Title: Statistical Mechanics (PHYS 602) - Lecture 4

Date: Oct 01, 2009 10:30 AM

URL: http://pirsa.org/09100123

Abstract:

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## More is the Same Phase Transitions and Mean Field Theories

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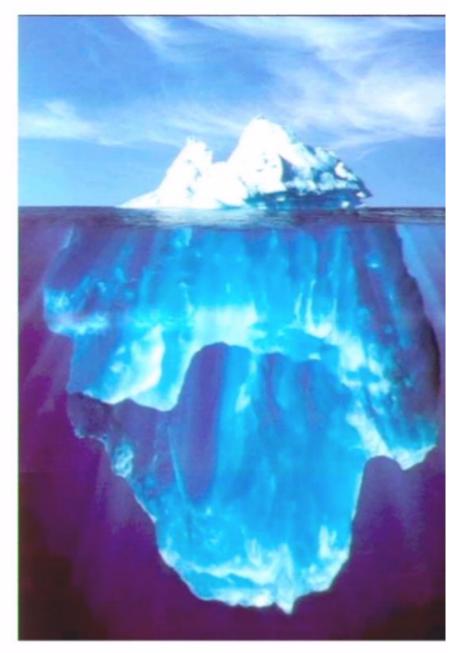
## Abstract

This talk summarizes concepts derived from the study of phase transitions mostly within condensed matter physics. In its original form, the talk was aimed equally at condensed matter physicists and philosophers of science. The latter group are particularly interested in the logical structure of science. This talk bears some traces of its history. The key technical ideas go under the names of ``singularity", ``order parameter", ``mean field theory", ``variational method", and ``correlation length". The key ideas here go under the names of 'mean field theory", "phase transitions", "universality", "variational

Pirsa: 0910012\method", and "scaling".

## Issues

Matter exists in different phases, different states of matter with qualitatively different properties: These phases are interesting in modern physics and provocative to modern philosophy. For example, no phase transition can ever occur in a finite system. Thus, in some sense phase transitions are not products of the finite world but of the human imagination.



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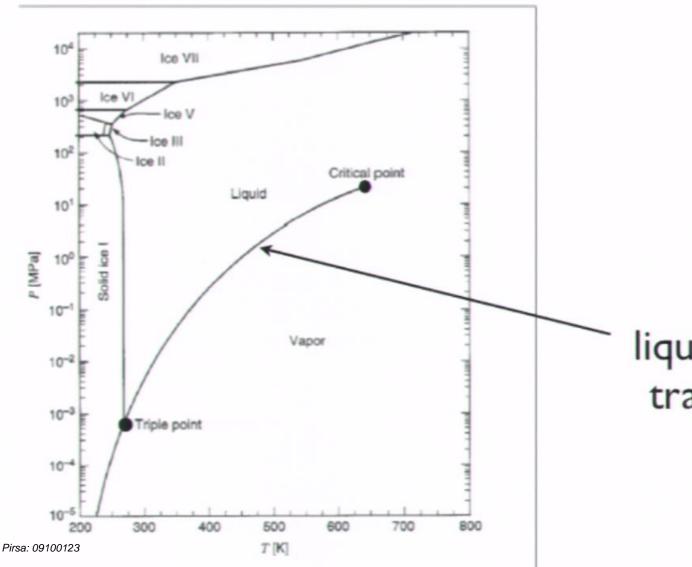
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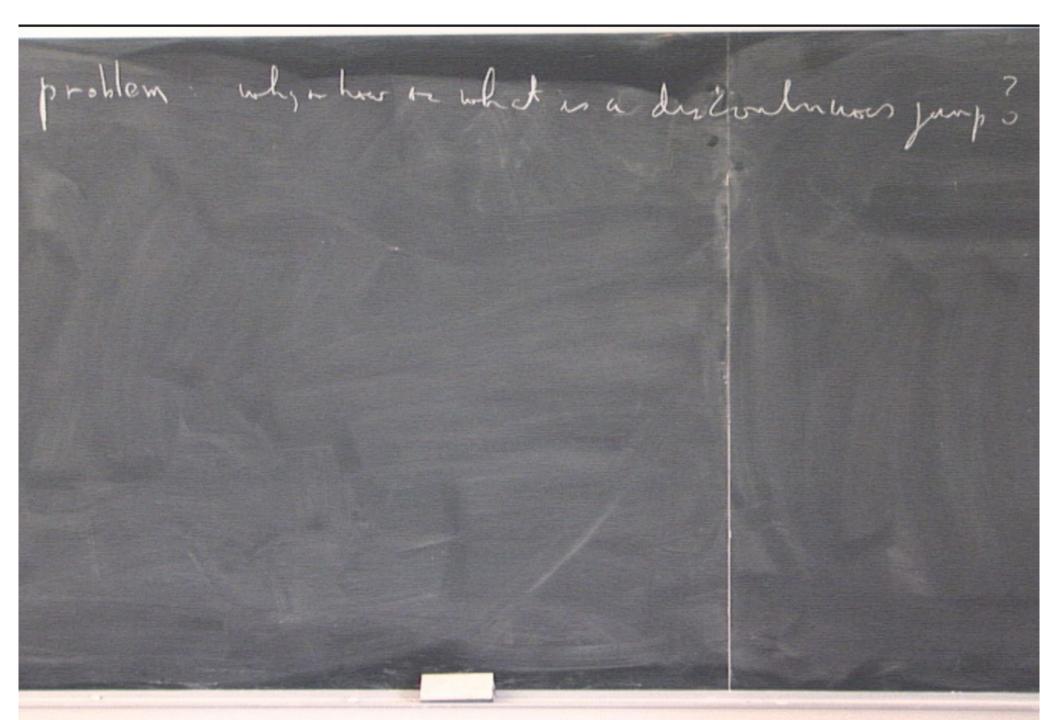
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## Phase Diagram for Water



