

Statistical Mechanics Notes for L. Susskind's Lecture Series, Part 10

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Abstract

This paper contains my notes on the tenth lecture of the 2013 Leonard Susskind's Statistical Mechanics Stanford Lecture Series. (He also made a 2009 video series on the same topic.) They can be found on YouTube. Our goal this time is to use the Ising model to form an analogy to the liquid-gas phase transition.

1 Getting Started

In what way is the Ising Model of magnetism also a model of a liquid-gas phase transition?

The model presented in the last lecture is somewhat accurate for large dimension d . In fact, there is no phase transition in 1d, but in 2d and higher there will be. The approximation we get in 3d is pretty accurate. In 3d, each atom has six neighbors. The Mean Field Approximation offers us a qualitative understanding of the basic principles involved.

At each point in the lattice, we associate a σ . If it is $+1$, the spin is up, if it is -1 the spin is down.

In the Ising model we looked at, we saw that we could think about the energy as residing in the connections between the sites (the bonds) rather than in the sites themselves.

$$E = -J \sum_{\text{links}} \sigma(i)\sigma(j), \quad (1)$$

where i, j refer to two ends of a link.

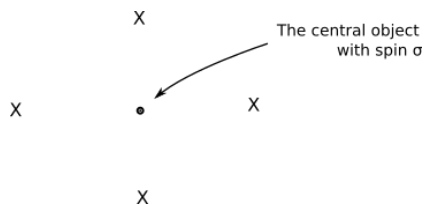


Figure 1. The Central Object and its nearest neighbors. (Only 2d shown.)

Now, to change two adjacent parallel spins to antiparallel spins, requires two units of energy. Thus, every broken bond cost an energy of $2J$.

$$E = -J \sum_{\text{links}} \sigma(i)\sigma(j) + \sum_{\text{sites}} h\sigma(i), \quad (2)$$

the h acting on the sites has a tendency to make the σ 's $+1$, whereas the tendency of the first term is to make the neighbors lie in the same direction.

The energy of the system is then

$$\begin{aligned}\bar{E} &= -2dJ\bar{\sigma}\sigma + h\sigma \\ &= [-2dJ\bar{\sigma} + h]\sigma.\end{aligned}\tag{3}$$

The value σ is itself an average, which we'll denote by $\bar{\bar{\sigma}}$. Hence,

$$\bar{\bar{\sigma}} = \tanh[-2dJ\bar{\sigma} + h]\beta.\tag{4}$$

Now, we make the Mean-Field Approximation $\bar{\bar{\sigma}} = \bar{\sigma}$.

$$\bar{\sigma} = \tanh[-2dJ\bar{\sigma} + h]\beta.\tag{5}$$

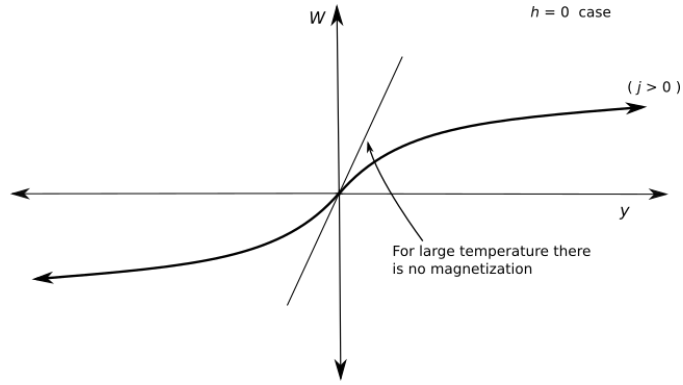


Figure 2. For large temperature there is no magnetization.

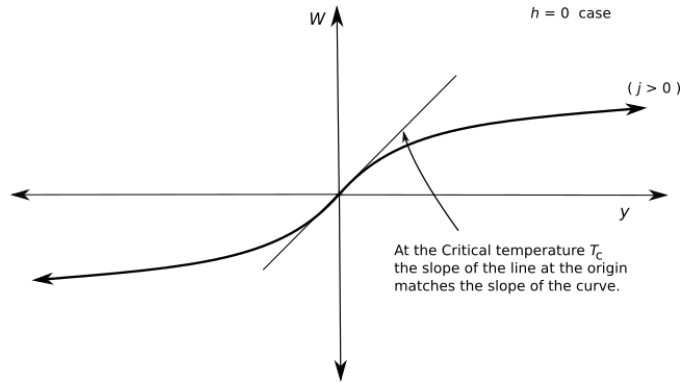


Figure 3. The Critical Temperature T_c is where the slope of the line is the slope of the tanh function at the origin.

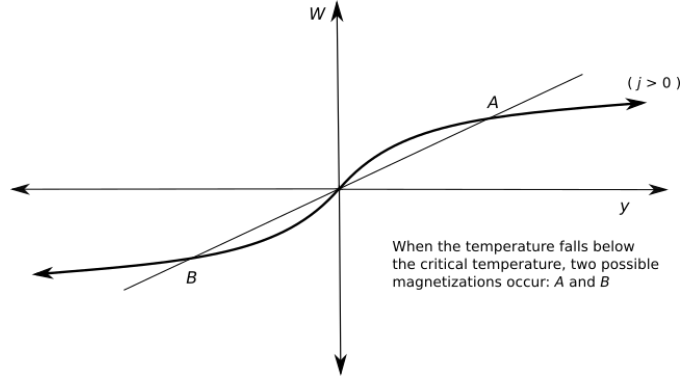


Figure 4. For temperatures below T_c magnetization will occur at either point A or point B .

