

G25.2651: Statistical Mechanics

Notes for Lecture 27

I. THE EXPONENTS ν AND η

Consider a spin-spin correlation function at zero field of the form

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{Q} \sum_{\sigma_1} \cdots \sum_{\sigma_N} \sigma_i \sigma_j e^{-\beta H}$$

If σ_i and σ_j occupy lattice sites at positions \mathbf{r}_i and \mathbf{r}_j , respectively, then at large spatial separation, with $r = |\mathbf{r}_i - \mathbf{r}_j|$, the correlation function depends only r and decays exponentially according to

$$G(r) \equiv \langle \sigma_i \sigma_j \rangle - \langle \sigma_i \rangle \langle \sigma_j \rangle \sim \frac{e^{-r/\xi}}{r^{d-2+\eta}}$$

for $T < T_c$. The quantity ξ is called the *correlation length*. Since, as a critical point is approached from above, long range order sets in, we expect ξ to diverge as $T \rightarrow T_c^+$. The divergence is characterized by an exponent ν such that

$$\xi \sim |T - T_c|^{-\nu}$$

At $T = T_c$, the exponential dependence of $G(r)$ becomes 1, and $G(r)$ decays in a manner expected for a system with long range order, i.e., as some small inverse power of r . The exponent η appearing in the expression for $G(r)$ characterizes this decay at $T = T_c$.

The exponents, ν and η cannot be determined from MFT, as MFT neglects all correlations. In order to calculate these exponents, a theory is needed that restores fluctuations at some level. One such theory is the so called *Landau-Ginzberg* theory. Although we will not discuss this theory in great detail, it is worth giving a brief introduction to it.

II. INTRODUCTION TO LANDAU-GINZBERG THEORY

The Landau-Ginzberg (LG) theory is a phenomenological theory meant to be used only near the critical point. Thus, it is formulated as a macroscopic theory. The basic idea of LG theory is to introduce a spin density field variable $S(\mathbf{x})$ defined by

$$S(\mathbf{x}) = \sum_{i=1}^N \sigma_i \delta(\mathbf{x} - \mathbf{x}_i)$$

Then the total magnetization is given by

$$M = \int d^d x S(\mathbf{x})$$

Since the free energy at zero field is $A = A(N, M, T)$, there should be a corresponding free energy density $A(T, S(\mathbf{x})) = a(\mathbf{x})$ such that

$$A(N, M, T) = \int d^d x a(\mathbf{x})$$

It is assumed that $a(\mathbf{x})$ can be represented as a power series according to

$$a(\mathbf{x}) = a_0 + a_1(T)S^2(\mathbf{x}) + a_2(T)S^4(\mathbf{x}) + \cdots$$

such that a_1 and a_2 are both positive for $T > T_c$ and a_1 vanishes at $T = T_c$. These conditions are analogous to those exhibited by the total free energy in MFT above and near the critical point (see previous lecture). By symmetry, all odd terms vanish and are, therefore, not explicitly included.

In the presence of a magnetic field $h(\mathbf{x})$, we have a Gibbs free energy density given by

$$g(\mathbf{x}) = a(\mathbf{x}) - h(\mathbf{x})S(\mathbf{x}) = a_0 + a_1(T)S^2(\mathbf{x}) + a_2(T)S^4(\mathbf{x}) - h(\mathbf{x})S(\mathbf{x})$$

In addition, a term $a_3(\nabla S)^2$ with $a_3 > 0$ is added to the free energy in order to damp out local fluctuations. If there are significant local fluctuations, then $(\nabla S)^2$ becomes large, so these field configurations contribute negligibly to the partition function, which is defined by

$$\begin{aligned} Z &= \int \mathcal{D}[S] \exp \left[-\beta \int d^d x g(\mathbf{x}) \right] \\ &= \int \mathcal{D}[S] \exp \left[-\beta \int d^d x (a_0 + a_1(T)S^2(\mathbf{x}) + a_2(T)S^4(\mathbf{x}) + a_3(\nabla S)^2 - h(\mathbf{x})S(\mathbf{x})) \right] \end{aligned}$$

Thus, the LG theory is a field theory. The form of this field theory is well known in quantum field theory, and is known as a d -dimensional scalar *Klein-Gordon* theory. In terms of Z , a correlation function at zero field can be defined by

$$\langle S(\mathbf{x})S(\mathbf{x}') \rangle = \frac{1}{\beta^2} \frac{\delta^2 \ln Z}{\delta h(\mathbf{x})\delta h(\mathbf{x}')} \Big|_{h=0}$$

Thus, by studying the behavior of the correlation function, the exponents ν and η can be determined.