liquid-gas phase transition line



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#### **Dual Couplings**

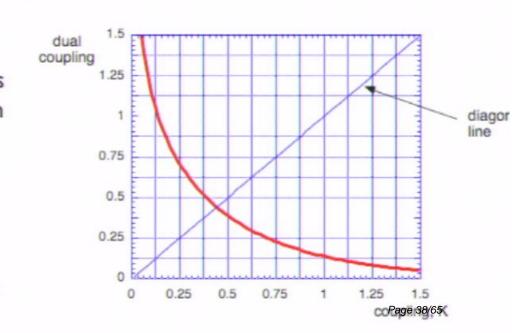
$$-\mathcal{H} = \widetilde{K}_0 \mathbf{1} + \widetilde{K} \tau_1 \qquad (4.22)$$

The quantity  $\tilde{K}$  is said to be the dual of K. For a simpler notation, we call this function by another name so that the dual of K is D(K) This name implies in part that the function D(K) has the property that if it is applied twice that you get precisely the same thing once more:

$$D(D(K))=K$$
 or  $D^{-1}(K)=D(K)$   
How would I find the function  $D(K)$ ?

$$\widetilde{K} = D(K) = -[\ln(\tanh K)]/2$$
  $\widetilde{K}_0 = [\ln(\sinh 2K)]/2$ 

This function has the property that when *K* is strong its dual is weak and *vice versa*. This property has proven to be very important in both statistical physics and particle physics. Often we know both a basic model and its dual. Often models are hard to solve in strong coupling. But the dual models have weak coupling when the basic model has strong coupling. So then we get an indirect Pirsa: 09100123 SOLUTION of the basic model.



## Solution of the one-dimensional Ising model

From equation 4.20, we find that the partition function of the one-dimensional Ising model is

$$Z = \text{trace } (e^{K}\mathbf{1} + e^{-K}\tau_{1})^{N}$$

But the trace is a sum over eigenvalues and the eigenvalues of  $\tau_1$ are plus or minus one. Thus, the answer is:

$$Z = (2\cosh K)^{N} + (2\sinh K)^{N}$$
(4.25)

If N is very large, the first term is much larger than the second and thus in this limit of large system size:

$$-\beta F = \ln Z = N \ln(2 \cosh K) \tag{4.26}$$

What quantum mechanics problem have we solved?

