# Supplement to Chapter 9

**REVIEW QUESTIONS**

**9.1** What does it mean to say that $f(x, y)$ is analytic at the point $(x, y)$?

**9.2** How is a phase transition point in the $p$-$T$ plane defined?

**9.3** Why are true phase transitions not possible in finite systems?

**9.4** How do we distinguish between first-order and second-order phase transitions?

**9.5** What is a critical point?

**9.6** What is meant, with regard to critical phenomena, by universality?

**9.7** How are the following critical exponents defined?

1. The order parameter exponent $\beta$.
2. The specific heat exponent $\alpha$.
3. The susceptibility exponent $\gamma$.
4. The critical isotherm exponent $\delta$.

**9.8** What is the fundamental assumption of simple Landau theory?

**9.9** In the Landau theory, what is the criterion for the critical temperature?

**9.10** What is the behavior of $\phi(T, M)$ as a function of $M$, for $T$ above and below $T_c$?

**9.11** Calculate the equilibrium value of $M$ as a function of $t$, near the critical point, using simple Landau theory.

**9.12** What is the value of the order parameter exponent $\beta$ in simple Landau theory?

**9.13** Calculate $E(T)$, for $T$ slightly less than $T_c$, in simple Landau theory, and use it to derive the specific heat exponent $\alpha$.

**9.14** Derive an equation for the magnetization $M$ near the critical temperature in a weak magnetic field, and use it to derive the susceptibility exponent $\gamma$ and the critical isotherm exponent $\delta$.

**9.15** How can one see that large-wavelength fluctuations are important at the critical point?

**9.16** In the Landau–Ginsburg theory, what is the probability of a magnetization pattern $M(\mathbf{r})$?

**9.17** How are the fluctuation amplitudes $M_{\mathbf{K}}$ related to the magnetization $M(\mathbf{r})$?

**9.18** Why is it legitimate to take only a finite number of fluctuation amplitudes in calculating critical phenomena?

**9.19** What is the partition function in the Landau–Ginsburg theory?

**9.20** What is the Gaussian approximation to $Z$?

**9.21** In the Gaussian approximation, calculate the specific heat.

**9.22** What happens to the specific heat at $t = 0$ in the Gaussian approximation?

**9.23** How is the critical dimension defined?

**9.24** Explain how the critical dimension was shown to be $D = 4$.

**9.25** What is the epsilon expansion?

**9.26** In a general, pictorial, way, describe a renormalization transformation.

**9.27** What is the energy exression for the chain of harmonic oscillators that was used to describe a renormalization transformation?

**9.28** Describe how the renormalization transformation $(K_1, K_2) \to (\tilde{K}_1 \tilde{K}_2)$, was derived for the harmonic chain.

**9.29** Derive the transformation $(K_1, K_2) \to (\tilde{K}_1, \tilde{K}_2)$ for the harmonic chain.

**9.30** What is a fixed point of a renormalization flow diagram?

**9.31** Why does any point $(K_1, K_2)$, with $K_1 > 0$ flow to a trivial fixed point $(K_1^*, 0)$?

**9.32** Describe the nontrivial fixed points of the renormalization flow for the harmonic chain.

**9.33** What is a scale-invariant probability distribution?

**9.34** What are the assumptions of Wilson's analysis of critical phenomena?

**9.35** What are stable and unstable fixed points?

**9.36** What kinds of fixed points are stable?

**9.37** Given that, under the scaling transformation $\mathbf{r} \to s\mathbf{r}$ and $M \to \gamma M$, the correlation function satisfies the equation $\langle \gamma M(s\mathbf{r}) \gamma M(s\mathbf{r}') \rangle = \langle M(\mathbf{r}) M(\mathbf{r}') \rangle$, derive the relationship between $\gamma$, $s$, and the correlation function exponent $\lambda$.

**9.38** Explain the meaning of all the terms [$\gamma$, $c(r)$, $s$, $K$, and $\tilde{K}$] in the renormalization relation $\gamma^2 c(sr|K) = c(r, \tilde{K})$.

**9.39** Describe the four steps in a momentum-space renormalization transformation for the Landau–Ginsburg theory.

**9.40** In terms of the parameters $x = A\Lambda^2/2\pi^2$, $y = 3b/2\pi^2$, and $\delta = s - 1$, the Wilson renormalization equations (in 3D) are

$$x \to x + (2x + y - xy)\delta \quad \text{and} \quad y \to y + (y - 3y^2)\delta$$

Derive the fixed point $(x^*, y^*)$.

**9.41** Derive the differential flow equations and give a rough sketch of the flowlines.

**9.42** Describe what modifications are necessary in order to go beyond first order in $\epsilon$ for the Landau–Ginsburg renormalization transformation.

**9.43** How are the fundamental exponents $y_t$ and $y_B$ defined?

**9.44** What is the basic assumption that leads to the scaling formulas for critical exponents in terms of $y_t$ and $y_B$?