For the choice $a_2 = 0$, the theory can be solved exactly analytically. This is known as the Gaussian model, for which

$$Z = \int \mathcal{D}[S] \exp \left[-\beta \int d^d x (a_0 + a_1(T)S^2(\mathbf{x}) + a_3(\nabla S)^2 - h(\mathbf{x})S(\mathbf{x})) \right]$$

which leads to values of η and ν of 0 and $1/2$, respectively. These values are known as the “classical” exponents. They are independent of the number of spatial dimensions d . Dependence on d comes in at higher orders in S . Comparing these to the exact exponents from the Onsager solution, which gives $\eta = 1/4$ and $\nu = 1$, it can be seen that the classical exponents are only qualitatively correct. Going to higher orders in the theory leads to improved results, although the theory cannot be solved exactly analytically. It can either be solved numerically using path integral Monte Carlo or Molecular Dynamics or analytically perturbatively using Feynman diagrams.

III. RENORMALIZATION GROUP AND THE SCALING HYPOTHESIS

A. General formulation

The renormalization group (RG) has little to do with “group theory” as it is meant mathematically. Also, there is no uniqueness to the renormalization group, so the use of “the” in this context is misleading. Rather, the RG is an idea that exploits the physics of systems near their critical point which leads to a procedure for finding the critical point. It also offers an explanation of universality, perhaps the closest thing there is to a proof of this concept. Finally, through the scaling hypothesis, it generates relations, called *scaling relations* satisfied by the critical exponents. It does not allow actual determination of specific exponents. However, given a numerical calculation or some other method of determining a small subset of exponents, the scaling relations can be used to determine the remaining exponents.

In order to see how the RG works, we will consider a specific example. Consider a square spin lattice:

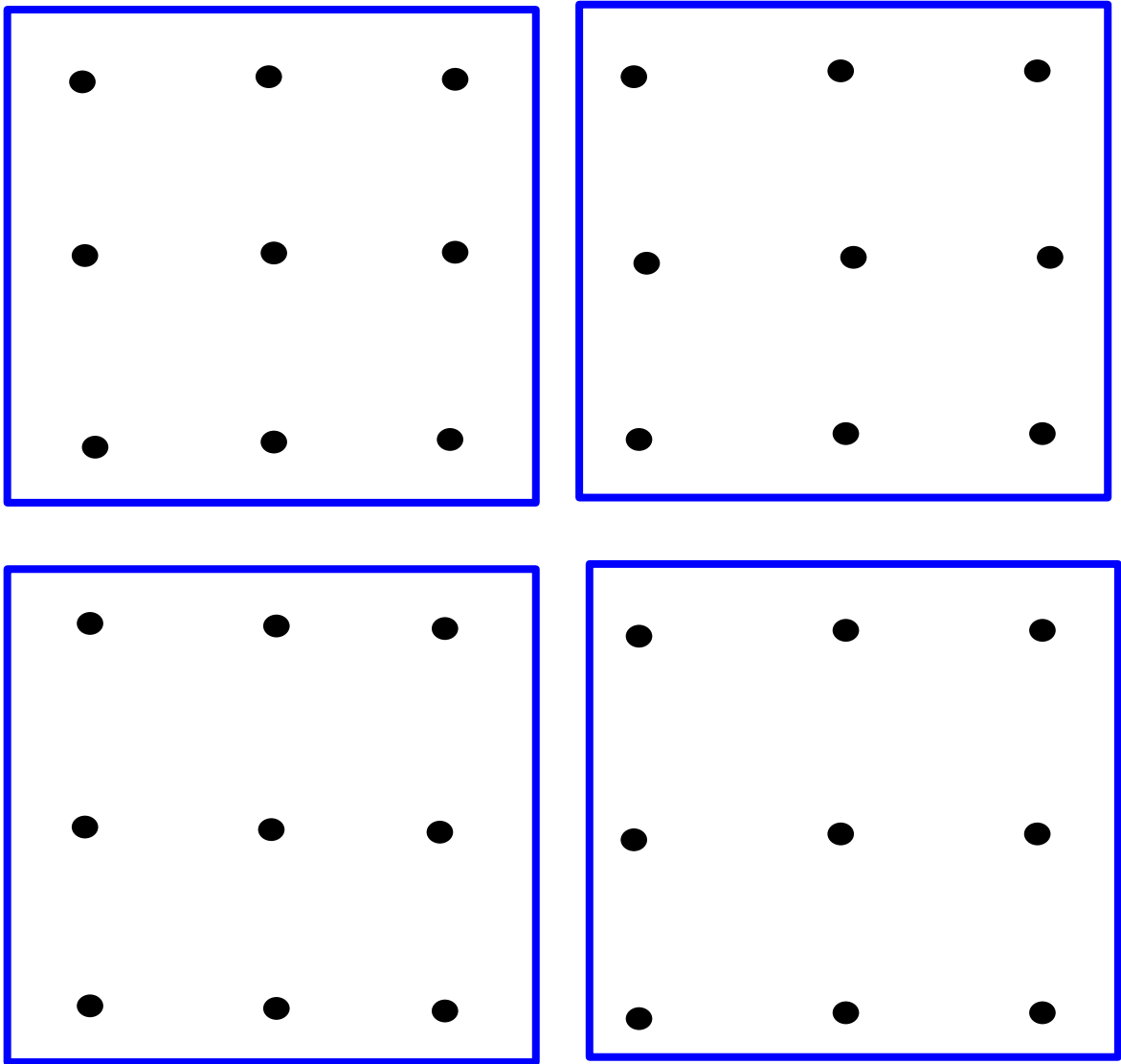


FIG. 1.

which has been separated into 3×3 blocks as shown. Consider defining a new spin lattice from the old by application of a coarse-graining procedure in which each 3×3 block is replaced by a single spin. The new spin is an up spin if the majority of spins in the block is up and down is the majority point down. The new lattice is shown below:



FIG. 2.

Such a transformation is called a *block spin transformation*. Near a critical point, the system will exhibit long-range ordering, hence the coarse-graining procedure should yield a new spin lattice that is statistically equivalent to the old spin lattice. If this is so, then the spin lattice is said to possess *scale invariance*.

What will be the Hamiltonian for the new spin lattice? To answer this, consider the partition function at $h = 0$ for the old spin lattice using the Ising Hamiltonian as the starting point:

$$Q = \sum_{\sigma_1} \dots \sum_{\sigma_N} e^{-\beta H_0(\sigma_1, \dots, \sigma_N)} \equiv \text{Tr}_{\sigma} e^{-\beta H_0(\sigma_1, \dots, \sigma_N)}$$

The block spin transformation can be expressed by defining, for each block, a transformation function:

$$T(\sigma'; \sigma_1, \dots, \sigma_9) = \begin{cases} 1 & \sigma' \sum_{i=1}^9 \sigma_i > 0 \\ 0 & \text{otherwise} \end{cases}$$

When inserted into the expression for the partition function, T acts to project out those configurations that are consistent with the block spin transformation, leaving a function of only the new spin variables $\{\sigma'_1, \dots, \sigma'_{N'}\}$, in terms of which a new partition function can be defined. To see how this works, let the new Hamiltonian be defined through:

$$e^{-\beta H'_0(\{\sigma'\})} = \text{Tr}_{\sigma} \left[\prod_{\text{blocks}} T(\sigma'; \sigma_1, \dots, \sigma_9) \right] e^{-\beta H_0(\{\sigma\})}$$

That this is a consistent definition follows from the fact that

$$\sum_{\sigma'} T(\sigma'; \sigma_1, \dots, \sigma_9) = 1$$

Thus, tracing both sides of the projected partition function expression over σ' yields:

$$\text{Tr}_{\sigma'} e^{-\beta H'_0(\{\sigma'\})} = \text{Tr}_{\sigma} e^{-\beta H_0(\{\sigma\})}$$

which states that the partition function is preserved by the block spin transformation, hence the physical properties are also preserved.

