L line, this the straight line and this is the tan hyperbolic, you know the tan hyperbolic very well because tan hyperbola set like this, and these are the solutions when they meet that is the solution of that and that is L_0 + and - solutions. Okay, so this is part of these things works out beautifully? So next go to the next page.

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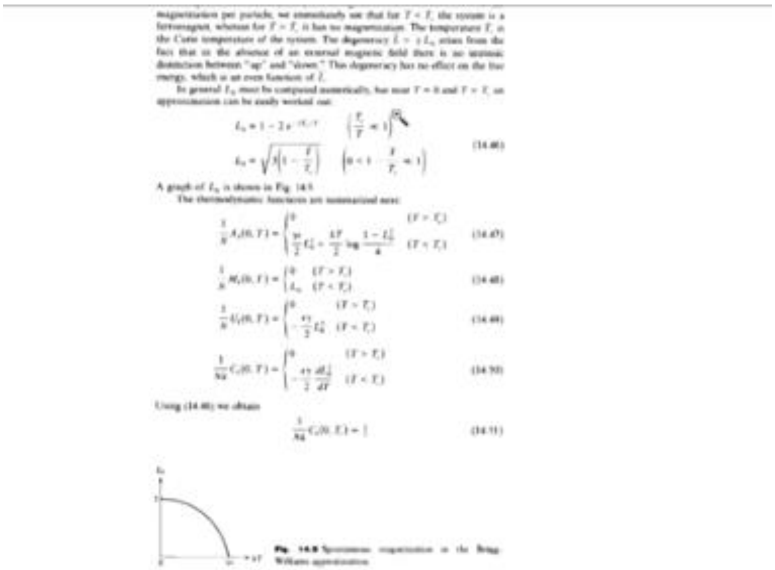

So one beautiful thing of that is the following, of all these calculations is the following; that in general can be, it can be obtained numerically and one finds numerically, some very interesting things comes out.

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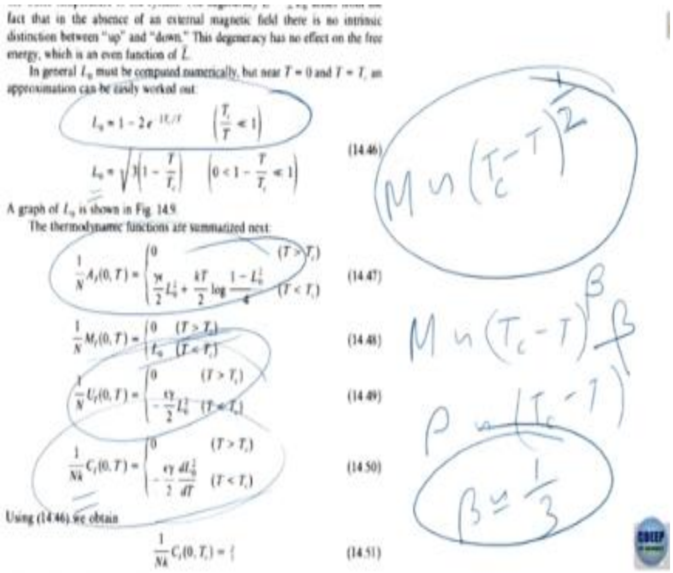

fact that in the absence of an external magnetic field there is no intrinsic distinction between "up" and "down." This degeneracy has no effect on the free energy, which is an even function of $\bar{L}$.

In general L_0 must be computed numerically, but near $T = 0$ and $T = T_c$ an approximation can be easily worked out:

$$L_0 \approx 1 - 2e^{-2T_c/T} \qquad \left(\frac{T_c}{T} \ll 1\right)$$

$$L_0 \approx \sqrt{3\left(1 - \frac{T}{T_c}\right)} \qquad \left(0 < 1 - \frac{T}{T_c} \ll 1\right) \tag{14.46}$$

A graph of L_0 is shown in Fig. 14.9.