**9.45** Derive the relation $\beta = (3 - y_B)/y_t$.

**9.46** Show that the susceptibility exponent $\gamma = (2y_B - 3)/y_t$.

**9.47** In the real-space renormalization method, how is the renormalized Hamiltonian $\tilde{H}(\tilde{\sigma}_1, \tilde{\sigma}_2, \ldots)$ defined?

**9.48** What is meant by the proliferation of interactions?

**9.49** What is meant by block spin ambiguity?

## EXERCISES

**Exercise 9.1** When we say that two atoms, let us say two oxygen atoms, are *hydrogen bonded*, we mean that there is a hydrogen atom located somewhere between the two atoms that is strongly bonded to one of them and weakly bonded to the other, the net effect being a weak bond between the two atoms. The hydrogen atom is not equally distant from the two bonded atoms, but is much closer to the atom to which it is strongly bonded. Ordinary water ice is a solid that is held together by hydrogen bonds. Each oxygen

**Fig. S9.1** A long chain of oxygen atoms, bonded by double hydrogen bonds, forms the imaginary substance, one-dimensional ice.

atom is strongly bonded to two hydrogens and weakly bonded to two others.

In Fig. S9.1 is a picture of a nonexistent substance, called *one-dimensional ice*. It is a very long chain of oxygen atoms, each connected to its nearest neighbors by double hydrogen bonds. As in real ice, there is a restriction that exactly two hydrogen atoms lie close to each oxygen atom. We can indicate the bonds by arrows, with the arrowhead pointing to the strongly bonded oxygen. Then each oxygen atom must have two arrows entering and two arrows leaving. The energy of the system can be written as the sum of the energies of the double bonds. We assume that the double bond patterns have energies as shown in Fig. S9.2.

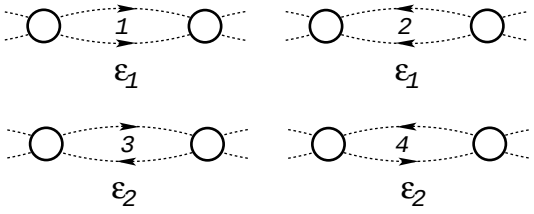


**Fig. S9.2** The energies of the four possible double bond patterns.

The hydrogen bonds are geometrically quite localized and directional, so that it makes sense to distinguish between the two patterns shown with energy $\varepsilon_2$. (a) Assuming that the number of oxygens, $N$, is very large, calculate the partition function and show that the system undergoes a first order phase transition at a finite temperature. (b) Determine the latent heat of transition per oxygen atom.

**Solution** (a) If the first two oxygen atoms have either of the bonding patterns (1) or (2), then every pair of atoms will have the same bonding pattern as the first pair. Thus there are two states of the system with energies $-N\varepsilon_1$. If the first pair of oxygen atoms has bonding pattern (3) or (4), then every other pair has one of those two patterns, but not necessarily the same one. Thus there are $2^N$ states of the system with energies $-N\varepsilon_2$. The partition function is therefore

$$\begin{aligned} Z &= 2e^{\beta N\varepsilon_1} + 2^N e^{\beta N\varepsilon_2} \\ &= 2\big(e^{\beta\varepsilon_1}\big)^N + \big(2e^{\beta\varepsilon_2}\big)^N \end{aligned} \tag{S9.1}$$

If $e^{\beta\varepsilon_1} > 2e^{\beta\varepsilon_2}$, then $2(e^{\beta\varepsilon_1})^N \gg (2e^{\beta\varepsilon_2})^N$, and the second term can be neglected. In the opposite case, in which $e^{\beta\varepsilon_1} < 2e^{\beta\varepsilon_2}$, the first term can be neglected. The transition temperature is determined by setting

$$e^{\beta\varepsilon_1} = 2e^{\beta\varepsilon_2} \tag{S9.2}$$

which gives

$$\tau_o = \frac{\varepsilon_1 - \varepsilon_2}{\log 2} \tag{S9.3}$$

Below $\tau_o$,

$$\phi(\beta) = \log 2 + N\beta\varepsilon_1 \tag{S9.4}$$

Above $\tau_o$,

$$\phi(\beta) = N(\log 2 + \beta\varepsilon_2) \tag{S9.5}$$

(b) The energy of the system, as a function of $\tau$, is

$$E = -\frac{\partial\phi}{\partial\beta} = \begin{cases} -N\varepsilon_1, & \tau < \tau_o \\ -N\varepsilon_2, & \tau > \tau_o \end{cases} \tag{S9.6}$$

The latent heat of the transition per oxygen atom is therefore $\varepsilon_1 - \varepsilon_2$.

**Exercise 9.2** In the one-dimensional ice system described in the last exercise assume that bonds (1) and (2) have a length (distance between neighboring oxygen atoms) of $\ell_1$ and bonds (3) and (4) have a length of $\ell_2$. The long molecule is held fixed at one end and a tension $F$ is applied at the other. It may be helpful to imagine that the force is being created by a very long spring, attached at one end, that can store energy. One now has two variables to describe the equilibrium states of the system, namely $\tau$ and $F$ (analogous to $T$ and $p$). (a) In the $\tau$–$F$ plane, determine the phase transition line. (b) Show that the phase transition line satisfies the Clausius–Clapeyron equation.