Transformations of this type should be chosen so as to preserve the functional form of the Hamiltonian, for if this is done, then the transformation can be iterated in exactly the same way for each new lattice produced by the previous iteration. The importance of being able to iterate the procedure is that, in a truly ordered state formed at a critical point, the iteration transformation will produce exactly the same lattice as the previous iteration, thus signifying the existence of a critical point. If the functional form of the Hamiltonian is preserved, then only its parameters are affected by the transformation, so we can think of the transformation as acting on these parameters. If the original Hamiltonian contains parameters $K_1, K_2, \dots, \equiv \mathbf{K}$ (e.g., the J coupling in Ising model), then the transformation yields a Hamiltonian with a new set of parameters $\mathbf{K}' = (K'_1, K'_2, \dots)$, such that the new parameters are functions of the old parameters

$$\mathbf{K}' = \mathbf{R}(\mathbf{K})$$

The vector function \mathbf{R} characterizes the transformation. These equations are called the *renormalization group equations* or *renormalization group transformations*. By iterating the RG equations, it is possible to determine if a system has an ordered phase or not and for what values of the parameters such a phase will occur.

B. Example: The one-dimensional Ising model

For the one-dimensional Ising model:

$$H_0 = -J \sum_{i=1}^N \sigma_i \sigma_{i+1}$$

Define:

$$\begin{aligned} \mathcal{H}_0 &= \beta H \\ K &= \beta J \end{aligned}$$

so that

$$\mathcal{H}_0 = -K \sum_{i=1}^N \sigma_i \sigma_{i+1}$$

and the partition function becomes

$$Q = \text{Tr}_{\sigma} e^{-\mathcal{H}_0}$$

We will consider a simple block spin transformation as illustrated below:

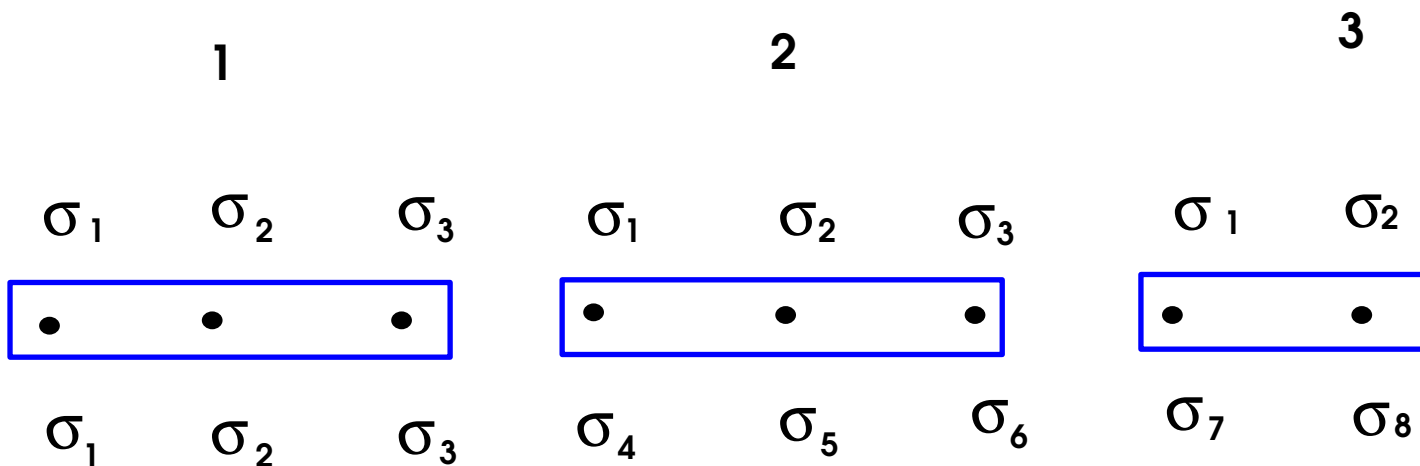


FIG. 3.