The thermodynamic functions are summarized next:

$$\frac{1}{N}A_I(0,T) = \begin{cases} 0 & (T > T_c) \\ \frac{\gamma\epsilon}{2}L_0^2 + \frac{kT}{2}\log\frac{1-L_0^2}{4} & (T < T_c) \end{cases} \tag{14.47}$$

$$\frac{1}{N}M_I(0,T) = \begin{cases} 0 & (T > T_c) \\ L_0 & (T < T_c) \end{cases} \tag{14.48}$$

$$\frac{1}{N}U_I(0,T) = \begin{cases} 0 & (T > T_c) \\ -\frac{\epsilon\gamma}{2}L_0^2 & (T < T_c) \end{cases} \tag{14.49}$$

$$\frac{1}{Nk}C_I(0,T) = \begin{cases} 0 & (T > T_c) \\ -\frac{\epsilon\gamma}{2}\frac{dL_0^2}{dT} & (T < T_c) \end{cases} \tag{14.50}$$

Using (14.46) we obtain

$$\frac{1}{Nk}C_I(0,T_c) = \frac{3}{2} \tag{14.51}$$

$M \sim (T_c - T)^{1/2}$

$M \sim (T_c - T)^{\beta}$

$\rho \sim (T_c - T)$

$\beta \simeq \frac{1}{3}$

That near the critical temperature when you are close to T$_C$, close to T$_C$ is a subject of great, great interest because of the critical, what is called the critical phenomena and we have done Landau theory of the critical phenomena somewhat. Then you find that numerically that this approximation then L$_0$ gives as like that when you are away from the critical point, but when you are very in a region close to critical point.

Then the order parameter or magnetization behaves as, $(T_C - T)^{1/2}$ this is that means the magnetisation varies sharply as a fractional exponent and this exponent is called in a critical phenomena magnetic is called exponent beta. We use the same beta in many, many different ways this is equation of state also this is the same way Rho varies as again TC-T.

Also the notation beta in Mean Field Theory, Landau Theory, Bragg Williams Theory all these cases this exponent beta is half which experimentally is found to be wrong, experiment you one found, yes there is a fractional exponent and the basic thing is current that they is a very singular behaviour it shows near the critical phenomena but this exponent is more like one-third. So this is called equation of state exponent and as I told you magnetization same as density in order disorder transition.

They gain the track probability of one being occupied by copper or magnetization or you can say composition, you know one minus other density of minus density of the copper minus density of the zinc, is exactly same thing. All now in need not be strictly one-third between varies from 0.36 to 0.31 and all these things. But essentially very, very similar, so this is the essence of the critical phenomena and the critical exponents and the critical exponents in many different forms.

But this magnetization and density is specific it also has a critical behaviour that we will be discussing little bit here. So now here the thermodynamic functions are summarized for these, so this is the magnetization the L_0 and so, this is the free energy and then you get the, as I said magnetization, this is the internal energy and this is the specific heat, that goes like that and they gives in the following fraction, it in this case it does not.

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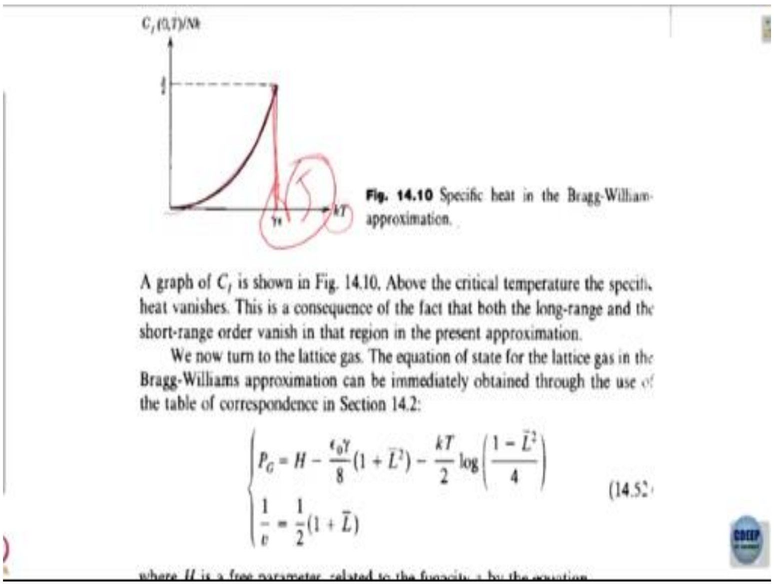

Fig. 14.10 Specific heat in the Bragg-Williams approximation.