**Solution** (a) We assume that $\ell_2 > \ell_1$. The system now has two macrostates—a *long state*, of length $N\ell_2$, and a *short state*, of length $N\ell_1$. The long state has $2^N$ corresponding microstates, while the short state has only 2. If we take the energy of the spring as zero when the ice molecule is in a long state, then the system in the short state has an extra energy of $N(\ell_2 - \ell_1)F = N\,\Delta\ell\,F$. The system now has two states of energy $-N(\varepsilon_1 - \Delta\ell\,F)$ and $2^N$ states of energy $-N\varepsilon_2$. Everything proceeds as before, except for the change of replacing $\varepsilon_1$ by $\varepsilon_1 - \Delta\ell\,F$. Letting $\Delta\varepsilon = \varepsilon_1 - \varepsilon_2$, the transition temperature is given by

$$\tau_o = \frac{\Delta\varepsilon - F\,\Delta\ell}{\log 2} \tag{S9.7}$$

The transition line in the $\tau$–$F$ plane is thus the straight line

$$\tau \log 2 + F\,\Delta\ell = \Delta\varepsilon \tag{S9.8}$$

(b) The entropy change in going from the short to the long state is

$$S_{\text{long}} - S_{\text{short}} = \log 2^N - \log 2 \approx N \log 2 \tag{S9.9}$$

The length change is

$$L_{\text{long}} - L_{\text{short}} = N\,\Delta\ell \tag{S9.10}$$

Solving Eq. (S9.8) for $F(\tau)$ gives

$$F = \frac{\Delta\varepsilon - \tau \log 2}{\Delta\ell} \tag{S9.11}$$

Thus

$$\frac{dF}{d\tau} = -\frac{\log 2}{\Delta\ell} = -\frac{S_{\text{long}} - S_{\text{short}}}{L_{\text{long}} - L_{\text{short}}} \tag{S9.12}$$

Comparing this with Eq. (6.90), one sees that they disagree in sign. This shows that the tension force $F$ corresponds to the negative of the compression force $p$.

**Exercise 9.3** According to the Landau–Ginsburg theory, the conditional canonical potential associated with a magnetization pattern $M(\mathbf{r})$ is

$$\phi(M) = \phi_o - \int_V \left(atM^2 + bM^4 + c|\nabla m|^2\right) d^3r \tag{S9.13}$$

For temperatures not too close to the critical temperature, the observed magnetization pattern would be one that maximizes the value of $\phi(M)$. In Problem 9.2, the reader was asked to show that the maximizing function, with any given boundary conditions, is a solution of the differential equation

$$-c\nabla^2 M + atM + 2bM^3 = 0 \tag{S9.14}$$

In this exercise we consider the case of temperatures below the critical temperature; that is, of negative $t$. If $t < 0$, then the absolute minimum of $\phi(M)$ is given by the trivial solution of Eq. (S9.14) in which $M(\mathbf{r}) = M_o$ is constant. The value of $M_o$ is given by Eq. (S9.14) without the gradient term.

$$-a|t|M_o + 2bM_o^3 = 0 \tag{S9.15}$$

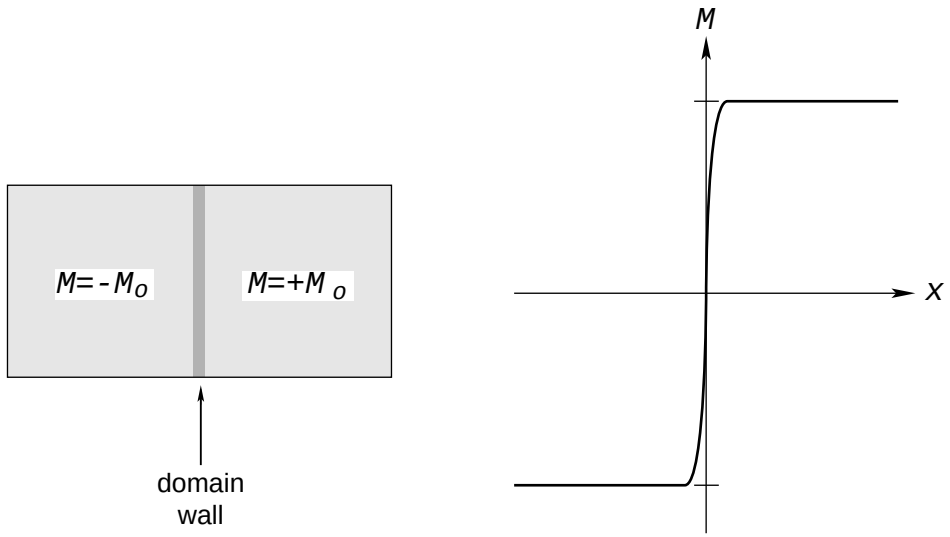


**Fig. S9.3** A ferromagnetic two-phase state. The down phase on the left is separated from the up phase on the right by a domain wall. The magnetization function is shown to the right. One can calculate the domain wall energy, using the Landau–Ginsburg theory.

or

$$M_o = \pm\sqrt{\frac{a|t|}{2b}} \tag{S9.16}$$

It is easy to see that the other solution of Eq. (S9.15), namely $M_o = 0$, gives a local minimum, rather than a maximum of $\phi(M)$.

