6
Lattice systems

6.1 Models and methods

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 then a matter of computational convenience.

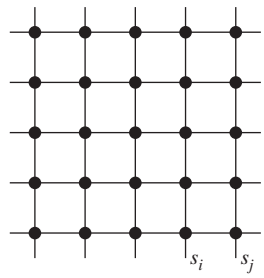

Fig. 6.1 Interacting "spins" $\{s_i\}$ defined on a square lattice.

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

$$\mathcal{H} = \sum_{\langle i,j \rangle} \hat{B}(\sigma_i, \sigma_j), \tag{6.1}$$

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

$$\hat{B}(\sigma, \sigma') = -\hat{g} - \frac{\hat{h}}{z}(\sigma + \sigma') - J\sigma\sigma'. \tag{6.2}$$

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

$$Z = \sum_{\{\sigma_i\}} \mathrm{e}^{-\beta\mathcal{H}} = \sum_{\{\sigma_i\}} \exp\left[K \sum_{\langle i,j \rangle} \sigma_i\sigma_j + h \sum_i \sigma_i + g \right], \tag{6.3}$$

where we have set $K = \beta J$, $h = \beta\hat{h}$, and $g = z\beta\hat{g}/2$ ($\beta = 1/k_{\mathrm{B}}T$, 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 $K_c = J/k_{\mathrm{B}}T_c$ 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

$$S_i \equiv (S_i^1, S_i^2, \cdots, S_i^n), \quad \text{with} \quad \sum_{\alpha=1}^{n} (S_i^\alpha)^2 = 1. \tag{6.4}$$

A nearest-neighbor interaction can be written as

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - \hat{\vec{h}} \cdot \sum_i \vec{S}_i. \tag{6.5}$$

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 $S_i \equiv 1, 2, \cdots, q$. The interactions between the spins are described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \delta_{S_i,S_j} - \hat{h} \sum_i \delta_{S_i,1}. \tag{6.6}$$

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 three 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 $q \geq 4$ 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, $s_i = -s, -s + 1, \cdots, +s$. A general nearest-neighbor Hamiltonian is

$$\mathcal{H} = \sum_{\langle i,j \rangle} \left(J_1 s_i s_j + J_2 (s_i s_j)^2 + \cdots + J_{2s} (s_i s_j)^{2s} \right) - \hat{h} \sum_i s_i. \tag{6.7}$$

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) ***Exact solutions*** can be obtained for a very limited subset of lattice models. These include many one dimensional systems that can be solved by the transfer matrix method described next, and the two-dimensional Ising model discussed in the next chapter.

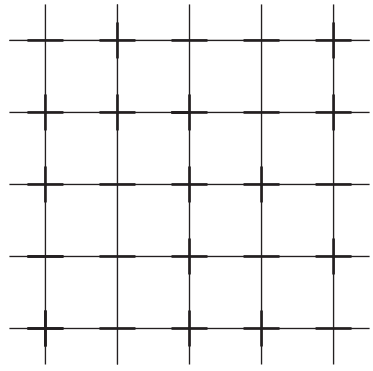

Fig. 6.2 A configuration of Ising spins on a square lattice.

(2) ***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 in this chapter.

(3) ***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 only be touched upon briefly.

(4) ***Series expansions:*** Low-temperature expansions start with the ordered ground state and examine the lowest energy excitations around it (see the next chapter). High temperature 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.

6.2 Transfer matrices

Consider a linear chain of N Ising spins ($\sigma_i = \pm 1$), with a nearest-neighbor coupling K, and a magnetic field h. To simplify calculations, we assume that the chain is closed upon itself such that the first and last spins are also coupled (periodic boundary conditions), resulting in the Hamiltonian

$$-\beta\mathcal{H} = K\left(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \cdots + \sigma_{N-1}\sigma_N + \sigma_N\sigma_1\right) + h\sum_{i=1}^{N}\sigma_i\ . \tag{6.8}$$

The corresponding partition function, obtained by summing over all states, can be expressed as the product of matrices, since

$$\begin{aligned} Z &= \sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1}\prod_{i=1}^{N}\exp\left[K\sigma_i\sigma_{i+1} + \frac{h}{2}\left(\sigma_i + \sigma_{i+1}\right)\right] \\ &\equiv \mathrm{tr}\left[\langle\sigma_1|T|\sigma_2\rangle\langle\sigma_2|T|\sigma_3\rangle\cdots\langle\sigma_N|T|\sigma_1\rangle\right] = \mathrm{tr}\left[T^N\right], \end{aligned} \tag{6.9}$$

where we have introduced the 2×2 *transfer matrix* T, with elements

$$\langle\sigma_i|T|\sigma_j\rangle = \exp\left[K\sigma_i\sigma_j + \frac{h}{2}(\sigma_i + \sigma_j)\right], \quad \text{i.e.} \quad T = \begin{pmatrix} \mathrm{e}^{K+h} & \mathrm{e}^{-K} \\ \mathrm{e}^{-K} & \mathrm{e}^{K-h} \end{pmatrix}. \tag{6.10}$$

The expression for trace of the matrix can be evaluated in the basis that diagonalizes T, in which case it can be written in terms of the two eigenvalues $\lambda_\pm$ as

$$Z = \lambda_+^N + \lambda_-^N = \lambda_+^N\left[1 + \left(\lambda_-/\lambda_+\right)^N\right] \approx \lambda_+^N. \tag{6.11}$$

We have assumed that $\lambda_+ > \lambda_-$, and since in the limit of $N \to \infty$ the larger eigenvalue dominates the sum, the free energy is

$$\beta f = -\ln Z/N = -\ln\lambda_+. \tag{6.12}$$

Solving the characteristic equation, we find the eigenvalues

$$\lambda_\pm = \mathrm{e}^K\cosh h \pm \sqrt{\mathrm{e}^{2K}\sinh^2 h + \mathrm{e}^{-2K}}. \tag{6.13}$$

We shall leave a discussion of the singularities of the resulting free energy (at zero temperature) to the next section, and instead look at the averages and correlations in the limit of $h = 0$.

To calculate the average of the spin at site i, we need to evaluate

$$\begin{aligned}\langle\sigma_i\rangle &= \frac{1}{Z}\sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1}\sigma_i\prod_{j=1}^{N}\exp\left(K\sigma_j\sigma_{j+1}\right)\\ &\equiv \frac{1}{Z}\mathrm{tr}\left[\langle\sigma_1|T|\sigma_2\rangle\cdots\langle\sigma_{i-1}|T|\sigma_i\rangle\sigma_i\langle\sigma_i|T|\sigma_{i+1}\rangle\cdots\langle\sigma_N|T|\sigma_1\rangle\right]\\ &= \frac{1}{Z}\,\mathrm{tr}\left[T^{i-1}\hat{\sigma}_z T^{N-i+1}\right]\\ &= \frac{1}{Z}\,\mathrm{tr}\left[T^N\hat{\sigma}_z\right],\end{aligned} \tag{6.14}$$

where have permuted the matrices inside the trace, and $\hat{\sigma}_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$ is the usual 2×2 Pauli matrix. One way to evaluate the final expression in Eq. (6.14) is to rotate to a basis where the matrix T is diagonal. For $h = 0$, this is accomplished by the unitary matrix $U = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$, resulting in

$$\langle\sigma_i\rangle = \frac{1}{Z}\,\mathrm{tr}\left[\begin{pmatrix}\lambda_+^N & 0\\ 0 & \lambda_-^N\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right] = \frac{1}{Z}\begin{pmatrix}0 & \lambda_+^N\\ \lambda_-^N & 0\end{pmatrix} = 0. \tag{6.15}$$

Note that under this transformation the Pauli matrix $\hat{\sigma}_z$ is rotated into $\hat{\sigma}_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$.

