8.334 Statistical Mechanics II: Statistical Physics of Fields Spring 2008

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V. Position Space Renormalization Group

V.A Lattice Models

While Wilson's perturbative RG provides a systematic approach to probing critical properties, carrying out the ϵ -expansion to high orders is quite cumbersome. Models defined on a discrete lattice provide a number of alternative computational routes that can complement the perturbative RG approach. Because of universality, we expect that all models with appropriate microscopic symmetries and range of interactions, no matter how simplified, lead to the same critical exponents. Lattice models are convenient for visualization, computer simulation, and series expansion purposes. We shall thus describe models in which an appropriate "spin" degree of freedom is placed on each site of a lattice, and the spins are subject to simple interaction energies. While such models are formulated in terms of explicit 'microscopic' degrees of freedom, depending on their degree of complexity, they may or may not provide a more accurate description of a specific material than the Landau–Ginzburg model. The point is that universality dictates that both descriptions describe the same *macroscopic* physics, and the choice of continuum or discrete models is a matter of computational convenience. Some commonly used lattice models are described here:

1. The Ising Model is the simplest and most widely applied paradigm in statistical mechanics. At each site *i* of a lattice, there is a spin σ_i which takes the two values of +1 or -1. Each state may correspond to one of two species in a binary mixture, or to empty and occupied cells in a lattice approximation to an interacting gas. The simplest possible short range interaction involves only neighboring spins, and is described by a Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} \hat{B}(\sigma_i, \sigma_j), \tag{V.1}$$

where the notation $\langle i, j \rangle$ is commonly used to indicate the sum over all *nearest neighbor* pairs on the lattice. Since $\sigma_i^2 = 1$, the most general interaction between two spins is

$$\hat{B}(\sigma,\sigma') = -\hat{g} - \frac{\hat{h}}{z}(\sigma+\sigma') - J\sigma\sigma'.$$
(V.2)

For N spins, there are 2^N possible *micro-states*, and the (Gibbs) partition function is

$$Z = \sum_{\{\sigma_i\}} e^{-\beta \mathcal{H}} = \sum_{\{\sigma_i\}} \exp\left[K \sum_{\langle i,j \rangle} \sigma_i \sigma_j + h \sum_i \sigma_i + g\right], \quad (V.3)$$

where we have set $K = \beta J$, $h = \beta \hat{h}$, and $g = \beta \hat{g}$ ($\beta = 1/k_B T$, and z is the number of bonds per site, i.e. the coordination number of the lattice). For h = 0 at T = 0, the ground state has a two fold degeneracy with all spins pointing up or down (K > 0). This order is destroyed at a critical $K_c = J/k_B T_c$ with a phase transition to a disordered state. The field h breaks the up-down symmetry and removes the phase transition. The parameter g merely shifts the origin of energy, and has no effect on the relative weights of microstates, or the macroscopic properties.

All the following models can be regarded as generalizations of the Ising model.

2. The O(n) model: Each lattice site is now occupied by an *n*-component unit vector, i.e.

$$S_i \equiv (S_i^1, S_i^2, \dots, S_i^n), \text{ with } \sum_{\alpha=1}^n (S_i^{\alpha})^2 = 1.$$
 (V.4)

A nearest–neighbor interaction can be written as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - \hat{\vec{h}} \cdot \sum_i \vec{S}_i.$$
(V.5)

In fact, the most general interaction consistent with spherical symmetry is $f(\vec{S}_i \cdot \vec{S}_j)$ for an arbitrary function f. Similarly, the *rotational symmetry* can be broken by a number of "fields" such as $\sum_i (\vec{h}_p \cdot \vec{S}_i)^p$. Specific cases are the Ising model (n = 1), the XY model (n = 2), and the Heisenberg model (n = 3).

3. The Potts model: Each site of the lattice is occupied by a q-valued spin $S_i \equiv 1, 2, \dots, q$. The interactions between the spins are described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{S_i,S_j} - \hat{h} \sum_i \delta_{S_i,1}.$$
 (V.6)

The field h now breaks the *permutation symmetry* amongst the q-states. The Ising model is recovered for q = 2, since $\delta_{\sigma,\sigma'} = (1 + \sigma\sigma')/2$. The 3 state Potts model can for example describe the distortion of a cube along one of its faces. Potts models with q > 2 represent new universality classes not covered by the O(n) model. Actually, the transitions for $q \ge 4$ in d = 2, and q > 3 in d = 3 are discontinuous.