A more interesting solution of Eq. (S9.14) is one that describes a two-phase state, such as that shown in Fig. S9.3. To describe such a state, one can take a function $M(x)$ that depends only on $x$ and has the form shown in the figure. (a) Assuming that $M(-x) = -M(x)$ and that $M(x) \to M_o$ as $x \to \infty$, determine an exact solution of Eq. (S9.14). (b) Using the solution obtained in (a), and the fact that the free energy is related to the canonical potential by $F = -\tau\phi$, determine the free energy per unit area associated with an interface between two magnetic domains of opposite magnetization.

**Solution** (a) For a function of $x$ alone, and for negative $t$, Eq. (S9.14) becomes

$$-c\frac{d^2M}{dx^2} - a|t|M + 2bM^3 = 0 \tag{S9.17}$$

The most obvious elementary function with the general characteristics shown in Fig. S9.3 is

$$M(x) = A\tanh(\alpha x) \tag{S9.18}$$

where $A$ and $\alpha$ are as yet undetermined. We will see that $A$ and $\alpha$ may be chosen so as to produce an exact solution of the nonlinear differential equation. Taking two derivatives, one obtains

$$\frac{d^2M}{dx^2} = -2A\alpha^2\frac{\tanh(\alpha x)}{\cosh^2(\alpha x)} \tag{S9.19}$$

Substituting this into Eq. (S9.17) gives the relation

$$2Ac\alpha^2\frac{\tanh(\alpha x)}{\cosh^2(\alpha x)} - a|t|\tanh(\alpha x) + 2bA^3\tanh^3(\alpha x) = 0 \tag{S9.20}$$

or

$$2c\alpha^2\mathrm{sech}^2(\alpha x) + 2bA^2\tanh^2(\alpha x) = a|t| \tag{S9.21}$$

But $\tanh^2(\alpha x) = 1 - \mathrm{sech}^2(\alpha x)$. Thus, if the constants $\alpha$ and $A$ are chosen so that

$$2c\alpha^2 = a|t| \quad \text{and} \quad 2bA^2 = a|t| \tag{S9.22}$$

then Eq. (S9.21) is satisfied. The second equation states that the asymptotic values of $M(x)$ are $\pm M_o$, as one could have guessed.

The thickness of the interface is approximately $2/\alpha$. But, by Eq. (S9.22),

$$\frac{2}{\alpha} = 2\sqrt{\frac{2c}{a|t|}} = 2\sqrt{2}\ell \tag{S9.23}$$

where $\ell = \sqrt{c/a|t|}$ is the correlation length, defined in Eq. (9.34). One should notice that, as the critical temperature is approached, the domain wall thickness increases in proportion to the correlation length.
(b) We consider a sample in the form of a long rectangular cylinder, with $L_y = L_z = 1\,\mathrm{m}$ and $L_x = 2L$, where $L$ is some very large number. The canonical potential of the uniformly magnetized state would be given by

$$\phi(M) = \phi_o - \int_{-L}^{L} (-a|t|M_o^2 + bM_o^4)\, dx \tag{S9.24}$$

The canonical potential per unit area of interface is the canonical potential of the nonuniform state minus the canonical potential of the uniform state. After we have made the subtraction (but not before), it is possible to let $L \to \infty$. Then

$$\Delta\phi(M) = -\int_{-\infty}^{\infty} \Big[-a|t|[M^2(x) - M_o^2\,] + b[M^4(x) - M_o^4\,] + c\Big(\frac{dM}{dx}\Big)^2\Big]\, dx \tag{S9.25}$$

Using the facts that $M(x) = M_o \tanh(\alpha x)$ and $M_o^2 = a|t|/2b$, we see that

$$\begin{aligned} -a|t|(M^2 - M_o^2) + b(M^4 - M_o^4) &= \frac{a^2t^2}{2b}\big[1 - \tanh^2(\alpha x)\big] - \frac{a^2t^2}{4b}\big[1 - \tanh^4(\alpha x)\big] \\ &= \frac{a^2t^2}{4b}\big[1 - \tanh^2(\alpha x)\big]^2 \\ &= \frac{a^2t^2}{4b}\mathrm{sech}^4(\alpha x) \end{aligned} \tag{S9.26}$$

and

$$c\Big(\frac{dM}{dx}\Big)^2 = \frac{ca|t|}{2b}\alpha^2\mathrm{sech}^4(\alpha x) = \frac{a^2t^2}{4b}\mathrm{sech}^4(\alpha x) \tag{S9.27}$$