The vanishing of the magnetization at zero field is of course expected by symmetry. A more interesting quantity is the two-spin correlation function

$$\begin{aligned}\langle\sigma_i\sigma_{i+r}\rangle &= \frac{1}{Z}\sum_{\sigma_1=\pm1}\sum_{\sigma_2=\pm1}\cdots\sum_{\sigma_N=\pm1}\sigma_i\sigma_{i+r}\prod_{j=1}^{N}\exp\left(K\sigma_j\sigma_{j+1}\right)\\ &= \frac{1}{Z}\,\mathrm{tr}\left[T^{i-1}\hat{\sigma}_z T^r\hat{\sigma}_z T^{N-i-r+1}\right] = \frac{1}{Z}\,\mathrm{tr}\left[\hat{\sigma}_z T^r\hat{\sigma}_z T^{N-r}\right].\end{aligned} \tag{6.16}$$

Once again rotating to the basis where T is diagonal simplifies the trace to

$$\begin{aligned}\langle\sigma_i\sigma_{i+r}\rangle &= \frac{1}{Z}\,\mathrm{tr}\left[\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\lambda_+^r & 0\\ 0 & \lambda_-^r\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\lambda_+^{N-r} & 0\\ 0 & \lambda_-^{N-r}\end{pmatrix}\right]\\ &= \frac{1}{Z}\,\mathrm{tr}\begin{pmatrix}\lambda_+^{N-r}\lambda_-^r & 0\\ 0 & \lambda_-^{N-r}\lambda_+^r\end{pmatrix} = \frac{\lambda_+^{N-r}\lambda_-^r + \lambda_-^{N-r}\lambda_+^r}{\lambda_+^N + \lambda_-^N}.\end{aligned} \tag{6.17}$$

Note that because of the periodic boundary conditions, the above answer is invariant under $r \to (N-r)$. We are interested in the limit of $N \gg r$, for which

$$\langle\sigma_i\sigma_{i+r}\rangle \approx \left(\frac{\lambda_-}{\lambda_+}\right)^r \equiv \mathrm{e}^{-r/\xi}, \tag{6.18}$$

with the correlation length

$$\xi = \left[\ln\left(\frac{\lambda_+}{\lambda_-}\right)\right]^{-1} = -\frac{1}{\ln\tanh K}. \tag{6.19}$$

The above transfer matrix approach can be generalized to any one dimensional chain with variables $\{s_i\}$ and nearest-neighbor interactions. The partition function can be written as

$$Z = \sum_{\{s_i\}} \exp\left[\sum_{i=1}^{N} B(s_i, s_{i+1})\right] = \sum_{\{s_i\}} \prod_{i=1}^{N} \mathrm{e}^{B(s_i, s_{i+1})}, \tag{6.20}$$

where we have defined a *transfer matrix* T with elements,

$$\langle s_i|T|s_j\rangle = \mathrm{e}^{B(s_i,s_j)}. \tag{6.21}$$

In the case of *periodic boundary conditions*, we then obtain

$$Z = \mathrm{tr}\left[T^N\right] \approx \lambda_{\max}^N. \tag{6.22}$$

Note that for $N \to \infty$, the trace is dominated by the largest eigenvalue $\lambda_{\max}$. Quite generally the largest eigenvalue of the transfer matrix is related to the free energy, while the correlation lengths are obtained from ratios of eigenvalues. *Frobenius' theorem* states that for any finite matrix with finite positive elements, the largest eigenvalue is always non-degenerate. This implies that $\lambda_{\max}$ 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).

While the above formulation is framed in the language of discrete variables $\{s_i\}$, the method can also be applied to continuous variables as illustrated by problems at the end of this chapter. As an example of the latter, let us consider three component *unit* spins $\vec{s}_i = \left(s_i^x, s_i^y, s_i^z\right)$, with the *Heisenberg model* Hamiltonian

$$-\beta\mathcal{H} = K\sum_{i=1}^{N} \vec{s}_i \cdot \vec{s}_{i+1}. \tag{6.23}$$

Summing over all spin configurations, the partition function can be written as

$$Z = \mathop{\mathrm{tr}}_{\vec{s}_i} \mathrm{e}^{K\sum_{i=1}^{N} \vec{s}_i\cdot\vec{s}_{i+1}} = \mathop{\mathrm{tr}}_{\vec{s}_i} \mathrm{e}^{K\vec{s}_1\cdot\vec{s}_2}\mathrm{e}^{K\vec{s}_2\cdot\vec{s}_3}\cdots\mathrm{e}^{K\vec{s}_N\cdot\vec{s}_1} = \mathrm{tr}\, T^N, \tag{6.24}$$

where $\langle\vec{s}_1|T|\vec{s}_2\rangle = \mathrm{e}^{K\vec{s}_1\cdot\vec{s}_2}$ is a transfer function. Quite generally we would like to bring T into the diagonal form $\sum_\alpha \lambda_\alpha|\alpha\rangle\langle\alpha|$ (in Dirac notation), such that

$$\langle\vec{s}_1|T|\vec{s}_2\rangle = \sum_\alpha \lambda_\alpha \langle\vec{s}_1|\alpha\rangle\langle\alpha|\vec{s}_2\rangle = \sum_\alpha \lambda_\alpha f_\alpha(\vec{s}_1) f_\alpha^*(\vec{s}_2). \tag{6.25}$$

From studies of plane waves in quantum mechanics you may recall that the exponential of a dot product can be decomposed in terms of the spherical harmonics $Y_{\ell m}$. In particular,

$$\mathrm{e}^{K\vec{s}_1\cdot\vec{s}_2} = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} 4\pi i^\ell j_\ell(-iK) Y_{\ell m}^*(\vec{s}_1) Y_{\ell m}(\vec{s}_2) \tag{6.26}$$

is precisely in the form of Eq. (6.25), from which we can read off the eigenvalues $\lambda_{\ell m}(K) = 4\pi i^\ell j_\ell(-iK)$, which do not depend on m. The partition function is now given by

$$Z = \operatorname{tr} T^N = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \lambda_{\ell m}^N = \sum_{\ell=0}^{\infty} (2\ell+1)\lambda_\ell^N \approx \lambda_0^N, \tag{6.27}$$

with $\lambda_0 = 4\pi j_0(-iK) = 4\pi \sinh K/K$ as the largest eigenvalue. The second largest eigenvalue is three fold degenerate, and given by $\lambda_1 = 4\pi j_1(-iK) = 4\pi\left[\cosh K/K - \sinh K/K^2\right]$.

6.3 Position space RG in one dimension

An exact RG treatment can be carried out for the Ising model with nearest-neighbor interactions (Eq. 6.1) 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.

$$Z = \sum_{\{\sigma_i | i=1,\cdots,N\}} \mathrm{e}^{-\beta \mathcal{H}[\sigma_i]} = \sum_{\left\{\sigma'_{i'} | i'=1,\cdots,N/b\right\}} \mathrm{e}^{-\beta \mathcal{H}'[\sigma'_{i'}]}. \tag{6.28}$$

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*.

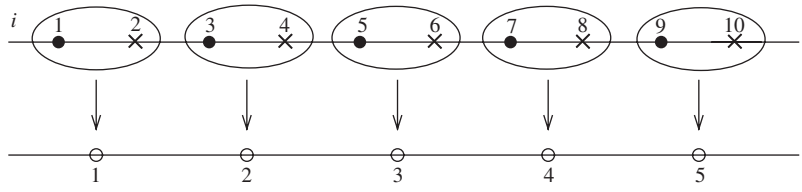

Fig. 6.3 Renormalization treatment of a one-dimensional chain via decimation by a factor of $b = 2$.