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## More about quantum from the Long Chain

We should be able to say more about quantum problems based upon the analysis of the long chain. For example let us imagine that we wish to calculate the average of some quantum operator, X(q), which happens to be diagonal in the q-representation. The text book goes through a long song and dance to prove a rather obvious result. You have seen that the trace in equation 4.10 pushes us into a sum over energy states, and if N is very large that sum reduces to a projection onto the ground state of the system. Specifically,

$$Z = \text{trace}_{q_1} \text{trace}_{q_2} \dots \text{trace}_{q_n} \prod_{j=1}^{N} \exp(w(q_j, q_{j+1}))$$
 (4.10)

becomes  $Z=\exp(-\tau\epsilon_0)$ 

So if we insert an X, for any any operator X, in that sum the result should give what happens to that X in the ground state, specifically

$$(1/Z) \operatorname{Trace}_{\{q\}} \exp[W\{q\}] X = <0 | X(q) | 0 >$$

In this way, we can use statistical mechanics to calculate the average of any operator in the ground state. If we do not take N to infinity, we can do the corresponding calculation to calculate the average of any operator at a inverse temperature ( $\beta$ - value) equal to N  $\tau$ .

By playing with the times in an appropriate fashion, we can even calculate time-dependent Pirsa: 09100123 correlation functions in the ground state or in a finite-temperature state.

## Statistical Correlations in a Long Chain

We should be able lots about the statistical mechanics of a the long chain with Ising style interactions. For example, let us calculate the average of the jth spin on a long chain or the correlations among the spins in the chain. Start from

$$Z = \text{Tr exp}\left[\sum_{j=1}^{N} K \sigma_{j+1} \sigma_{j}\right]$$

$$< \sigma_{k} >= (1/Z) \text{Tr} \sigma_{k} \exp\left[\sum_{j=1}^{N} K \sigma_{j+1} \sigma_{j}\right]$$

$$< \sigma_{k} \sigma_{k+r} >= (1/Z) \text{Tr} \sigma_{k} \sigma_{k+r} \exp\left[\sum_{j=1}^{N} K \sigma_{j+1} \sigma_{j}\right]$$

Here Tr means "sum over all the N spin-values". We use periodic boundary conditions. In this equation all the  $\sigma$ 's are numbers, and they commute with each other.

We can make the calculation easier by replacing all the couplings by their expressions in terms of Pauli spins matrices giving these three calculations as, first,

$$Z=\operatorname{trace}_{\mathsf{T}} \prod_{j=1}^{\mathsf{N}} \exp\left(\widetilde{\mathsf{K}}_0 + \widetilde{\mathsf{K}}\mathsf{T}_1\right) = \operatorname{trace}_{\mathsf{T}} \exp[\mathsf{N} \left(\widetilde{\mathsf{K}}_0 + \widetilde{\mathsf{K}}\mathsf{T}_1\right)]$$

$$= (2 \cosh \mathsf{K})^\mathsf{N} + (2 \sinh \mathsf{K})^\mathsf{N} \qquad \approx (2 \cosh \mathsf{K})^\mathsf{N}$$

The  $\approx$  is an approximate equality which holds for large N. Note that in this limit the Pirsa: 09100123 term with eigenvalue of  $T_1 = 1$  dominates because the dual coupling is positive.