A graph of C_I is shown in Fig. 14.10. Above the critical temperature the specifi heat vanishes. This is a consequence of the fact that both the long-range and the short-range order vanish in that region in the present approximation.

We now turn to the lattice gas. The equation of state for the lattice gas in the Bragg-Williams approximation can be immediately obtained through the use o the table of correspondence in Section 14.2:

$$\begin{cases} P_G = H - \dfrac{\epsilon_0\gamma}{8}(1+\bar{L}^2) - \dfrac{kT}{2}\log\left(\dfrac{1-\bar{L}^2}{4}\right) \\ \dfrac{1}{v} = \dfrac{1}{2}(1+\bar{L}) \end{cases} \tag{14.52}$$

where H is a free parameter related to the fugacity z by the equation

So specific in the Bragg Williams approximation type does not diverge, but it increases like that. So this gamma J, if I increase the, this is combined gamma J as I increase the temperature $K_B T$ and it goes and saturates to high do like that it increases like that, and then similarly one can go to lattice gas. This property comes from this; Solution comes from this solution here, this thing.

You can figure it out so that we just described in the previous page, similar behaviour you get indeed lattice gas, very similar equations that table of correspondence is given, and this is just exactly the same one model maps into the other model predictions are exactly the same.

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Same will be binary alloy. So now this is what it is this beautiful thing given here where I have been referring to all this time.

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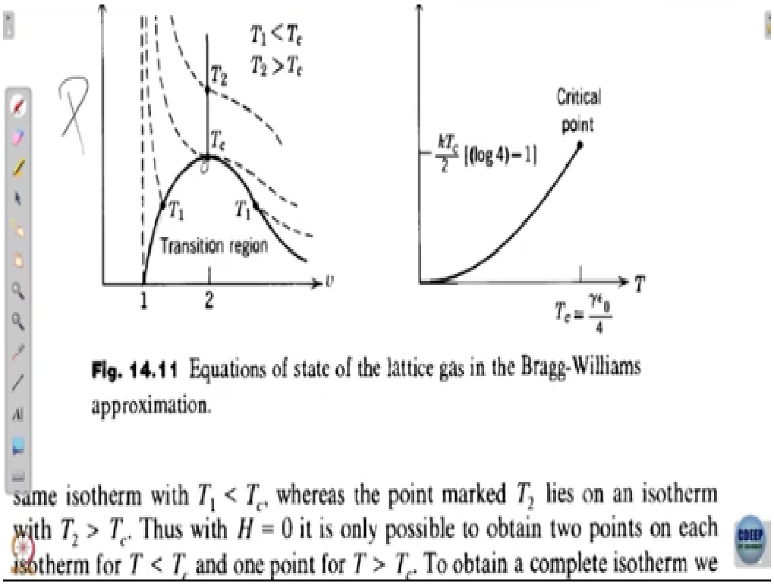

Fig. 14.11 Equations of state of the lattice gas in the Bragg-Williams approximation.

same isotherm with $T_1 < T_c$, whereas the point marked T_2 lies on an isotherm with $T_2 > T_c$. Thus with $H = 0$ it is only possible to obtain two points on each isotherm for $T < T_c$ and one point for $T > T_c$. To obtain a complete isotherm we

That, these the gas liquid all of you know Van Der Waals, that pressure versus volume, pressure versus volume, volume is isotherm and this is the critical point when this is the inverse parabola that I was drawing as density versus temperature, if I plot against temperature I get that the top is the critical point and the lattice gas equation of state in the lattice gas and same in the this is the Mean Field Theory or simplest type of Mean Field theory Bragg Williams approximation not too simple as we have seen.

But it captures some aspects of the critical phenomena but does not as beautiful full aspect of critical phenomena which requires far more work and the same thing you get from Van Der Waals the same thing you get from Landau Theory and you need to do lot more work to go beyond this level of approximation.

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So next one level what does better with the considerable more work is the Bethe approximation, but we are not going to do that so we will stop here.