Thus

$$\begin{aligned} \Delta\phi(M) &= -\frac{a^2t^2}{2b}\int_{-\infty}^{\infty} \mathrm{sech}^4(\alpha x)\, dx \\ &= -\frac{2a^2t^2}{3b}\alpha \\ &= -\frac{\sqrt{2}(a|t|)^{5/2}}{3\sqrt{c}} \end{aligned} \tag{S9.28}$$

The interface free energy per unit area is therefore

$$\Delta F = \frac{\sqrt{2}\tau(a|t|)^{5/2}}{3\sqrt{c}} \tag{S9.29}$$

Notice that the interface free energy needed to create a smaller domain of reversed polarization within a larger domain of a given polarization goes to zero at the critical temperature. This is the magnetic equivalent of the fact that the surface tension of a liquid drop vanishes at the critical point. Both effects show why fluctuations become so important near the critical point.

**Exercise 9.4** In Section 9.19, it was suggested that renormalization theory is, in some sense, a generalization of the Central Limit Theorem. If that is so, then the Gaussian probability density that appears in the CLT should be the solution of some appropriately constructed fixed-point problem. Given a sequence of random variables $x_1, x_2, \ldots$ that satisfy the conditions of the CLT, construct a reasonable renormalization procedure whose fixed point gives the unique Gaussian probability density predicted by that theorem.

**Solution** The statistically independent random variables $x_1, x_2, \ldots$ have probability distributions $P_1(x_1)$, $P_2(x_2), \ldots$ that satisfy the conditions that $\bar{x}_n = 0$ and

$$\lim_{N\to\infty}\Big(\frac{\Delta x_1^2 + \cdots + \Delta x_N^2}{N}\Big) = a^2 \tag{S9.30}$$

We construct a single renormalization step by defining new random variables that are weighted sums of pairs of neighboring variables. That is,

$$y_1 = \lambda(x_1 + x_2), \quad y_2 = \lambda(x_3 + x_4), \quad y_3 = \lambda(x_5 + x_6), \ldots \tag{S9.31}$$

A second renormalization would produce the sequence of random variables

$$\begin{aligned} z_1 &= \lambda(y_1 + y_2) = \lambda^2(x_1 + x_2 + x_3 + x_4) \\ z_2 &= \lambda(y_3 + y_4) = \lambda^2(x_5 + x_6 + x_7 + x_8) \end{aligned} \tag{S9.32}$$

After $n$ steps, each variable would represent the sum of $2^n$ of the original variables, multiplied by a scaling factor $\lambda^n$. If a fixed point exists, then it must be possible to choose the scaling factor $\lambda$ so that the probability distributions for the variables are unaffected by the renormalization transformation when $n$ is sufficiently large. It is clear from Eq S9.31 that, because the original variables were statistically independent, the renormalized variables $y_1, y_2, \ldots$ are also statistically independent. Thus each renormalization retains the property of independence.

If we write the $n$th renormalization transformation as $u_1, u_2, \ldots \to \tilde{u}_1, \tilde{u}_2, \ldots$, where $\tilde{u}_1 = \lambda(u_1 + u_2)$, etc., then Eq. (1.51) says that the probability distribution for $\tilde{u}_1$ is related to those for $u_1$ and $u_2$ by

$$\tilde{P}_1(\tilde{u}_1) = \int \delta\big(\tilde{u}_1 - \lambda(u_1 + u_2)\big) P_1(u_1) P_2(u_2)\, du_1\, du_2 \tag{S9.33}$$

The fixed-point property is that, as $n \to \infty$, all probability distributions approach some limit function $P(u)$. By Eq. (S9.33), $P(u)$ must satisfy the relation

$$P(u) = \int \delta\big(u - \lambda(u_1 + u_2)\big) P(u_1) P(u_2)\, du_1\, du_2 \tag{S9.34}$$

The Fourier transform of $P(u)$, which we write as $Q(k)$, is defined by

$$\begin{aligned} Q(k) &= \int e^{iku} P(u)\, du \\ &= \int e^{iku} \delta\big(u - \lambda(u_1 + u_2)\big) P(u_1) P(u_2)\, du\, du_1\, du_2 \\ &= \int e^{ik\lambda u_1} P(u_1)\, du_1 \int e^{ik\lambda u_2} P(u_2)\, du_2 \\ &= Q(\lambda k) Q(\lambda k) \\ &= Q^2(\lambda k) \end{aligned} \tag{S9.35}$$

Before we try to determine the probability density function $P(u)$, let us try to determine the scaling factor $\lambda$. After $n$ renormalization steps,

$$u_1 = \lambda^n(x_1 + \cdots + x_N) \tag{S9.36}$$

where $N = 2^n$. But then, by the Law of Large Numbers, the uncertainty in $u_1$ is

$$\begin{aligned}\Delta u_1 &= \lambda^n \Delta(x_1 + \cdots + x_N) \\ &= \lambda^n \sqrt{N} a \\ &= (\sqrt{2}\lambda)^n a\end{aligned} \tag{S9.37}$$