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

$$Z = \sum_{\{\sigma_i\}} \exp\left[\sum_{i=1}^{N} B(\sigma_i, \sigma_{i+1})\right] = \sum_{\left\{\sigma'_i\right\}}^{N/2} \sum_{\{s_i\}}^{N/2} \exp\left[\sum_{i=1}^{N/2} \left[B(\sigma'_i, s_i) + B(s_i, \sigma'_{i+1})\right]\right]. \tag{6.29}$$

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

$$e^{-\beta\mathcal{H}'[\sigma'_i]} \equiv \prod_{i=1}^{N/2}\left[\sum_{s_i=\pm1} e^{\left[B(\sigma'_i,s_i)+B(s_i,\sigma'_{i+1})\right]}\right] \equiv e^{\sum_{i=1}^{N/2} B'(\sigma'_i,\sigma'_{i+1})}, \tag{6.30}$$

where following Eq. (6.2)

$$B(\sigma_1,\sigma_2) = g + \frac{h}{2}(\sigma_1+\sigma_2) + K\sigma_1\sigma_2, \tag{6.31}$$

and

$$B'(\sigma'_1,\sigma'_2) = g' + \frac{h'}{2}(\sigma'_1+\sigma'_2) + K'\sigma'_1\sigma'_2 \tag{6.32}$$

are the most general interaction forms for Ising spins.

Following Eq. (6.30), the renormalized interactions are obtained from

$$\begin{aligned} R(\sigma'_1,\sigma'_2) &\equiv \exp\left[K'\sigma'_1\sigma'_2 + \frac{h'}{2}(\sigma'_1+\sigma'_2) + g'\right] \\ &= \sum_{s_1=\pm1} \exp\left[Ks_1(\sigma'_1+\sigma'_2) + \frac{h}{2}(\sigma'_1+\sigma'_2) + hs_1 + 2g\right]. \end{aligned} \tag{6.33}$$

To solve for the renormalized interactions it is convenient to set

$$\begin{cases} x = e^K, \quad y = e^h, \quad z = e^g \\ x' = e^{K'}, \quad y' = e^{h'}, \quad z' = e^{g'}. \end{cases} \tag{6.34}$$

The four possible configurations of the bond are

$$\begin{cases} R(+,+) = x'y'z' = z^2y(x^2y + x^{-2}y^{-1}) \\ R(-,-) = x'y'^{-1}z' = z^2y^{-1}(x^{-2}y + x^2y^{-1}) \\ R(+,-) = x'^{-1}z' = z^2(y + y^{-1}) \\ R(-,+) = x'^{-1}z' = z^2(y + y^{-1}). \end{cases} \tag{6.35}$$

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

$$\begin{cases} z'^4 = z^8(x^2y + x^{-2}y^{-1})(x^{-2}y + x^2y^{-1})(y + y^{-1})^2 \\ y'^2 = y^2\dfrac{x^2y + x^{-2}y^{-1}}{x^{-2}y + x^2y^{-1}} \\ x'^4 = \dfrac{(x^2y + x^{-2}y^{-1})(x^{-2}y + x^2y^{-1})}{(y + y^{-1})^2}. \end{cases} \tag{6.36}$$

Taking the logarithms, we find recursion relations of the form

$$\begin{cases} g' = 2g + \delta g(K,h) \\ h' = h + \delta h(K,h) \\ K' = K'(K,h). \end{cases} \tag{6.37}$$

The parameter g is just an additive constant to the Hamiltonian. It does not affect 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. (6.36) imply $y' = 1$, and

$$e^{4K'} = \left(\frac{e^{2K} + e^{-2K}}{2}\right)^2, \quad \Longrightarrow \quad K' = \frac{1}{2}\ln\cosh 2K. \tag{6.38}$$

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 $K' \approx \ln\left(e^{2K}/2\right)/2 \approx K - \ln 2/2$ is somewhat smaller. This fixed point is thus unstable with an infinite correlation length.

Fig. 6.4 Fixed points and RG flows for the coupling K in one dimension.

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 of Eq. (6.38) 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 $h^* = 0$ and $K^* \to \infty$ which has two unstable directions in the (K, h) parameter space.

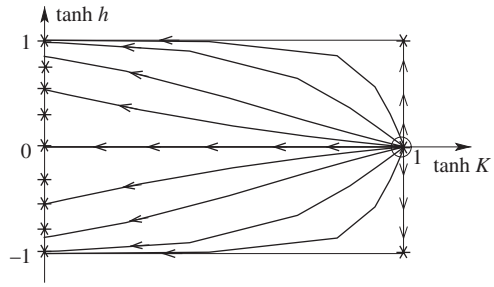

Fig. 6.5 Fixed points and RG flows in the space of coupling $(\tanh h, \tanh K)$ in one dimension.

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

$$\begin{cases} x'^4 \approx x^4/4 \\ y'^2 \approx y^4 \end{cases} \quad \Longrightarrow \quad \begin{cases} e^{-K'} = \sqrt{2}e^{-K} \\ h' = 2h. \end{cases} \tag{6.39}$$

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 ($b = 2$)

$$\begin{aligned}\xi\left(e^{-K}, h\right) &= 2\xi\left(\sqrt{2}e^{-K}, 2h\right) \\ &= 2^{\ell}\xi\left(2^{\ell/2}e^{-K}, 2^{\ell}h\right).\end{aligned} \tag{6.40}$$

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

$$\xi\left(e^{-K}, h\right) = e^{2K} g_{\xi}\left(he^{2K}\right). \tag{6.41}$$

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

$$f_{\text{sing}}(K, h) \propto \xi^{-1} = e^{-2K} g_f\left(he^{2K}\right). \tag{6.42}$$

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

$$\chi(K) \sim \left.\frac{\partial^2 f}{\partial^2 h}\right|_{h=0} \sim e^{2K}. \tag{6.43}$$

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 $\eta = 1$.

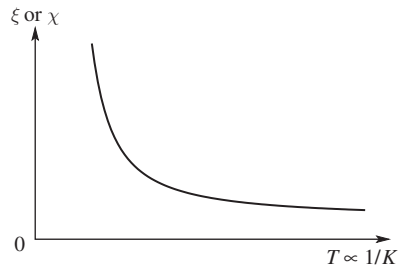

Fig. 6.6 The susceptibility (and correlation length) diverge similarly at zero temperature in the one-dimensional Ising model.

The transfer matrix method also provides an alternative RG scheme for all general one-dimensional chains with nearest-neighbor interactions. 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 from

$$e^{B(s_i', s_j')} \equiv \langle s_i'|T'|s_j'\rangle = \langle s_i'|T^b|s_j'\rangle. \tag{6.44}$$

6.4 The Niemeijer–van Leeuwen cumulant approximation

Unfortunately, the decimation procedure cannot be performed exactly in higher dimensions. For example, the square lattice can be divided into two sublattices. For an RG with $b = \sqrt{2}$, we can start by decimating the spins on one sublattice. The interactions between the four spins surrounding each decimated spin are obtained by generalizing Eq. (6.33). If initially $h = g = 0$, we obtain

$$R(\sigma_1', \sigma_2', \sigma_3', \sigma_4') = \sum_{s=\pm 1} \mathrm{e}^{Ks(\sigma_1'+\sigma_2'+\sigma_3'+\sigma_4')} = 2\cosh\left[K(\sigma_1'+\sigma_2'+\sigma_3'+\sigma_4')\right]. \quad (6.45)$$

Clearly the four spins appear symmetrically in the above expression, and hence are subject to the same two-body interaction. This implies that new interactions along the diagonals of the renormalized lattice are also generated, and the nearest-neighbor form of the original Hamiltonian is not preserved. There is also a four-point interaction, and

$$R = \exp\left[g' + K'(\sigma_1'\sigma_2' + \sigma_2'\sigma_3' + \sigma_3'\sigma_4' + \sigma_4'\sigma_1' + \sigma_1'\sigma_3' + \sigma_2'\sigma_4') + K_4'\sigma_1'\sigma_2'\sigma_3'\sigma_4'\right]. \quad (6.46)$$

The number (and range) of new interactions increases with each RG step, and some truncating approximation is necessary. Two such schemes are described in the following sections.