4. Spin s-models: The spin at each site takes the 2s + 1 values, $s_i = -s, -s + 1, \dots, +s$. A general nearest-neighbor Hamiltonian is

$$\mathcal{H} = \sum_{\langle i,j \rangle} \left(J_1 s_i s_j + J_2 (s_i s_j)^2 + \dots + J_{2s} (s_i s_j)^{2s} \right) - \hat{h} \sum_i s_i.$$
(V.7)

The Ising model corresponds to s = 1/2, while s = 1 is known as the Blume–Emery–Griffith (BEG) model. It describes a mixture of non-magnetic (s = 0), and magnetic ($s = \pm 1$) elements. This model exhibits a tricritical point separating continuous and discontinuous transitions. However, since the ordered phase breaks an up–down symmetry, the phase transition belongs to the Ising universality class for all values of s.

Some of the computational tools employed in the study of discrete models are:

1. *Position space renormalizations:* These are implementations of Kadanoff's RG scheme on lattice models. Some approximation is usually necessary to keep the space of interactions tractable. Most such approximations are uncontrolled; a number of them will be discussed here.

2. Series expansions: Low-temperature expansions start with the ordered ground state and examine the lowest energy excitations around it. High temperatures expansions begin with the collection of non-interacting spins at infinite temperature and include the interactions between spins perturbatively. Critical behavior is then extracted from the singularities of such series.

3. *Exact solutions* can be obtained for a very limited subset of lattice models. These include one dimensional chains which will be solved by the transfer matrix method in recitations, and the two dimensional Ising model as described later in the course.

4. Monte-Carlo simulations: The aim of such methods is to generate configurations of spins that are distributed with the correct Boltzmann weight $\exp(-\beta \mathcal{H})$. There are a number of methods, most notably the Metropolis algorithm, for achieving this aim. Various expectation values and correlation functions are then directly computed from these configurations. With the continuing increase of computer power, numerical simulations have become increasingly popular. Limitations of the method are due to the size of systems that can be studied, and the amount of time needed to ensure that the correctly weighted configurations are generated. There is an extensive literature on numerical simulations which will not be further discussed in this course.

V.B Exact treatment in d = 1

An exact RG treatment can be carried out for the Ising model with nearest neighbor interactions (eq.(V.1)) in one dimension. The basic idea is to find a transformation that reduces the number of degrees of freedom by a factor b, while preserving the partition function, i.e.

$$Z = \sum_{\{\sigma_i | i=1,\cdots,N\}} e^{-\beta \mathcal{H}[\sigma_i]} = \sum_{\{\sigma'_{i'} | i'=1,\cdots,N/b\}} e^{-\beta \mathcal{H}'[\sigma'_{i'}]}.$$
 (V.8)

There are many mappings $\{\sigma_i\} \mapsto \{\sigma'_{i'}\}$, that satisfy this condition. The choice of the transformation is therefore guided by the simplicity of the resulting RG. With b = 2, for example, one possible choice is to group pairs of neighboring spins and define the renormalized spin as their average. This majority rule, $\sigma'_i = (\sigma_{2i-1} + \sigma_{2i})/2$, is in fact not very convenient as the new spin has three possible values $(0, \pm 1)$ while the original spins are two valued. We can remove the ambiguity by assigning one of the two spins, e.g. σ_{2i-1} , the role of tie-breaker whenever the sum is zero. In this case the transformation is simply $\sigma'_i = \sigma_{2i-1}$. Such an RG procedure effectively removes the even numbered spins, $s_i = \sigma_{2i}$ and is usually called a *decimation*. Note that since $\sigma' = \pm 1$ as in the original model, no renormalization factor ζ , is necessary in this case. Since the interaction is over adjacent neighbors, the partition function can be written as

$$Z = \sum_{\{\sigma_i\}}^{N} \exp\left[\sum_{i=1}^{N} B(\sigma_i, \sigma_{i+1})\right] = \sum_{\{\sigma'_i\}}^{N/2} \sum_{\{s_i\}}^{N/2} \exp\left[\sum_{i=1}^{N/2} \left[B(\sigma'_i, s_i) + B(s_i, \sigma'_{i+1})\right]\right].$$
 (V.9)