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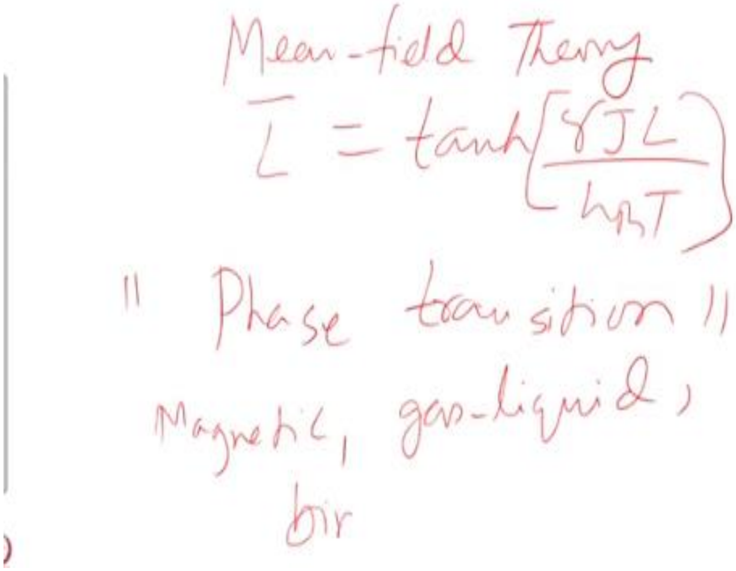

Mean-field Theory

$$\bar{L} = \tanh\left[\frac{\gamma J \bar{L}}{k_B T}\right]$$

" Phase transition "

Magnetic, gas-liquid,

bin

As for mean Field theory goes, so what did we achieve? We got a beautiful equation in average or L, we also got a equation, similar equation dependence of the magnetic field which is a little bit more complex not too much and both has to be solved numerically, but in some cases as you showed that one can do after doing the numerical work there are some idea what one can do.

And one get the magnetisation as a function of temperature in a critical exponent beta equal to half which is we call Mean Field exponent and that does not do a good job but what is the beauty of the whole thing is that, it does describe the phase transition.

It does capture many, many aspects of phase transition of three systems; which is magnetic, gas –liquid, then binary alloy, order disorder transition in binary alloys. All the three so it shows that these three systems to a certain level is isomorphic and this was further in a beautiful paper that I recommend people to study by;

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Yang and Lee (1952)

Yang and Lee 1952 in Physical Review he further pushed this analogy between Ising and lattice gas and binary alloy. Actually some of these things follows what we have done follows from these classic paper of Yang and Lee and these two gentlemen got the Nobel Prize for what their work on parity but in 1952 they wrote to Physical Review papers one after another where they mapped the Mayer’s Theories, so they connected the Ising model of Mayer’s theory and they showed that the cluster integrals that we do in Mayer theory are can be expressed in terms of zeros of the grand canonical partition function and huge number of results were done together and all these build things of Ising, Ising model binary alloy all these things were put together in a pop making paper of in these two papers and, you know what level Mean Field Theory working, what level not working.

So that along with Mayer’s theory and Ising model, Yang Lee to those two papers played essentially the starting point or launching point sometimes obtained tends to our study of the phase transitions and critical point. So we might come returned later to the critical phenomena and a little bit more we already have done the Landau Theory and we have done the concept of order parameter.

And you see here already that in the free energy then ultimately described in terms of a L square term and L is the magnetization and Landau theory or a parameter is the magnetisation, so Landau theories expansion of free energy in terms of L Square L for is fully consistent with the Bragg Williams. Or other way around though Bragg Williams has a microscopic basis it starts with the Hamiltonian but Landau's just writes down the free energy expansion.

So it is quite satisfying to see that the Landau Theory is recovered in a more consistent theoretical framework. And so the concept of order parameter that we introduced in Landau Theory which is same as a long range order parameter here, which is same as the magnetization, which is same as the density, which is same as the mole fraction. So Bragg Williams approximation gives us a beautiful understanding of the free energy.

That is happening the flattening of the free energy surface all these things comes out of the Bragg Williams what is periodically assumed Bragg Williams arguments and the basic physics by Landau. Okay, so we will stop here now we will probably get to use Lee and Yang again and we get to use Ising model again in future course. We stop here and now thank you.