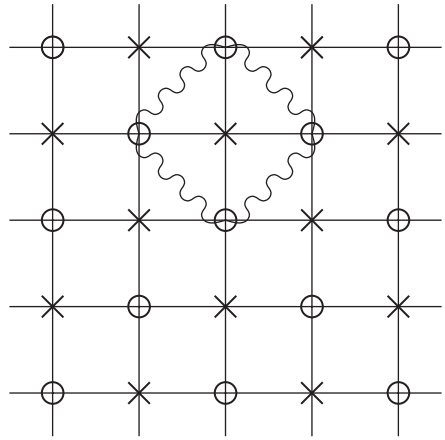

Fig. 6.7 Removal of a spin in two (and higher) dimensions results in more than nearest-neighbor interactions.

One of the earliest approaches was developed by Niemeijer and van Leeuwen (NvL) for treating the Ising model on a *triangular lattice*, subject to the usual nearest-neighbor Hamiltonian $-\beta\mathcal{H} = K\sum_{\langle ij\rangle}\sigma_i\sigma_j$. The original lattice sites are grouped into *cells* of three spins (e.g. in alternating up pointing triangles). Labeling the three spins in cell α as $\{\sigma_\alpha^1, \sigma_\alpha^2, \sigma_\alpha^3\}$, we can use a *majority rule* to define the renormalized cell spin as

$$\sigma_\alpha' = \mathrm{sign}\left[\sigma_\alpha^1 + \sigma_\alpha^2 + \sigma_\alpha^3\right]. \quad (6.47)$$

(There is no ambiguity in the rule for any odd number of sites, and the renormalized spin is two-valued.) The renormalized interactions corresponding to the above map are obtained from the constrained sum

$$\mathrm{e}^{-\beta\mathcal{H}'[\sigma'_\alpha]} = \sum_{\{\sigma^i_\alpha \mapsto \sigma'_\alpha\}}{}' \mathrm{e}^{-\beta\mathcal{H}[\sigma^i_\alpha]}. \tag{6.48}$$

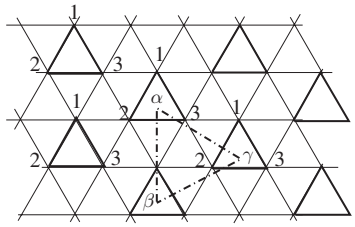

Fig. 6.8 Each cell spin is assigned from the majority of its three site spins.

To truncate the number of interactions in the renormalized Hamiltonian, NvL introduced a perturbative scheme by setting $\beta\mathcal{H} = \beta\mathcal{H}_0 + \mathcal{U}$. The unperturbed Hamiltonian

$$-\beta\mathcal{H}_0 = K\sum_\alpha \left(\sigma^1_\alpha\sigma^2_\alpha + \sigma^2_\alpha\sigma^3_\alpha + \sigma^3_\alpha\sigma^1_\alpha\right) \tag{6.49}$$

involves only *intracell interactions*. Since the cells are decoupled, this part of the Hamiltonian can be treated exactly. The remaining *intercell interactions* are treated as a perturbation

$$-\mathcal{U} = K\sum_{\langle\alpha,\beta\rangle}\left(\sigma^{(1)}_\beta\sigma^{(2)}_\alpha + \sigma^{(1)}_\beta\sigma^{(3)}_\alpha\right). \tag{6.50}$$

The sum is over all neighboring cells, each connected by two bonds. (The actual spins involved depend on the relative orientations of the cells.) Equation (6.48) is now evaluated perturbatively as

$$\mathrm{e}^{-\beta\mathcal{H}'[\sigma'_\alpha]} = \sum_{\{\sigma^i_\alpha \mapsto \sigma'_\alpha\}}{}' \mathrm{e}^{-\beta\mathcal{H}_0[\sigma^i_\alpha]}\left[1 - \mathcal{U} + \frac{\mathcal{U}^2}{2} - \cdots\right]. \tag{6.51}$$

The renormalized Hamiltonian is given by the cumulant series

$$\beta\mathcal{H}'[\sigma'_\alpha] = -\ln Z_0[\sigma'_\alpha] + \langle\mathcal{U}\rangle_0 - \frac{1}{2}\left(\langle\mathcal{U}^2\rangle_0 - \langle\mathcal{U}\rangle_0^2\right) + \mathcal{O}(\mathcal{U}^3), \tag{6.52}$$

where $\langle\ \rangle_0$ refers to the expectation values with respect to $\beta\mathcal{H}_0$, with the restriction of fixed $[\sigma'_\alpha]$, and Z_0 is the corresponding partition function.

To proceed, we construct a table of all possible configurations of spins within a cell, their renormalized value, and contribution to the cell energy:

	σ'_α	σ^1_α	σ^2_α	σ^3_α	$\exp[-\beta\mathcal{H}_0]$	
	$+$	$+$	$+$	$+$	e^{3K}	
	$+$	$-$	$+$	$+$	e^{-K}	
	$+$	$+$	$-$	$+$	e^{-K}	
	$+$	$+$	$+$	$-$	e^{-K}	
	$-$	$-$	$-$	$-$	e^{3K}	
	$-$	$+$	$-$	$-$	e^{-K}	
	$-$	$-$	$+$	$-$	e^{-K}	
	$-$	$-$	$-$	$+$	e^{-K}	

The restricted partition function is the product of contributions from the independent cells,

$$Z_0[\sigma'_\alpha] = \prod_\alpha \left[{\sum_{\{\sigma^i_\alpha \mapsto \sigma'_\alpha\}}}' e^{K(\sigma^1_\alpha\sigma^2_\alpha + \sigma^2_\alpha\sigma^3_\alpha + \sigma^3_\alpha\sigma^1_\alpha)} \right] = \left(e^{3K} + 3e^{-K}\right)^{N/3}. \tag{6.53}$$

It is *independent* of $[\sigma'_\alpha]$, thus contributing an additive constant to the Hamiltonian. The first cumulant of the interaction is

$$-\langle \mathcal{U} \rangle_0 = K \sum_{\langle \alpha,\beta \rangle} \left[\langle \sigma^1_\beta \rangle_0 \langle \sigma^2_\alpha \rangle_0 + \langle \sigma^1_\beta \rangle_0 \langle \sigma^3_\alpha \rangle_0 \right] = 2K \sum_{\langle \alpha,\beta \rangle} \langle \sigma^i_\alpha \rangle_0 \left\langle \sigma^j_\beta \right\rangle_0, \tag{6.54}$$

where we have taken advantage of the equivalence of the three spins in each cell. Using the table, we can evaluate the restricted average of site spins as

$$\langle \sigma^i_\alpha \rangle_0 = \left\{ \begin{array}{ll} \dfrac{+e^{3K} - e^{-K} + 2e^{-K}}{e^{3K} + 3e^{-K}} & \text{for } \sigma'_\alpha = +1 \\ \dfrac{-e^{3K} + e^{-K} - 2e^{-K}}{e^{3K} + 3e^{-K}} & \text{for } \sigma'_\alpha = -1 \end{array} \right\} \equiv \frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \sigma'_\alpha. \tag{6.55}$$

Substituting in Eq. (6.54) leads to

$$-\beta\mathcal{H}'[\sigma'_\alpha] = \frac{N}{3} \ln\left(e^{3K} + 3e^{-K}\right) + 2K \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right)^2 \sum_{\langle \alpha\beta \rangle} \sigma'_\alpha \sigma'_\beta + \mathcal{O}(\mathcal{U}^2). \tag{6.56}$$

At this order, the renormalized Hamiltonian involves only nearest-neighbor interactions, with the recursion relation

$$K' = 2K \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}} \right)^2. \tag{6.57}$$

(1) Equation (6.57) has the following *fixed points:*

(a) The high-temperature sink at $K^* = 0$. If $K \ll 1$, $K' \approx 2K(2/4)^2 = K/2 < K$, i.e. this fixed point is *stable*, and has zero correlation length.