Summing over the decimated spins, $\{s_i\}$, leads to

$$e^{-\beta \mathcal{H}'[\sigma_i']} \equiv \prod_{i=1}^{N/2} \left[\sum_{s_i=\pm 1} e^{\left[B(\sigma_i', s_i) + B(s_i, \sigma_{i+1}')\right]} \right] \equiv e^{\sum_{i=1}^{N/2} B'(\sigma_i', \sigma_{i+1}')}, \quad (V.10)$$

where following eq. (V.2),

$$B(\sigma_1, \sigma_2) = g + \frac{h}{2}(\sigma_1 + \sigma_2) + K\sigma_1\sigma_2, \qquad (V.11)$$

and

$$B'(\sigma'_1, \sigma'_2) = g' + \frac{h'}{2}(\sigma'_1 + \sigma'_2) + K'\sigma'_1\sigma'_2, \qquad (V.12)$$

are the most general interaction forms for Ising spins.

Following eq. (V.10), the renormalized interactions are obtained from

$$R(\sigma'_{1}, \sigma'_{2}) \equiv \exp\left[K'\sigma'_{1}\sigma'_{2} + \frac{h'}{2}(\sigma'_{1} + \sigma'_{2}) + g'\right]$$

= $\sum_{s_{1}=\pm 1} \exp\left[Ks_{1}(\sigma'_{1} + \sigma'_{2}) + \frac{h}{2}(\sigma'_{1} + \sigma'_{2}) + hs_{1} + 2g\right].$ (V.13)

To solve for the renormalized interactions it is convenient to set

$$\begin{cases} x = e^{K}, & y = e^{h}, & z = e^{g} \\ x' = e^{K'}, & y' = e^{h'}, & z' = e^{g'} \end{cases}.$$
 (V.14)

The four possible configurations of the bond are

$$\begin{cases} R(+,+) = x'y'z' = z^2y(x^2y + x^{-2}y^{-1}) \\ R(-,-) = x'y'^{-1}z' = z^2y^{-1}(x^{-2}y + x^2y^{-1}) \\ R(+,-) = x'^{-1}z' = z^2(y + y^{-1}) \\ R(-,+) = x'^{-1}z' = z^2(y + y^{-1}) \end{cases}$$
(V.15)

The last two equations are identical, resulting in three equations in three unknowns, with the solutions,

$$\begin{cases} z'^{4} = z^{8} (x^{2}y + x^{-2}y^{-1})(x^{-2}y + x^{2}y^{-1})(y + y^{-1})^{2} \\ y'^{2} = y^{2} \frac{x^{2}y + x^{-2}y^{-1}}{x^{-2}y + x^{2}y^{-1}} \\ x'^{4} = \frac{(x^{2}y + x^{-2}y^{-1})(x^{-2}y + x^{2}y^{-1})}{(y + y^{-1})^{2}} \end{cases}$$
(V.16)

Taking the logarithms, we find recursion relations of the form

$$\begin{cases} g' = 2g + \delta g(K, h) \\ h' = h + \delta h(K, h) \\ K' = K'(K, h) \end{cases}$$
(V.17)

The parameter g is just an additive constant to the Hamiltonian. It does not effect the probabilities and hence does not appear in the recursion relations for K and h. $\delta g(K, h)$ is the contribution of the decimated spins to the overall free energy.

1. Fixed points: The h = 0 subspace is closed by symmetry, and it can be checked that for y = 1 eqs.(V.16) imply y' = 1, and

$$e^{4K'} = \left(\frac{e^{2K} + e^{-2K}}{2}\right)^2, \qquad \Longrightarrow \qquad K' = \frac{1}{2}\ln\cosh 2K.$$
 (V.18)

The recursion relation for K has the following fixed points:

- (a) An infinite temperature fixed point at $K^* = 0$, which is the *sink* for the disordered phase. If K is small, $K' \approx \ln(1 + 4K^2/2)/2 \approx K^2$, is even smaller, indicating that this is a *stable* fixed point with zero correlation length.
- (b) A zero temperature fixed point at $K^* \to \infty$, describing the ordered phase. For a large but finite K, the renormalized interaction $K' \approx \ln(e^{2K}/2)/2 \approx K \ln 2/2$, is somewhat smaller. This fixed point is thus unstable with an infinite correlation length.