In order for this to be independent of $n$, we must choose $\lambda = 1/\sqrt{2}$. Thus Eq. (S9.35) can be written as

$$Q(k) = Q^2(k/\sqrt{2}) \tag{S9.38}$$

If we let $F(k) = \log Q(k)$, then

$$F(k) = 2F(k/\sqrt{2}) \tag{S9.39}$$

An obvious solution to this functional equation is $F(k) = Ak^2$. From the results of Exercise 1.31, we know that $F(0) = 0$, $F'(0) = 0$, and $F''(0) = -a^2$. To show that $F(k) = -\frac{1}{2}ak^2$ is the only solution, we let $F(k) = -\frac{1}{2}ak^2 G(k)$, where $G(0) = 1$. Equation (S9.39) then says that

$$-\tfrac{1}{2}ak^2 G(k) = -\tfrac{1}{2}ak^2 G(k/\sqrt{2}) \tag{S9.40}$$

or

$$G(k) = G(k/\sqrt{2}) \tag{S9.41}$$

Beginning with any value of $k$, we can use this repeatedly to get

$$G(k) = G(k/2^K) \to G(0) = 1 \tag{S9.42}$$

This tells us that $Q(k) = \exp(-\frac{1}{2}ak^2)$ and, taking the Fourier transform,

$$\begin{aligned}P(u) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-iku} e^{-\frac{1}{2}ak^2} dk \\ &= e^{-u^2/2a} \int e^{-\frac{1}{2}a(k+iu/a)^2} dk \\ &= \frac{e^{-u^2/2a}}{\sqrt{2\pi a}}\end{aligned} \tag{S9.43}$$

which is exactly the result predicted by the Central Limit Theorem.

**Exercise 9.5** The Ising model and the Landau–Ginsburg theory describe systems with a real scalar order parameter, namely, the magnetization $M$. Such a system is said to have a one-component order parameter. In contrast, a ferromagnetic system in which the magnetization is a vector $\mathbf{M}$ has a three-component order parameter. By a long, complicated analysis, using quantum field theory, it is possible to express the fundamental critical exponents $y_t$ and $y_B$ [see Eq. (9.120)] for a system with an $n$-component order parameter as an expansion in the parameter $\epsilon = 4 - D$, where $D$ is the dimensionality of the system. Through second order, the formulas are

$$y_t = 2 - \frac{n+2}{n+8}\epsilon - \frac{(n+2)(13n+44)}{2(n+8)^3}\epsilon^2 \tag{S9.44}$$

and

$$y_B = 3 - \frac{1}{2}\epsilon - \frac{n+2}{4(n+8)}\epsilon^2 \tag{S9.45}$$

(a) For a one-component order parameter, in 3D, calculate $y_t$ and $y_B$ to second order. (b) Use the result obtained in (a) to compute the magnetization exponent $\beta$.

**Solution** (a) Setting $n$ and $\epsilon$ equal to one in Eqs. (S9.44) and (S9.45) gives

$$y_t = 2 - \frac{1}{3} - \frac{19}{162} = \frac{251}{162} \approx 1.55 \tag{S9.46}$$

and

$$y_B = 3 - \frac{1}{2} - \frac{1}{12} = \frac{29}{12} \approx 2.42 \tag{S9.47}$$

(b) When these values are used in Eq. (9.126), one obtains

$$\beta = \frac{3 - y_B}{y_t} = 0.374 \tag{S9.48}$$

**Exercise 9.6** For a one-dimensional Ising lattice, with periodic boundary conditions, and $\beta V = K$, the probability of a configuration is

$$P(\sigma_1, \sigma_2, \ldots, \sigma_N) = Ce^{K(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \cdots + \sigma_N\sigma_1)} \tag{S9.49}$$

Assume that $N$ is an even number and, by summing over the even spins $\sigma_2$, $\sigma_4, \ldots$, determine the probability distribution for the odd spins $\sigma_1$, $\sigma_3, \ldots$.

**Solution** Following the analysis of Exercise 8.11, we can write the probability in the form

$$P(\sigma_1, \sigma_2, \ldots) = CM(\sigma_1, \sigma_2)M(\sigma_2, \sigma_3)\cdots M(\sigma_N, \sigma_1) \tag{S9.50}$$

where the $2 \times 2$ matrix $M$ is

$$M = \begin{bmatrix} e^K & e^{-K} \\ e^{-K} & e^K \end{bmatrix} \tag{S9.51}$$

Summing over the even spins will simply replace the product of $N$ matrices $M$ in Eq. (S9.50) by a product of $N/2$ matrices $M^2$. That is,

$$P(\sigma_1, \sigma_3, \sigma_5, \ldots) = CM^2(\sigma_1, \sigma_3)M^2(\sigma_3, \sigma_5)\cdots M^2(\sigma_{N-1}, \sigma_1) \tag{S9.52}$$

where

$$M^2 = \begin{bmatrix} e^K & e^{-K} \\ e^{-K} & e^K \end{bmatrix}\begin{bmatrix} e^K & e^{-K} \\ e^{-K} & e^K \end{bmatrix} = 2\begin{bmatrix} \cosh(2K) & 1 \\ 1 & \cosh(2K) \end{bmatrix} \tag{S9.53}$$