(b) The low-temperature sink at $K^* = \infty$. If $K \gg 1$, then $K' \approx 2K > K$, i.e. unlike the one-dimensional case, this fixed point is also stable with zero correlation length.

(c) Since both of the above fixed points are stable, there must be at least one unstable fixed point at finite $K' = K = K^*$. From Eq. (6.57), the fixed point position satisfies

$$\frac{1}{\sqrt{2}} = \frac{e^{3K^*} + e^{-K^*}}{e^{3K^*} + 3e^{-K^*}}, \quad \Longrightarrow \quad \sqrt{2}e^{4K^*} + \sqrt{2} = e^{4K^*} + 3. \tag{6.58}$$

The fixed point value

$$K^* = \frac{1}{4}\ln\left(\frac{3-\sqrt{2}}{\sqrt{2}-1}\right) \approx 0.3356 \tag{6.59}$$

can be compared to the exactly known value of 0.2747 for the triangular lattice.

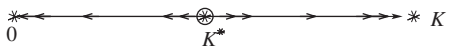

Fig. 6.9 Fixed points and RG flows for the coupling K in two dimensions.

(2) Linearizing the recursion relation around the non-trivial fixed point yields,

$$\left.\frac{\partial K'}{\partial K}\right|_{K^*} = 2\left(\frac{e^{4K^*}+1}{e^{4K^*}+3}\right)^2 + 32K^*e^{4K^*}\frac{(e^{4K^*}+1)}{(e^{4K^*}+3)^3} \approx 1.624. \tag{6.60}$$

The fixed point is indeed unstable as required by the continuity of flows. This RG scheme removes 1/3 of the degrees of freedom, and corresponds to $b = \sqrt{3}$. The thermal eigenvalue is thus obtained as

$$b^{y_t} = \left.\frac{\partial K'}{\partial K}\right|_{K^*} \quad \Longrightarrow \quad y_t \approx \frac{\ln(1.624)}{\ln(\sqrt{3})} \approx 0.883. \tag{6.61}$$

This can be compared to the exactly known value of $y_t = 1$, for the two-dimensional Ising model. It is certainly better than the mean-field (Gaussian) estimate of $y_t = 2$. From this eigenvalue we can estimate the exponents

$$\nu = 1/y_t \approx 1.13 \quad (1), \quad \text{and} \quad \alpha = 2 - 2/y_t = -0.26 \quad (0),$$

where the exact values are given in the brackets.

(3) To complete the calculation of exponents, we need the *magnetic eigenvalue* y_h, obtained after adding a magnetic field to the Hamiltonian, i.e. from

$$\beta\mathcal{H} = \beta\mathcal{H}_0 + \mathcal{U} - h\sum_i \sigma_\alpha^i. \tag{6.62}$$

Since the fixed point occurs for $h^* = 0$, the added term can also be treated perturbatively, and to the lowest order

$$\beta\mathcal{H}' = \beta\mathcal{H}_0 + \langle\mathcal{U}\rangle_0 - h\sum_\alpha \left\langle(\sigma_\alpha^1 + \sigma_\alpha^2 + \sigma_\alpha^3)\right\rangle_0 , \tag{6.63}$$

where the spins are grouped according to their cells. Using Eq. (6.55),

$$\beta\mathcal{H}' = \ln Z_0 + K' \sum_{\langle\alpha,\beta\rangle} \sigma'_\alpha\sigma'_\beta - 3h\sum_\alpha \left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}}\right)\sigma'_\alpha, \tag{6.64}$$

thus identifying the renormalized magnetic field as

$$h' = 3h\left(\frac{e^{3K} + e^{-K}}{e^{3K} + 3e^{-K}}\right). \tag{6.65}$$

In the vicinity of the unstable fixed point

$$b^{y_h} = \left.\frac{\partial h'}{\partial h}\right|_{K^*} = 3\,\frac{e^{4K^*} + 1}{e^{4K^*} + 3} = \frac{3}{\sqrt{2}}, \tag{6.66}$$

and

$$y_h = \frac{\ln\left(3/\sqrt{2}\right)}{\ln\left(\sqrt{3}\right)} \approx 1.37. \tag{6.67}$$

This is lower than the exact value of $y_h = 1.875$. (The Gaussian value of $y_h = 2$ is closer to the correct result in this case.)

(4) NvL carried out the approach to the second order in $\mathcal{U}$. At this order two additional interactions over further neighbor spins are generated. The recursion relations in this three parameter space have a non-trivial fixed point with one unstable direction. The resulting eigenvalue of $y_t = 1.053$ is tantalizingly close to the exact value of 1, but this agreement is likely accidental.

6.5 The Migdal–Kadanoff bond moving approximation

Consider a $b = 2$ RG for the Ising model on a square lattice, in which every other spin along each lattice direction is decimated. As noted earlier, such decimation generates new interactions between the remaining spins. One way of overcoming this difficulty is to simply remove the bonds not connected to the retained spins. The renormalized spins are then connected to their nearest neighbors by two successive bonds. Clearly after decimation, the renormalized bond is given by the recursion relation in Eq. (6.38), characteristic of a one dimensional chain. The approximation of simply removing the unwanted bonds weakens the system to the extent that it behaves one dimensionally. This is remedied by using the unwanted bonds to strengthen those that are left behind. The spins that are retained are now connected by a pair of double bonds (of strength $2K$), and the decimation leads to

$$K' = \frac{1}{2}\ln\cosh(2 \times 2K)\,. \tag{6.68}$$

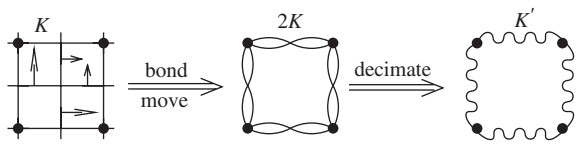

Fig. 6.10 The bond moving scheme for the Migdal–Kadanoff RG for $b = 2$ in dimension $d = 2$.

(1) Fixed points of this recursion relation are located at

(a) $K^* = 0$: For $K \ll 1$, $K' \approx \ln(1 + 8K^2)/2 \approx 4K^2 \ll K$, i.e. this fixed point is stable.

(b) $K^* \to \infty$: For $K \gg 1$, $K' \approx \ln(\mathrm{e}^{4K}/2)/2 \approx 2K \gg K$, indicating that the low-temperature sink is also stable.

(c) The domains of attractions of the above sinks are separated by a third fixed point at

$$\mathrm{e}^{2K^*} = \frac{\mathrm{e}^{4K^*} + \mathrm{e}^{-4K^*}}{2} \quad \Longrightarrow \quad K^* \approx 0.305, \tag{6.69}$$

which can be compared with the exact value of $K_c \approx 0.441$.

(2) Linearizing Eq. (6.68) near the fixed point gives

$$b^{y_t} = \left.\frac{\partial K'}{\partial K}\right|_{K^*} = 2\tanh 4K^* \approx 1.6786 \quad \Longrightarrow \quad y_t \approx 0.747, \tag{6.70}$$

compared to the exact value of $y_t = 1$.