The figure shows the one-dimension spin lattice numbered in two different ways – one a straight numbering and one using blocks of three spins, with spins in each block numbered 1-3. The block spin transformation to be employed here is that the spin of a block will be determined by the value of the spin in the center of the block. Thus, for block 1, it is the value of spin 2, for block 2, it is the value of spin 5, etc. This rather undemocratic choice should be reasonable at low temperature, where local ordering is expected, and spins close to the center spin would be expected to be aligned with it, anyway. The transformation function, T for this case is

$$T(\sigma'; \sigma_1, \sigma_2, \sigma_3) = \delta_{\sigma' \sigma_2}$$

The new lattice will look like:

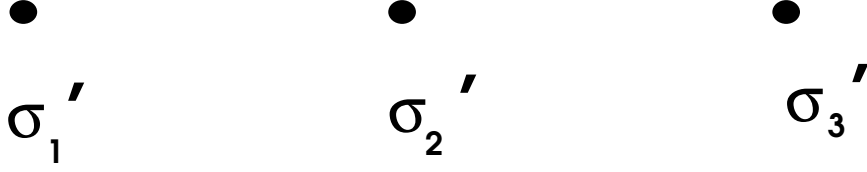


FIG. 4.

with $\sigma'_1 = \sigma_2$, $\sigma'_2 = \sigma_5$, etc.

The new Hamiltonian is computed from

$$\begin{aligned} e^{-cH_{z'}(\{\sigma'\})} &= \sum_{\sigma_1} \sum_{\sigma_2} \sum_{\sigma_3} \cdots \sum_{\sigma_N} (\delta_{\sigma'_1 \sigma_2} \delta_{\sigma'_2 \sigma_5} \cdots) e^{K\sigma_1 \sigma_2} e^{K\sigma_2 \sigma_3} e^{K\sigma_3 \sigma_4} e^{K\sigma_4 \sigma_5} \cdots \\ &= \sum_{\sigma_1} \sum_{\sigma_3} \sum_{\sigma_4} \sum_{\sigma_6} \cdots e^{K\sigma_1 \sigma'_1} e^{K\sigma'_1 \sigma_3} e^{K\sigma_3 \sigma_4} e^{K\sigma_4 \sigma'_2} \cdots \end{aligned}$$

The idea is then to find a K' such that when the sum over σ_3 and σ_4 are performed, the new interaction between σ'_1 and σ'_2 is of the form $\exp(K'\sigma'_1 \sigma'_2)$, which preserves the functional form of the old Hamiltonian. The sum over σ_3 and σ_4 is

$$\sum_{\sigma_3} \sum_{\sigma_4} e^{K\sigma'_1 \sigma_3} e^{K\sigma_3 \sigma_4} e^{K\sigma_4 \sigma'_2}$$

Note that $\sigma_3 \sigma_4 = \pm 1$. Then, since

$$\begin{aligned} e^\theta &= \cosh\theta + \sinh\theta = \cosh\theta [1 + \tanh\theta] \\ e^{-\theta} &= \cosh\theta - \sinh\theta = \cosh\theta [1 - \tanh\theta] \end{aligned}$$

we can express $\exp(K\sigma_3 \sigma_4)$ as

$$e^{K\sigma_3 \sigma_4} = \cosh K [1 + \sigma_3 \sigma_4 \tanh K]$$

Letting $x = \tanh K$, the product of the three exponentials becomes:

$$\begin{aligned} e^{K\sigma'_1 \sigma_3} e^{K\sigma_3 \sigma_4} e^{K\sigma_4 \sigma'_2} &= \cosh^3 K (1 + \sigma'_1 \sigma_3 x)(1 + \sigma_3 \sigma_4 x)(1 + \sigma_4 \sigma'_2 x) \\ &= \cosh^3 K (1 + \sigma'_1 \sigma_3 x + \sigma_3 \sigma_4 x + \sigma_4 \sigma'_2 x + \sigma'_1 \sigma_3^2 \sigma_4 x^2 + \sigma'_1 \sigma_3 \sigma_4 \sigma'_2 x^2 + \sigma_3 \sigma_4^2 \sigma'_2 x^2 + \sigma'_1 \sigma_3^2 \sigma_4^2 \sigma'_2 x^3) \end{aligned}$$