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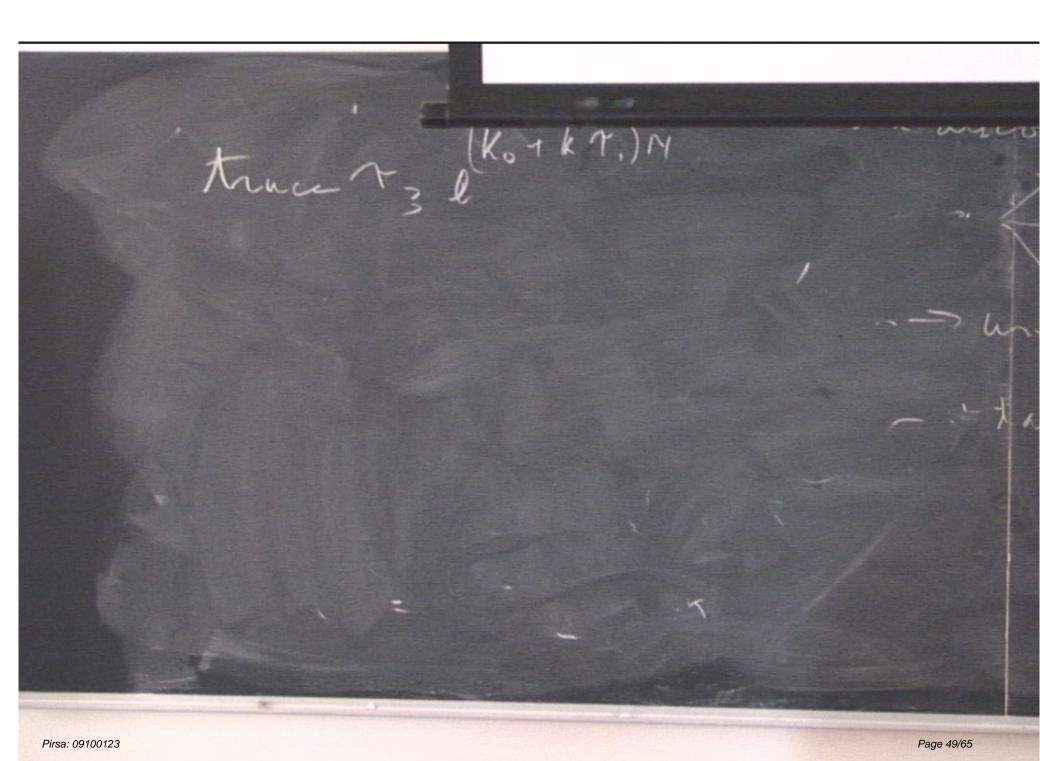
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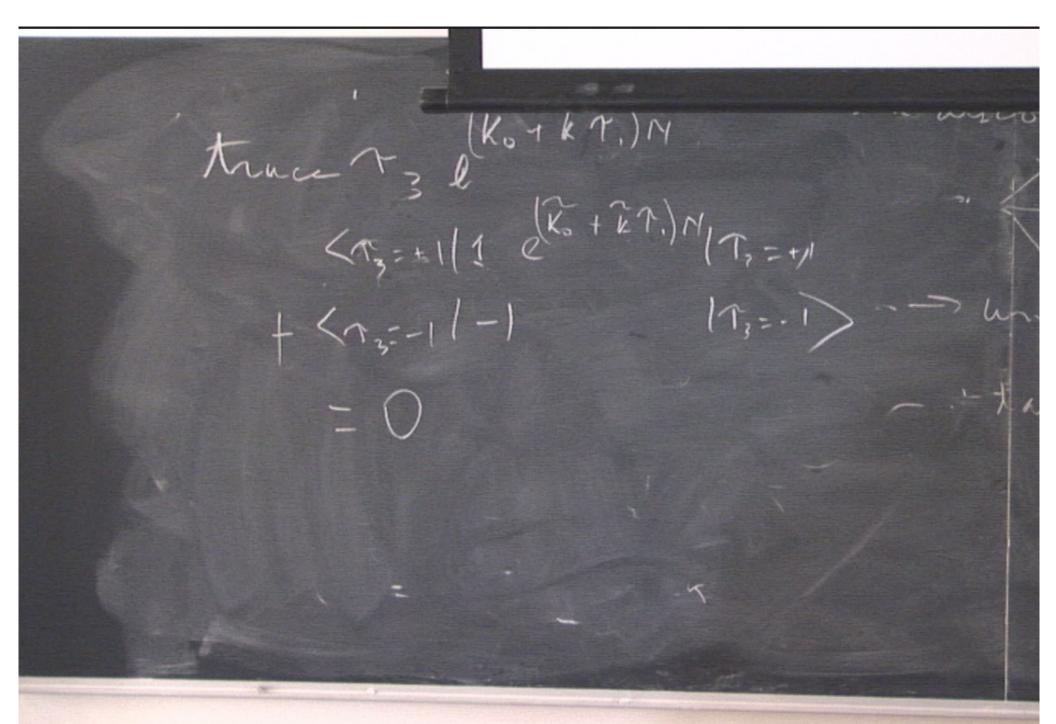
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$$=(2\;\operatorname{cosh}\;\mathsf{K})^{\mathsf{N}}+(2\;\operatorname{sinh}\;\mathsf{K})^{\mathsf{N}}\qquad \approx \;(2\;\operatorname{cosh}\;\mathsf{K})^{\mathsf{N}}$$

The  $\approx$  is an approximate equality which holds for large N. Note that in this limit the Pirsa: 09100123 term with eigenvalue of  $T_1 = 1$  dominates because the dual coupling is positive.