The bond moving procedure can be extended to *higher dimensions*. For a hypercubic lattice in d-dimensions, the bond moving step strengthens each bond by a factor of 2^{d-1}. After decimation, the recursion relation is

$$K' = \frac{1}{2}\ln\cosh\left[2 \times 2^{d-1}K\right]. \tag{6.71}$$

The high and low temperature sinks at $K^* = 0$ and $K^* \to \infty$ are stable since

$$K \ll 1 \quad \Longrightarrow \quad K' \approx \frac{1}{2}\ln(1 + 2^{2d-1}K^2) \approx 2^{2(d-1)}K^2 \ll K, \tag{6.72}$$

and

$$K \gg 1 \quad \Longrightarrow \quad K' \approx \frac{1}{2}\ln\frac{\mathrm{e}^{2^d k}}{2} \approx 2^{d-1}K \gg K. \tag{6.73}$$

(Note that the above result correctly identifies the lower critical dimension of the Ising model, in that the low-temperature sink is stable only for $d > 1$.) The intervening fixed point has an eigenvalue

$$2^{y_t} = \left.\frac{\partial K'}{\partial K}\right|_{K^*} = 2^{d-1}\tanh\left(2^d K^*\right). \tag{6.74}$$

The resulting values of $K^* \approx 0.065$ and $y_t \approx 0.934$ for $d = 3$ can be compared with the known values of $K_c \approx 0.222$ and $y_t \approx 1.59$ on a cubic lattice. Clearly the approximation gets worse at higher dimensions. (It fails to identify an upper critical dimension, and as $d \to \infty$, $K^* \to 2^{2(1-d)}$ and $y_t \to 1$.)

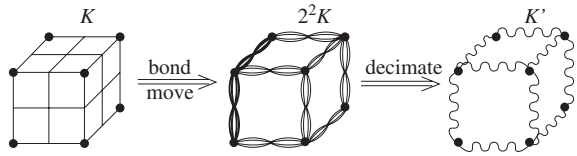

Fig. 6.11 The bond moving scheme for the Migdal–Kadanoff RG for $b = 2$ in dimension $d = 3$.

The Migdal–Kadanoff scheme can also be applied to more general spin systems. For a one-dimensional model described by the set of interactions $\{K\}$, the transfer matrix method in Eq. (6.44) allows construction of recursion relations from

$$T'_b(\{K'\}) = T(\{K\})^b.$$

For a d-dimensional lattice, the bond moving step strengthens each bond by a factor of b^{d-1}, and the generalized Migdal–Kadanoff recursion relations are

$$T'_b(\{K'\}) = T(\{b^{d-1}K\})^b. \tag{6.75}$$

The above equations can be used as a quick way of estimating phase diagrams and exponents. The procedure is exact in $d = 1$, and does progressively worse in higher dimensions. It thus complements mean-field (saddle point) approaches that are more reliable in higher dimensions. Unfortunately, it is not possible to develop a systematic scheme to improve upon its results. The RG procedure also allows evaluation of free energies, heat capacities, and other thermodynamic functions. One possible worry is that the approximations used to construct RG schemes may result in unphysical behavior, e.g. negative values of response functions C and χ. In fact most of these recursion relations (e.g. Eq. 6.75) are exact on *hierarchical* (Berker) lattices. The realizability of such lattices ensures that there are no unphysical consequences of the recursion relations.

6.6 Monte Carlo simulations

Another advantage of discrete spins on a lattice is that they are easily amenable to numerical simulations. The rapid advances of computer processing power, and the advent of clever schemes have made numerical methods quite popular and attractive, to the extent that the study of simulations may be regarded as a field onto itself. As such, the description in this section is intended only as a brief introduction to the topic, and the interested reader should consult the many specialized books devoted to this subject.

Let us consider a system with many degrees of freedom, e.g. a set of $N \gg 1$ spins denoted by $\{\underline{s}\}$, distributed according to the Boltzmann weights

$$P(\underline{s}) = \frac{1}{Z} \exp[-\beta \mathcal{H}(\underline{s})]. \tag{6.76}$$

We are interested in calculating the expectation value of some quantity $\mathcal{O}$, which is in principle obtained as

$$\langle \mathcal{O} \rangle = \mathrm{tr}_{\underline{\mathrm{S}}} \left[\mathcal{O}(\underline{\mathrm{s}}) P(\underline{\mathrm{s}}) \right], \tag{6.77}$$

where $\mathrm{tr}_{\underline{\mathrm{S}}}$ indicates summing over all possible values of $\{\underline{\mathrm{s}}\}$. Unfortunately, even for a discrete spin the number of terms in the sum is prohibitively large for interesting values of N, growing as q^N if each spin can be in one of q states. Monte Carlo procedures aim at evaluating the sum approximately by summing over a representative sample of configurations $\{\underline{\mathrm{s}}_\alpha\}$, as

$$\langle \mathcal{O} \rangle \approx \overline{\mathcal{O}} = \frac{1}{M} \sum_{\alpha=1}^{M} \mathcal{O}(\underline{\mathrm{s}}_\alpha). \tag{6.78}$$

The number of samples M is typically much smaller than the total number of states. The difficult part is to ensure that these M samples are chosen properly.

The question is now how to generate configurations that are weighted according to the distribution in Eq. (6.76). This is achieved by stochastically changing one configuration to another. Let us denote the microstates of the system by $\alpha = 1, 2, \cdots, q^N$, and indicate by $\Pi_{\alpha\beta}$ the probability that the state α is changed to state β in the next *time step*. Note that while it is helpful to maintain the mental image of the system evolving in time, the stochastic dynamic rules are an artificial set of steps for generating the desired configurations. Since $\Pi_{\alpha\beta}$ are transition probabilities, they are constrained by

$$\Pi_{\alpha\alpha} = 1 - \sum_{\beta \neq \alpha} \Pi_{\alpha\beta}. \tag{6.79}$$

The above transition rules are an example of a *Markov process*, in which the state of a system depends on the preceding step(s). Let us assume that initially (at time $t = 0$) the probability to select a state α is $P_\alpha(0)$, e.g. $P_\alpha(0) = 1/q^N$ if all states are equally likely. These probabilities change at the next step of the Markov chain ($t = 1$), and are now given by

$$P_\alpha(1) = \sum_{\beta=1}^{q^N} P_\beta(0) \Pi_{\beta\alpha}. \tag{6.80}$$

In terms of the vector of probabilities $\vec{P}$ and the transition matrix Π this is just

$$\vec{P}(1) = \vec{P}(0) \cdot \Pi. \tag{6.81}$$

Similarly, after t steps, we have

$$\vec{P}(t) = \vec{P}(0) \cdot \Pi^t. \tag{6.82}$$

After many steps of the stochastic dynamics, the probabilities converge to steady-state values $\vec{P}^*$ which form a left eigenvector of the matrix Π,[1] since

$$\vec{P}(t) = \vec{P}(0) \cdot \Pi^t \approx \vec{P}^* \quad \Leftrightarrow \quad \vec{P}^* = \vec{P}^* \cdot \Pi. \tag{6.83}$$

Having established that irrespective of the initial choice, the Markov probabilities converge to a unique set, how can we choose the transition rates to insure that the final probabilities are the Boltzmann weights in Eq. (6.76)? The change in the probability of state α in one step is given by

$$P_\alpha(t+1) - P_\alpha(t) = \sum_{\beta \neq \alpha} \left[P_\beta(t) \Pi_{\beta\alpha} - P_\alpha(t) \Pi_{\alpha\beta} \right]. \tag{6.84}$$

For the pair of states α and β, the first term in the square brackets is the increase in probability due to transitions from β to α, the second is the decrease due to transitions in the opposite direction. The probabilities are thus unchanged if these "probability currents" are equal for every pair, i.e.

$$P_\alpha \Pi_{\alpha\beta} = P_\beta \Pi_{\beta\alpha}. \tag{6.85}$$

This is known as the condition of *detailed balance*, which in the case of Boltzmann weights implies

$$\frac{\Pi_{\alpha\beta}}{\Pi_{\beta\alpha}} = \frac{P_\beta}{P_\alpha} = \exp\left[-\beta \left(E_\beta - E_\alpha \right) \right]. \tag{6.86}$$

Note that since $\sum_\beta \Pi_{\alpha\beta} = 1$, summing Eq. (6.85) over β gives

$$\left(\vec{P} \cdot \Pi \right)_\alpha = \sum_\beta P_\beta \Pi_{\beta\alpha} = P_\alpha \sum_\beta \Pi_{\alpha\beta} = P_\alpha, \tag{6.87}$$

as expected, the detailed balance condition ensures that $\vec{P}$ is the left eigenvector of the transition matrix, corresponding to its steady state.