**Exercise 9.7** Determine the value of $\tilde{K}$ as a function of $K$, for which we can write the matrix $M^2$ in the form

$$M^2 = C\begin{bmatrix} e^{\tilde{K}} & e^{-\tilde{K}} \\ e^{-\tilde{K}} & e^{\tilde{K}} \end{bmatrix} \tag{S9.54}$$

**Solution** Comparing Eqs. (S9.53) and (S9.54) gives two equations for $C$ and $\tilde{K}$.

$$Ce^{\tilde{K}} = 2\cosh(2K) \tag{S9.55}$$

and

$$Ce^{-\tilde{K}} = 2 \tag{S9.56}$$

Since we are not interested in determining the constant $C$, we divide the first equation by the second to obtain

$$e^{2\tilde{K}} = \cosh(2K) \tag{S9.57}$$

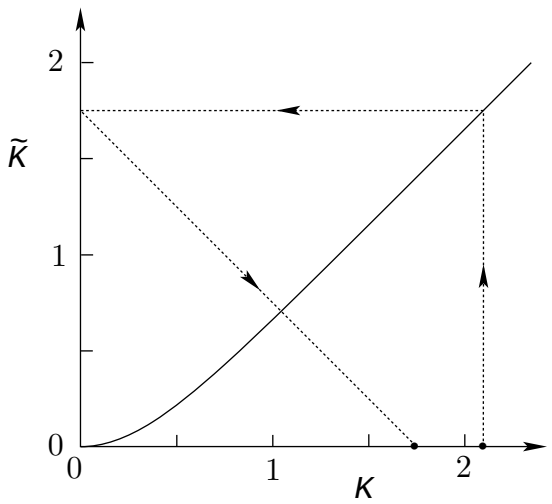


**Fig. S9.4** The curve shown is $\tilde{K}(K)$. The renormalization flow of any point on the $K$ axis can be calculated by first projecting the point upward onto the curve, then horizontally onto the $\tilde{K}$ axis, and finally at 45 degrees back onto the $K$ axis. Due to the fact that the curve is always below a 45 degree line through the origin, any point on the $K$ axis moves toward the origin under repeated renormalization.

or

$$\tilde{K} = \tfrac{1}{2}\log\cosh(2K) \tag{S9.58}$$

For positive $K$, the flow diagram for this transformation is shown in Fig. S9.4. The flow diagram for negative values of $K$ is left as a problem for the reader (Problem 9.9). This procedure, in which the spin variables in the renormalized probability distribution are not, in any sense, averages over a block of the original spin variables, but are simply a subset of the original spin variables, is called a *decimation transformation.*

**Exercise 9.8** The previous exercise shows that the probability distribution for the variables $(\sigma_1, \sigma_3, \sigma_5, \ldots)$ is of the form

$$P(\sigma_1, \sigma_3, \sigma_5, \ldots) = Ce^{\tilde{K}(\sigma_1\sigma_3 + \cdots)} \tag{S9.59}$$

Is it now correct to search for critical points of the 1D Ising model by looking for solutions of the equation

$$K = \tfrac{1}{2}\log\cosh(2K) \tag{S9.60}$$

which is just Eq. (S9.58) with $\tilde{K}$ set equal to $K$?

**Solution** No. That simple procedure is guaranteed to miss any critical points that exist in the model. Actually, since the 1D Ising model has no critical points, the false procedure would not really miss anything, but it is nevertheless important to understand why it is wrong.

The transformation from $K$ to $\tilde{K}$ allows the probability distribution for the renormalized variables

$$(\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_3, \ldots) \equiv (\sigma_1, \sigma_3, \sigma_5, \ldots) \tag{S9.61}$$

to be written in the same form as the probability distribution for the original variables $(\sigma_1, \sigma_2, \sigma_3, \ldots)$, except that $K$ is replaced by $\tilde{K}$. This immediately implies that the correlation functions satisfy the renormalization relation

$$\langle\tilde{\sigma}_1\tilde{\sigma}_2\rangle_{\tilde{K}} = \langle\sigma_1\sigma_2\rangle_K \tag{S9.62}$$

and, for any $n$,

$$\langle\tilde{\sigma}_1\tilde{\sigma}_{n+1}\rangle_{\tilde{K}} = \langle\sigma_1\sigma_{n+1}\rangle_K \tag{S9.63}$$

where

$$\langle\sigma_i\sigma_j\rangle_K \equiv \sum_{\{\sigma\}} \sigma_i\sigma_j e^{K(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \cdots)}/Z(K) \tag{S9.64}$$