We make the change in variables

$$y = 2\beta dj \bar{\sigma} . \quad (6)$$

Thus, (5) becomes

$$\frac{y}{2\beta dj} = \tanh y , \quad (7)$$

Now, we have the two coupled equations to solve simultaneously, either graphically or numerically:

$$W = \frac{1}{2\beta dj} y = \frac{T}{2dj} y , \quad (8a)$$

$$W = \tanh y . \quad (8b)$$

A straight line through the origin of slope 1 will only intersect the $\tanh y$ function at the origin. But as soon as the slope is greater than 1 or less than 1, the line will also intersect the $\tanh y$ function other than at the origin. The point P in Figure 2 is one such intersection point.

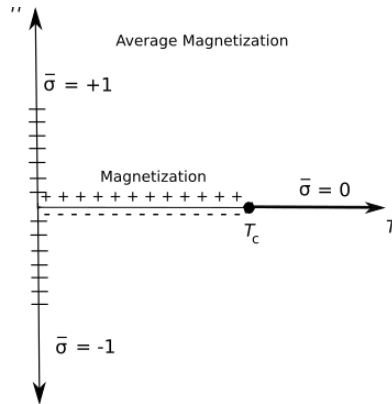


Figure 5. For temperatures below T_c magnetization will occur.

We can determine the critical temperature T_c by setting the slope of the line equal to unity:

$$\frac{T_c}{2dj} = 1 , \quad (9)$$

from which we get that

$$T_c = 2dj. \quad (10)$$

2 Chemical Potential and Phase Change

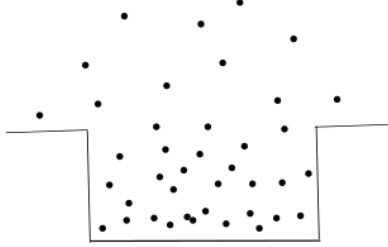


Figure 6. The number of particles N in the open box can change.

The particles going in and out of the box in Figure 6 have a vertical potential to deal with.

$$Z = \sum_{P, X, N} e^{-\beta \bar{E} + N\mu\beta}. \quad (11)$$

The chemical potential μ per particle is the term in the energy which depends on the number of particles in the box. Thus the chemical potential is the variable to change to affect the density of the fluid. For fixed volume of the box, that means changing the average number of particles in the box.

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In a liquid-gas transition, you take your box, keep it at a fixed temperature, and start varying the chemical potential.

- Density is a natural function of chemical potential.
- At some point in this change, the density of the fluid abruptly changes from gas to liquid (or vice versa).
- What are the conditions needed to setup a liquid-gas phase transition?
 - Hardcore repulsion between molecules when very close.
 - Some attraction at distance.

Lattice-Occupation Rules:

- At each site of the lattice, you can have a particle or not.
- At a given site, $\sigma = +1$ means there's a particle there (σ up).
- At a given site, $\sigma = -1$ means there's no particle there (σ down).

For the “attraction at a distance” requirement, we will use the Ising Model.

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$$E \sim \sum_{\text{links}} -j\sigma_i\sigma_j. \quad (12)$$

We will define the zero of energy to be when there are no particles inhabiting the lattice. Changing one down spin to an up spin is equivalent to placing one particle in a lattice site.

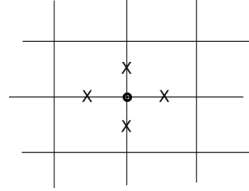


Figure 7. In 2d if we flip one spin, we break four bonds.

In Figure 7, the central object represents just one spin to flip, which will change the energy by

$$\Delta E = 2J/\text{bond} = 8J. \quad (13)$$

So, one particle has energy $8J$. If we put in two widely separated particles or merely diagonally separated, the energy change is $16J$. But if the two are neighbors, the energy change is $16J - 4J = 12J$, because the bond between them is not broken.

Therefore, something interesting happens when two widely separated particles get within a single bond length of each other: The common energy is decreased by four units, which acts like an attractive potential.

Does this system have a chemical potential? The chemical potential is just the energy of having a particle present. So the answer is yes, because just to have a particle in one site with no other particles around gives $8J$ units of energy.

Is there a way to vary the chemical potential without varying J ? Yes, we can apply an external magnetic field, h . Then,

$$E \sim \sum_{\text{links}} -j\sigma_i\sigma_j + \sum_{\text{sites}} h\sigma_i. \quad (14)$$

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So, for every isolated site that goes from down to up, gives us $2h$.

The average number of particles per site is given as

$$\frac{1 + \bar{\sigma}}{2} \quad \text{where} \quad \bar{\sigma} = \begin{cases} +1 \\ -1 \end{cases}. \quad (15)$$

Therefore, the density of particles ρ is proportional to this:

$$\rho \propto \frac{1 + \bar{\sigma}}{2}. \quad (16)$$

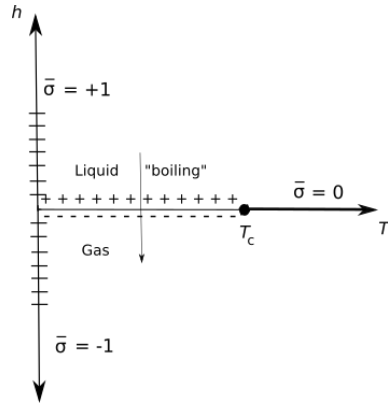


Figure 8. The arrow represents the boiling process, meaning that the occupied sites, represented by pluses, are replaced by unoccupied sites, represented by minues.