A popular method for implementing the detailed balance condition is the *Metropolis algorithm:* Let us attempt a transition from state α to state β. This transition is always accepted if it lowers the energy, and with a probability $\exp\left[-\beta \left(E_\beta - E_\alpha \right) \right] < 1$ if it increases the energy, i.e.

$$\Pi_{\alpha\beta} = q_{\alpha\beta} \begin{cases} 1 & \text{for } E_\alpha > E_\beta \\ \exp\left[-\beta \left(E_\beta - E_\alpha \right) \right] < 1 & \text{for } E_\alpha < E_\beta. \end{cases} \tag{6.88}$$

[1] Note the similarities to the transfer matrix approach described earlier in this chapter. In both cases we are interested in a matrix with non-negative elements raised to a large power. For the transition probability matrix, Eq. (6.79) implies that the vector of unit values is a right eigenvector of the matrix with eigenvalue 1. According to Frobenius' theorem, this is the non-degenerate largest eigenvalue of the matrix. The corresponding unique left eigenvector with eigenvalue one is the above steady-state probability $\vec{P}^*$. (More rigorously, the Markov process is called irreducible and converges to a unique limit, if for some finite power n, all elements of the matrix Π^n are positive.)

In the limit of zero temperature only moves that reduce the energy are accepted and the system proceeds towards a local energy minimum. At finite temperature moves that increase the energy are sometimes accepted. The factor of $q_{\alpha\beta}$ is the frequency with which the move from α to β is attempted. Since the energy change has the opposite sign for the transition in the reverse direction (from β to α) the acceptance criteria are reversed. If $q_{\alpha\beta} = q_{\beta\alpha}$, it is easy to see that Eq. (6.86) is satisfied irrespective of the energy change.

As a concrete example, let us consider simulating a system of N Ising spins, in which at each step we attempt to flip ($\sigma_i \to -\sigma_i$) a randomly chosen spin. (In this case, the attempt frequency is $q_{\alpha\beta} = 1/N$ for states related by a single spin flip.) This change is accepted if the resulting energy change ΔE is negative, and otherwise accepted with probability $\exp(-\beta\Delta E)$. For Ising models with short-range interactions calculating ΔE is very fast, since we only need to consider the bonds emanating from the flipped spin. We can start from a randomly generated initial state, and apply the stochastic (Monte Carlo) rule many times. The average of the quantity $\mathcal{O}$ is then estimated as

$$\langle \mathcal{O} \rangle \approx \overline{\mathcal{O}} = \frac{1}{T} \sum_{t=\tau}^{T+\tau} \mathcal{O}[\sigma(t)]. \tag{6.89}$$

The first few steps are strongly influenced by the initial condition and must be discarded. The *equilibration time* τ is not known *a priori*, and will be discussed further in chapter 9. Typically it grows as some power of the correlation length, and thus as a polynomial in N at the critical point. The relaxation time τ also determines the accuracy of the estimate in Eq. (6.89): States separated by a few time steps are highly correlated, and thus the number of independent configurations appearing in the above sum is of the order of T/τ. The relaxation time also depends on the set of attempted moves for transitions, and there are schemes for accelerating equilibration by clever choices of moves. There is also an interesting way to employ Monte Carlo simulations for a position space renormalization group calculation which will not be discussed here.

Problems for chapter 6

1. *Cumulant method:* Apply the Niemeijer–van Leeuwen first order cumulant expansion to the Ising model on a *square* lattice with $-\beta\mathcal{H} = K\sum_{\langle ij\rangle} \sigma_i\sigma_j$, by following these steps:

(a) For an RG with $b = 2$, divide the bonds into *intracell* components $\beta\mathcal{H}_0$, and *intercell* components $\mathcal{U}$.

(b) For each cell α, define a renormalized spin $\sigma'_\alpha = \text{sign}(\sigma^1_\alpha + \sigma^2_\alpha + \sigma^3_\alpha + \sigma^4_\alpha)$. This choice becomes ambiguous for configurations such that $\sum_{i=1}^4 \sigma^i_\alpha = 0$. Distribute the weight of these configurations equally between $\sigma'_\alpha = +1$ and -1 (i.e. put a factor of 1/2 in addition to the Boltzmann weight). Make a table for all possible configurations of a cell, the internal probability $\exp(-\beta\mathcal{H}_0)$, and the weights contributing to $\sigma'_\alpha = \pm 1$.

(c) Express $\langle \mathcal{U} \rangle_0$ in terms of the cell spins σ'_α, and hence obtain the recursion relation $K'(K)$.

(d) Find the fixed point K^*, and the thermal eigenvalue y_t.

(e) In the presence of a small magnetic field $h \sum_i \sigma_i$, find the recursion relation for h, and calculate the magnetic eigenvalue y_h at the fixed point.

(f) Compare K^*, y_t, and y_h to their exact values.

2. *Migdal–Kadanoff method:* Consider Potts spins $s_i = (1, 2, \cdots, q)$, on sites i of a hypercubic lattice, interacting with their nearest neighbors via a Hamiltonian

$$-\beta\mathcal{H} = K \sum_{\langle ij \rangle} \delta_{s_i, s_j} \ .$$

(a) In $d = 1$ find the exact recursion relations by a $b = 2$ renormalization/decimation process. Indentify all fixed points and note their stability.

(b) Write down the recursion relation $K'(K)$ in d-dimensions for $b = 2$, using the Migdal–Kadanoff bond moving scheme.

(c) By considering the stability of the fixed points at zero and infinite coupling, prove the existence of a non-trivial fixed point at finite K^* for $d > 1$.

(d) For $d = 2$, obtain K^* and y_t, for $q = 3$, 1, and 0.

3. *The Potts model:* The *transfer matrix* procedure can be extended to the Potts models, where the spin s_i on each site takes q values $s_i = (1, 2, \cdots, q)$; and the Hamiltonian is $-\beta\mathcal{H} = K \sum_{i=1}^{N} \delta_{s_i, s_{i+1}} + K\delta_{s_N, s_1}$.

(a) Write down the transfer matrix and diagonalize it. Note that you do not have to solve a q_{th} order secular equation as it is easy to guess the eigenvectors from the symmetry of the matrix.

(b) Calculate the free energy per site.

(c) Give the expression for the correlation length ξ (you don't need to provide a detailed derivation), and discuss its behavior as $T = 1/K \to 0$.

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4. *The spin-1 model:* Consider a linear chain where the spin s_i at each site takes on three values $s_i = -1,\ 0,\ +1$. The spins interact via a Hamiltonian

$$-\beta\mathcal{H} = \sum_i K s_i s_{i+1}.$$

(a) Write down the transfer matrix $\langle s|T|s' \rangle = \mathrm{e}^{Kss'}$ explicitly.

(b) Use symmetry properties to find the largest eigenvalue of T and hence obtain the expression for the free energy per site $(\ln Z/N)$.

(c) Obtain the expression for the correlation length ξ, and note its behavior as $K \to \infty$.

(d) If we try to perform a renormalization group by decimation on the above chain we find that additional interactions are generated. Write down the simplest generalization of $\beta\mathcal{H}$ whose parameter space is closed under such RG.

5. *Clock model:* Each site of the lattice is occupied by a q-valued spin $s_i \equiv 1, 2, \cdots, q$, with an underlying translational symmetry modulus q, i.e. the system is invariant under $s_i \to (s_i + n)_{\mathrm{mod}q}$. The most general Hamiltonian subject to this symmetry with nearest-neighbor interactions is

$$\beta\mathcal{H}_C = -\sum_{\langle i,j\rangle} J(|s_i - s_j|_{\mathrm{mod}q}),$$

where $J(n)$ is any function, e.g. $J(n) = J\cos(2\pi n/q)$. *Potts models* are a special case of clock models with full *permutation symmetry*, and the Ising model is obtained in the limit of $q = 2$.