## Average magnetization in a Long Chain

We know the answer: the system has full symmetry between spin up and spin down so that the average magnetization must be zero. Nonetheless, let's calculate

 $Z<\sigma_j>= \operatorname{trace}_{\mathsf{T}} \{\exp \left[-H \,\mathsf{T}(j-1)\right] \,\mathsf{T}_3 \,\exp \left[-H \,\mathsf{T}(N-j+1)\right] \}$ Since we can rearrange terms under a trace, as trace (ab)=trace (ba), this expression simplifies to =  $\operatorname{trace}_{\mathsf{T}} \{ \,\mathsf{T}_3 \,\exp \left[-H \,\mathsf{T} N\right] \} = \operatorname{trace}_{\mathsf{T}} \{ \,\mathsf{T}_3 \,\exp \left[-(K_0+K \,\mathsf{T}_1 \,N)\right] \}$ 

To evaluate the last expression we must take diagonal matrix elements of  $\tau_3$  between eigenstates of  $\tau_1$ . Both such matrix elements are zero. why? Because  $\tau_3$  acts to change the value of  $\tau_1$  so that  $\tau_3$   $|\tau_1=1> = |\tau_1=-1>$  so that  $|\tau_3|$   $|\tau_1=1> = |\tau_1=-1>=0$ . Therefore the entire result is zero and the average has the value zero, as expected.

$$\langle \sigma_j \rangle = 0$$

At zero magnetic field, the magnetization of the one-dimensional Ising model is zero. Thus, this Ising model has no ordered state. In fact no one-dimensional system with finite interactions has one. This model is always in the disordered phase at all finite temperatures.

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# Correlations in Large N limit

Let N be large. Z simplifies to  $Z = \exp(N\tilde{K}_0 + N\tilde{K})$  since the  $\tau_1$ =1 term dominates the trace We start from\*

$$Z < \sigma_j \sigma_{j+r} > = \operatorname{trace}_T \{ e^{-(j-1)H} \tau_3 e^{-rH} \tau_3 e^{-(N-j-r+1)H} \}, \quad \text{for large } N$$

\* Note how the ordering in space converts into an ordering in time.

Since we can rearrange terms under a trace, as trace (ab)=trace (ba), this expression simplifies to

$$(trace_{\tau} e^{-NH}) < \sigma_j \sigma_{j+r} > = trace_{\tau} \{e^{-(N-r)H} \tau_3 e^{-rH} \tau_3 \},$$
 so that

The  $K_0$  term is the same on both sides of the equation. It cancels. For large N, the  $\tau_1$  =1 term dominates both traces. Since the effect of  $\tau_3$  is to change the eigenvalue of  $\tau_1$  this result is

$$\exp[\widetilde{K}N] < \sigma_j \sigma_{j+r} > \approx \{\exp[\widetilde{K}N] \exp[-2 \widetilde{K}r] \}, \quad \text{for large } N$$
 Consequently

$$\langle \sigma_j \sigma_{j+r} \rangle \approx \exp[-2 \tilde{K} r]$$
, for large N iii. 7

The result is that correlations fall off exponentially with distance, with the typical falloff distance, denoted as  $\xi$ , being the distance between lattice Pirsa: 09100123 points (usually called a) times 1/(2D(K))=1/(2K).

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#### Correlation Length

$$<\sigma_j\sigma_{j+r}>=exp(-2r\tilde{K})$$
 =exp  $(-ar/\xi)$ 

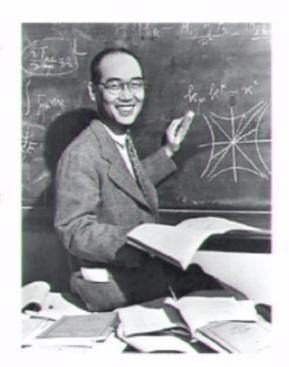
Here ar is distance between the sites of the two spins.