Clearly any finite interaction renormalizes to zero, indicating that the one dimensional chain is always disordered at sufficiently long length scales. The absence of any other fixed point is apparent by noting that the recursion relation eq.(V.18) can alternatively be written as $\tanh K' = (\tanh K)^2$.

2. Flow diagrams indicate that in the presence of a field h, all flows terminate on a line of fixed points with $K^* = 0$ and arbitrary h^* . These fixed points describe *independent* spins and all have zero correlation length. The flows originate from the fixed point at $K^* = h^* = 0$ which has two unstable directions in the (K, h) parameter space.

3. Linearizing the recursion relations around this fixed point $(x \to \infty)$ yields,

$$\begin{cases} x'^4 \approx x^4/4 \\ y'^2 \approx y^4 \end{cases}, \qquad \Longrightarrow \qquad \begin{cases} e^{-K'} = \sqrt{2}e^{-K} \\ h' = 2h \end{cases}.$$
(V.19)

We can thus regard e^{-K} and h as scaling fields. Since $\xi' = \xi/2$, the correlation length in the vicinity of the fixed point satisfies the homogeneous form (b = 2)

$$\xi(e^{-K},h) = 2\xi(\sqrt{2}e^{-K},2h)$$

= $2^{\ell}\xi(2^{\ell/2}e^{-K},2^{\ell}h).$ (V.20)

The second equation is obtained by repeating the RG procedure ℓ times. Choosing ℓ such that $2^{\ell/2}e^{-K} \approx 1$, we obtain the scaling form

$$\xi\left(e^{-K},h\right) = e^{2K}g_{\xi}\left(he^{2K}\right). \tag{V.21}$$

The correlation length diverges on approaching T = 0 for h = 0. However, its divergence is not a power law of temperature. There is thus an ambiguity in identifying the exponent ν related to the choice of the measure of vicinity to T = 0 (1/K or e^{-K}). The hyperscaling assumption states that the singular part of the free energy in d dimensions is proportional to ξ^{-d} . Hence we expect

$$f_{\text{sing.}}(K,h) \propto \xi^{-1} = e^{-2K} g_f(he^{2K}).$$
 (V.22)

At zero field, the magnetization is always zero, while the susceptibility behaves as

$$\chi(K) \sim \left. \frac{\partial^2 f}{\partial^2 h} \right|_{h=0} \sim e^{2K}.$$
 (V.23)

On approaching zero temperature, the divergence of the susceptibility is proportional to that of the correlation length. Using the general forms, $\langle s_i, s_{i+x} \rangle \sim e^{-x/\xi}/x^{d-2+\eta}$, and $\chi \sim \int d^d \mathbf{x} \langle s_0 s_{\mathbf{x}} \rangle_c \sim \xi^{2-\eta}$, we conclude that $\eta = 1$.

The one dimensional Ising model can be solved exactly by a *transfer matrix method* which will be described in more detail in the recitations. The results of the direct solution are in full agreement with those of the RG. The transfer matrix approach can be applied to any one dimensional chain with nearest neighbor interactions, since the partition function can be written as

$$Z = \sum_{\{s_i\}} \exp\left[\sum_{i=1}^N B(s_i, s_{i+1})\right] = \sum_{\{s_i\}} \prod_{i=1}^N e^{B(s_i, s_{i+1})}.$$
 (V.24)

Defining a transfer matrix,

$$\langle s_i | T | s_j \rangle = e^{B(s_i, s_j)}, \tag{V.25}$$

and with *periodic boundary conditions*, we obtain

$$Z = \operatorname{tr}\left[T^{N}\right] \approx \lambda_{\max}^{N}.$$
 (V.26)

Note that for $N \to \infty$, the trace is dominated by the largest eigenvalue λ_{\max} . Frobenius's theorem states that for any finite matrix with finite positive elements, the largest eigenvalue is always non-degenerate. This implies that λ_{\max} and Z are analytic functions of the parameters appearing in B, and that one dimensional models can exhibit singularities (and hence a phase transition) only at zero temperature (when some matrix elements become infinite). The transfer matrix method also provides an alternative RG scheme for all such one dimensional chains. For decimation by a factor b, we can use $Z = \text{tr}\left[\left(T^b\right)^{N/b}\right]$ to construct the rescaled bond energy as

$$e^{B(s'_i,s'_j)} \equiv \left\langle s'_i | T' | s'_j \right\rangle = \left\langle s'_i | T^b | s'_j \right\rangle. \tag{V.27}$$