(a) For a closed linear chain of N clock spins subject to the above Hamiltonian show that the partition function $Z = \mathrm{tr}\,[\exp(-\beta\mathcal{H})]$ can be written as

$$Z = \mathrm{tr}\,[\langle s_1|T|s_2\rangle\langle s_2|T|s_3\rangle \cdots \langle s_N|T|s_1\rangle],$$

where $T \equiv \langle s_i|T|s_j\rangle = \exp\left[J(s_i - s_j)\right]$ is a $q \times q$ transfer matrix.

(b) Write down the transfer matrix explicitly and diagonalize it. Note that you do not have to solve a qth order secular equation; because of the translational symmetry, the eigenvalues are easily obtained by discrete Fourier transformation as

$$\lambda(k) = \sum_{n=1}^{q} \exp\left[J(n) + \frac{2\pi i n k}{q}\right].$$

(c) Show that $Z = \sum_{k=1}^{q} \lambda(k)^N \approx \lambda(0)^N$ for $N \to \infty$. Write down the expression for the free energy per site $\beta f = -\ln Z/N$.

(d) Show that the correlation function can be calculated from

$$\left\langle \delta_{s_i, s_{i+\ell}} \right\rangle = \frac{1}{Z}\sum_{\alpha=1}^{q} \mathrm{tr}\left[\Pi_\alpha T^\ell \Pi_\alpha T^{N-\ell}\right],$$

where Π_α is a projection matrix. Hence show that $\left\langle \delta_{s_i, s_{i+\ell}} \right\rangle_c \sim [\lambda(1)/\lambda(0)]^\ell$. (You do not have to explicitly calculate the constant of proportionality.)

6. *XY model:* Consider two component unit spins $\vec{s}_i = (\cos\theta_i, \sin\theta_i)$ in one dimension, with the nearest-neighbor interactions described by $-\beta\mathcal{H} = K\sum_{i=1}^{N} \vec{s}_i \cdot \vec{s}_{i+1}$.

(a) Write down the transfer matrix $\langle\theta|T|\theta'\rangle$, and show that it can be diagonalized with eigenvectors $f_m(\theta) \propto \mathrm{e}^{\mathrm{i}m\theta}$ for integer m.

(b) Calulate the free energy per site, and comment on the behavior of the heat capacity as $T \propto K^{-1} \to 0$.

(c) Find the correlation length ξ, and note its behavior as $K \to \infty$.

7. *One-dimensional gas:* The transfer matrix method can also be applied to a one dimensional gas of particles with short-range interactions, as described in this problem.

(a) Show that for a potential with a hard core that screens the interactions from further neighbors, the Hamiltonian for N particles can be written as

$$\mathcal{H} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=2}^{N} \mathcal{V}(x_i - x_{i-1}).$$

The (indistinguishable) particles are labeled with coordinates $\{x_i\}$ such that

$$0 \le x_1 \le x_2 \le \cdots \le x_N \le L,$$

where L is the length of the box confining the particles.

(b) Write the expression for the partition function $Z(T, N, L)$. Change variables to $\delta_1 = x_1$, $\delta_2 = x_2 - x_1$, $\cdots$, $\delta_N = x_N - x_{N-1}$, and carefully indicate the allowed ranges of integration and the constraints.

(c) Consider the Gibbs partition function obtained from the Laplace transformation

$$\mathcal{Z}(T, N, P) = \int_0^\infty \mathrm{d}L \exp(-\beta P L) Z(T, N, L),$$

and by extremizing the integrand find the standard formula for P in the canonical ensemble.

(d) Change variables from L to $\delta_{N+1} = L - \sum_{i=1}^{N} \delta_i$, and find the expression for $\mathcal{Z}(T, N, P)$ as a product over one-dimensional integrals over each δ_i.

(e) At a fixed pressure P, find expressions for the mean length $L(T, N, P)$, and the density $n = N/L(T, N, P)$ (involving ratios of integrals which should be easy to interpret).

Since the expression for $n(T, P)$ in part (e) is continuous and non-singular for any choice of potential, there is in fact no condensation transition for the one-dimensional gas. By contrast, the approximate van der Waals equation (or the mean-field treatment) incorrectly predicts such a transition.

(f) For a hard sphere gas, with minimum separation a between particles, calculate the equation of state $P(T, n)$.

8. *Potts chain (RG):* Consider a one-dimensional array of N Potts spins $s_i = 1, 2, \cdots, q$, subject to the Hamiltonian $-\beta\mathcal{H} = J \sum_i \delta_{s_i, s_{i+1}}$.

(a) Using the transfer matrix method (or otherwise) calculate the partition function Z, and the correlation length ξ.

(b) Is the system critical at zero temperature for antiferromagnetic couplings $J < 0$?

(c) Construct a renormalization group (RG) treatment by eliminating every other spin. Write down the recursion relations for the coupling J, and the additive constant g.
(d) Discuss the fixed points, and their stability.
(e) Write the expression for $\ln Z$ in terms of the additive constants of successive rescalings.
(f) Show that the recursion relations are simplified when written in terms of $t(J) \equiv \mathrm{e}^{-1/\xi(J)}$.
(g) Use the result in (f) to express the series in (e) in terms of t. Show that the answer can be reduced to that obtained in part (a), upon using the result

$$\sum_{n=0}^{\infty} \frac{1}{2^{n+1}} \ln\left(\frac{1+t^{2^n}}{1-t^{2^n}}\right) = -\ln(1-t).$$

(h) Repeat the RG calculation of part (c), when a small symmetry breaking term $h\sum_i \delta_{s_i,1}$ is added to $-\beta\mathcal{H}$. You will find that an additional coupling term $K\sum_i \delta_{s_i,1}\delta_{s_{i+1},1}$ is generated under RG. Calculate the recursion relations in the three parameter space (J, K, h).
(i) Find the magnetic eigenvalues at the zero temperature fixed point where $J \to \infty$, and obtain the form of the correlation length close to zero temperature.

9. *Cluster RG:* Consider Ising spins on a *hexagonal lattice* with nearest-neighbor interactions J.

(a) Group the sites into clusters of four in preparation for a position space renormalization group with $b = 2$.
(b) How can the majority rule be modified to define the renormalized spin of each cluster?
(c) For a scheme in which the central site is chosen as the tie-breaker, make a table of all possible configurations of site-spins for a given value of the cluster-spin.
(d) Focus on a pair of neighboring clusters. Indicate the contributions of intracluster and intercluster bonds to the total energy.
(e) Show that in zero magnetic field, the Boltzmann weights of parallel and anti-parallel clusters are given by

$$R(+,+) = x^8 + 2x^6 + 7x^4 + 14x^2 + 17 + 14x^{-2} + 7x^{-4} + 2x^{-6},$$

and

$$R(+,-) = 9x^4 + 16x^2 + 13 + 16x^{-2} + 9x^{-4} + x^{-8},$$

where $x = \mathrm{e}^J$.
(f) Find the expression for the resulting recursion relation $J'(J)$.
(g) Estimate the critical *ferromagnetic* coupling J_c, and the exponent ν obtained from this RG scheme, and compare with the exact values.

(h) What are the values of the magnetic and thermal exponents (y_h, y_t) at the zero temperature ferromagnetic fixed point?

(i) Is the above scheme also applicable for antiferromagnetic interactions? What symmetry of the original problem is not respected by this transformation?

10. *Transition probability matrix:* Consider a system of two Ising spins with a coupling K, which can thus be in one of four states.

(a) Explicitly write the 4×4 transition matrix corresponding to single spin flips for a Metropolis algorithm. Verify that the equilibrium weights are indeed a left eigenvector of this matrix.

(b) Repeat the above exercise if both single spin and double spin flips are allowed. The two types of moves are chosen randomly with probabilities p and $q = 1 - p$.