The result is that correlations fall off exponentially with distance, with the typical falloff distance, denoted as  $\xi$ , being the distance between lattice points (usually called a) times 1/(2D(K))=1/(2K). This falloff distance is very important in field theory, particle physics, and phase transition theory. In the latter context it is called the coherence length. It is also called the Yukawa distance because it first came up in Hideki Yukjawa's description of mesons. Here, in the one dimensional Ising model, we have a very large coherence length for large K. Specifically

$$1/(2\tilde{K}) = \xi/a \rightarrow \exp(2K)/2 \text{ as } K \rightarrow \infty$$

while is very small in the opposite limit of small K.

$$\xi/a \rightarrow 1/(-\ln(2K))$$
 as  $K \rightarrow 0$ 



Hideki Yukawa

Large correlation lengths, or equivalently small masses, play an important role in statistical and particle physics since they indicate a near-by phase transition or change in behavior.

Firsa: 09100123  $\xi$  = correlation length= a/[2D(K)] = a/(2K)

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#### Correlation Length

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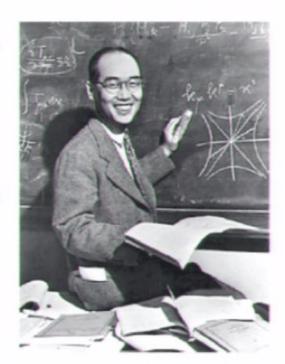
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#### Bloch Walls in 1 d

In the Ising model at large values of the coupling, K, the spins tend to line up.



However, with a cost in probability  $\exp(-2K)$  a whole region might flip its spins, producing a defect called a Bloch wall



This kind of defect produces the decay of correlations in the Ising model at low temperatures. In any long Ising chain, many such defects will be randomly placed and ruin any possibility of correlations over infinitely long distances.

This is the simplest example of what is called a topological excitation, a defect which breaks the ordering in the system by separating two regions with different kinds of order. Since ordering is crucial in many situations, so are topological excitations.

Notice that, at low temperatures, this kind of excitation is much more likely than a Pirsa: 09100123 simple flip of a single spin. The wall costs a factor of exp(-K); the flip costs exp(-2K).

\*\*\*\*

#### Renormalization for 1D ising,

following ideas of Kenneth Wilson, this calculation is due to David Nelson and myself

$$Z = \sum_{\sigma_1, \sigma_2, \dots} \exp(W_K \{ \sigma \}) = \sum_{\sigma_1, \sigma_2, \dots} \exp(K\sigma_1\sigma_2 + K\sigma_2\sigma_3 + \dots)$$

Rearrange calculation: Rename spins separated by two lattice sites: let  $\mu_1=\sigma_1$ ;  $\mu_2=\sigma_3$ ,  $\mu_3=\sigma_5$ , ....; and sum over every other spin,  $\sigma_2$ ,  $\sigma_4$  .....

$$Z = \sum_{\mu_1, \mu_2, \dots} \sum_{\sigma_2, \sigma_4, \dots} \exp(K\mu_1 \sigma_2 + K\sigma_2 \mu_2 + \dots) = \sum_{\mu_1, \mu_2, \dots} \exp(w'\{\mu\})$$

Note that sum over  $\sigma_2$ ,  $\sigma_4$ ..... generates only nearest neighbor interactions for the  $\mu$ 's

$$w'\{\mu\} = const + K' \mu_1 \mu_2 + K' \mu_2 \mu_3 + ...$$

K´ describes same system as before, with a new separation between lattice sites, which is twice as big as the old separation. Since the physical system is the same, physical quantities like the correlation length and the entropy are unchanged, but their description in terms of couplings and lattice constants has changed. In particular, the new lattice spacing is a´ = 2a, but the correlation length is exactly the same  $\xi$ ´ =  $\xi$ . Since we know that the correlation length is given by

 $\xi = a/[2D(K)]$ , we know that the new coupling obeys a/[2D(K)] = a'/[2D(K')] we find that the new coupling obeys D(K') = 2D(K) before we do any detailed Pirsa: \*\*Opena\*\*rmalization calculations. Since D is a decreasing function of K we know that Page 62/65 the new, renormalized, coupling is smaller than the old one.

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# Ising Model in d=2

$$-H/(kT) = K \sum_{nn} \sigma_r \sigma_s + h \sum_r \sigma_r$$

 $\sigma_r = \pm 1$ 

nn indicates a sum over nearest neighboirs

square lattice



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Onsager calculated partition function and phase transition for this situation

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Nearest neighbor structure s's are nearest neighbors to r Bonds= $\exp(K\sigma\sigma')$  connect nearest neighbors