When summed over σ_3 and σ_4 , most terms in the above expression will cancel, yielding the following expression:

$$\sum_{\sigma_3} \sum_{\sigma_4} e^{K\sigma'_1 \sigma_3} e^{K\sigma_3 \sigma_4} e^{K\sigma_4 \sigma'_2} = 2 \cosh^3 K [1 + \sigma'_1 \sigma'_2 x^3] \equiv \cosh K' [1 + \sigma'_1 \sigma'_2 x']$$

where the last expression puts the interaction into the original form with a new coupling constant K' . One of the possible choices for the new coupling constant is

$$\begin{aligned} \tanh K' &= \tanh^3 K \\ K' &= \tanh^{-1} [\tanh^3 K] \end{aligned}$$

This, then, is the RG equation for this particular block spin transformation. With this identification of K' , the new Hamiltonian can be shown to be

$$\mathcal{H}'_0(\{\sigma'\}) = N' g(K) - K' \sum_{i=1}^{N'} \sigma'_i \sigma'_{i+1}$$

where the spin-independent function $g(K)$ is given by

$$g(K) = -\frac{1}{3} \ln \left[\frac{\cosh^3 K}{\cosh K'} \right] - \frac{2}{3} \ln 2$$

Thus, apart from the additional term, the new Hamiltonian is exactly the same functional form as the original Hamiltonian but with a different set of spin variables and a different coupling constant.

The transformation can now be applied to the new Hamiltonian, yielding the same relation between the new and old coupling constants. This is equivalent to iterating the RG equation. Since the coupling constant K depends on temperature through $K = J/kT$, the purpose of the iteration would be to find out if, for some value of K , there is an ordered phase. In an ordered phase, the transformed lattice would be exactly the same as the old lattice, and hence the same coupling constant and Hamiltonian would result. Such points are called *fixed points* of the RG equations and are generally given by the condition

$$\mathbf{K} = \mathbf{R}(\mathbf{K})$$

The fixed points correspond to critical points. For the one-dimensional Ising model, the fixed point condition is

$$K = \tanh^{-1} [\tanh^3 K]$$

or, in terms of $x = \tanh K$,

$$x = x^3$$

Since K is restricted to $K \geq 0$, the only solutions to this equation are $x = 0$ and $x = 1$, which are the fixed points of the RG equation.

To see what these solutions mean, consider the RG equation away from the fixed point:

$$x' = x^3$$

Since $K = J/kT$, at high T , $K \rightarrow 0$ and $x = \tanh K \rightarrow 0^+$. At low temperature, $K \rightarrow \infty$ and $x \rightarrow 1^-$. Viewing the RG equation as an iteration or recursion of the form

$$x_{n+1} = x_n^3$$

if we start at $x_0 = 1$, each successive iteration will yield 1. However, for any value of x less than 1, the iteration eventually goes to 0 in some finite (though perhaps large) number of iterations of the RG equation. This can be illustrated pictorially as shown below:

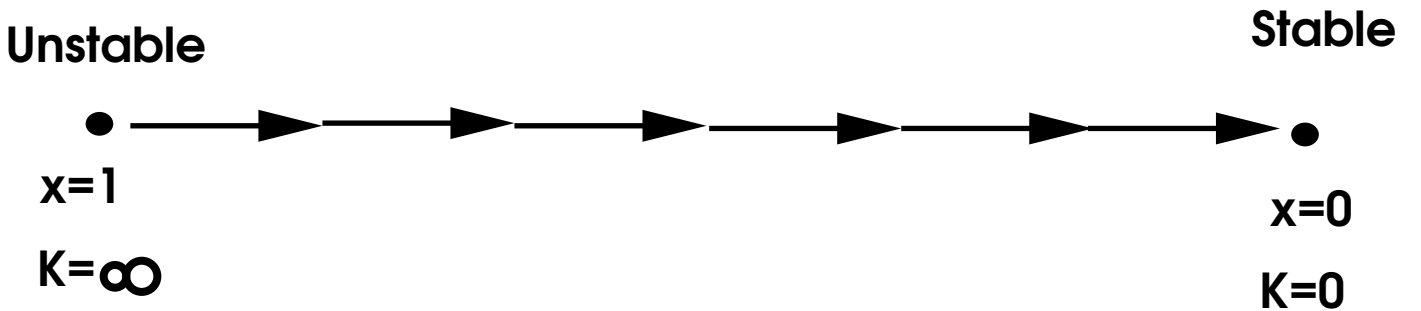


FIG. 5.

The iteration of the RG equation produces an *RG flow* through coupling constant space. The fixed point at $x = 1$ is called an *unstable fixed point* because any perturbation away from it, if iterated through the RG equation, flows away from this point to the other fixed point, which is called a *stable fixed point*. As the stable fixed point is approached, the coupling constant gets smaller and smaller until, at the fixed point, it is 0. The absence of a fixed point for any finite, nonzero value of temperature tells us that there can be no ordered phase in one dimension, hence no critical point in one dimension. If there were a critical point at a temperature T_c , then, at that point, long range order would set in, and there would be a fixed point of the RG equation at $K_c = J/kT_c$. Note, however, that at $T = 0$, $K = \infty$, there is perfect ordering in one dimension. Although this is physically meaningless, it suggests that ordered phases and critical points will be associated with the unstable fixed points of the RG equations.

Another way to see what the $T = 0$ unstable fixed point means is to study the correlation length. The correlation is a quantity that has units of length. However, if we choose to measure it in units of the lattice spacing, then the correlation length will be a number that can only depend on the coupling constant K or $x = \tanh K$:

$$\xi = \xi(x)$$

Under an RG transformation, the lattice spacing increases by a factor of 3 as a result of coarse graining. Thus, the correlation length, in units of the lattice spacing, must decrease by a factor of 3 in order for the same physical distance to be maintained:

$$\xi(x') = \frac{1}{3}\xi(x)$$

In general, for block containing b spins, the correlation length transforms as

$$\xi(x') = \frac{1}{b}\xi(x)$$

A function satisfying this equation is

$$\xi(x) \sim \frac{1}{\ln x}$$

Since, for arbitrary b , the RG equation is

$$x' = x^b$$

we have

$$\begin{aligned} \xi(x') &= \xi(x^b) \\ &\sim \frac{1}{\ln x^b} \\ &= \frac{1}{b \ln x} \\ &= \frac{1}{b} \xi(x) \end{aligned}$$

so that

$$\xi(K) \sim \frac{1}{\ln \tanh K} \rightarrow \infty \text{ as } T \rightarrow 0$$

so that at $T = 0$ the correlation length becomes infinite, indicating an ordered phase.

Note, also, that at very low T , where K is large, motion toward the stable fixed point is initially extremely slow. To see this, rewrite the RG equation as

$$\begin{aligned} \tanh K' &= \tanh^3 K \\ &= \tanh K \tanh^2 K \\ &= \tanh K \left[\frac{\cosh(2K) - 1}{\cosh(2K) + 1} \right] \end{aligned}$$

Notice that the term in brackets is extremely close to 1 if K is large. To leading order, we can say

$$K' \sim K$$

Since the interactions between blocks are predominantly mediated by interactions between boundary spins, which, for one dimension, involves a single spin pair between blocks, we expect that a block spin transformation in 1 dimension yields a coupling constant of the same order as the original coupling constant when T is low enough that there is alignment between the blocks and the new lattice is similar to the original lattice. This is reflected in the above statement.