[In Eq. (S9.64), we have not indicated the dependence of $\langle\sigma_i\sigma_j\rangle_K$ on the lattice length $N$, because, for large $N$, the correlation function becomes independent of $N$, and, in renormalization theory, we are interested only in the properties of the system in the large-$N$ limit.] If a solution of the equation $\tilde{K}(K^*) = K^*$ existed, then it would imply that the renormalized variables $(\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_3, \ldots)$ had the same probability distribution as the original variables, and therefore that

$$\langle\tilde{\sigma}_1\tilde{\sigma}_{n+1}\rangle_{K^*} = \langle\sigma_1\sigma_{n+1}\rangle_{K^*} \tag{S9.65}$$

or that, in terms of the original variables,

$$\langle\sigma_1\sigma_{2n+1}\rangle_{K^*} = \langle\sigma_1\sigma_{n+1}\rangle_{K^*} \tag{S9.66}$$

By this simple procedure, we are looking for states in which the correlation function does not change with distance *at all*. We are thus guaranteed to come up with only the following two trivial cases.

1. $K = 0$ (equivalent to $T = \infty$), where $\langle\sigma_1\sigma_{n+1}\rangle = 0$ for all $n$.
2. $K = \infty$ (equivalent to $T = 0$), where $\langle\sigma_1\sigma_{n+1}\rangle = 1$ for all $n$.

To search for critical points we should be looking for cases in which the correlation function falls off as some inverse power of $n$. That is, for solutions of [see Eq. (9.74)]

$$\langle\sigma_1\sigma_{n+1}\rangle \sim \frac{C}{n^\lambda} \tag{S9.67}$$

where $\lambda > 0$. Equation (S9.66) would then be replaced by the less demanding equation,

$$\langle\sigma_1\sigma_{2n+1}\rangle = \frac{1}{2^\lambda}\langle\sigma_1\sigma_{n+1}\rangle \tag{S9.68}$$

In using a decimation transformation with discrete variables, one cannot expect nontrivial critical points to be revealed by simple fixed points of the renormalization flow.

The next few exercises present some typical, but very small, real-space renormalization calculations, of gradually increasing complexity, on two-dimensional Ising lattices.

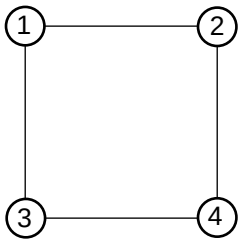


**Fig. S9.5** A $2 \times 2$ square lattice.

**Exercise 9.9** We consider a square Ising lattice with a Hamiltonian that contains nearest-neighbor (NN), next-nearest-neighbor (NNN), and four-spin interaction terms. That is,

$$-\beta E = H = K_1 \sum_{\text{NN}} \sigma_i\sigma_j + K_2 \sum_{\text{NNN}} \sigma_i\sigma_j + K_3 \sum_{\text{sq}} \sigma_i\sigma_j\sigma_k\sigma_l \tag{S9.69}$$

The first sum is taken over all bonds, the second sum over the diagonals of all squares, and the third sum over the corner spins of all squares. (a) For a $2 \times 2$ lattice, number the spins as shown in Fig. S9.5, and write the value of $H$ as an explicit function of $\sigma_1$, $\sigma_2$, $\sigma_3$, and $\sigma_4$. (b) Let $z(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = e^H$, and evaluate $z(+,+,+,+)$, $z(+,+,+,-)$, $z(+,+,-,-)$, and $z(+,-,-,+)$ in terms of $K_1$, $K_2$, and $K_3$. Using rotational and spin-flip symmetries, one could calculate the value of $z(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ for any other configuration in terms

of the four values listed here. (c) Calculate the partition function and the probability for any configuration of the $2 \times 2$ lattice in terms of $K_1$, $K_2$, and $K_3$. (d) Express the Hamiltonian parameters $K_1$, $K_2$, and $K_3$ in terms of the probabilities $P(+,+,+,+)$, $P(+,+,+,-)$, $P(+,+,-,-)$, and $P(+,-,-,+)$.

**Solution** (a)

$$\sum_{\text{NN}} \sigma_i \sigma_j = \sigma_1\sigma_2 + \sigma_3\sigma_4 + \sigma_1\sigma_3 + \sigma_2\sigma_4 \tag{S9.70}$$

$$\sum_{\text{NNN}} \sigma_i \sigma_j = \sigma_1\sigma_4 + \sigma_2\sigma_3 \tag{S9.71}$$

and

$$\sum_{\text{sq}} \sigma_i \sigma_j \sigma_k \sigma_l = \sigma_1\sigma_2\sigma_3\sigma_4 \tag{S9.72}$$

and, therefore,

$$H = K_1(\sigma_1\sigma_2 + \sigma_3\sigma_4 + \sigma_1\sigma_3 + \sigma_2\sigma_4) + K_2(\sigma_1\sigma_4 + \sigma_2\sigma_3) + K_3\sigma_1\sigma_2\sigma_3\sigma_4 \tag{S9.73}$$

(b) From Eq S9.73, $z(+,+,+,+) = \exp(4K_1+2K_2+K_3)$, $z(+,+,+,-) = \exp(-K_3)$, $z(+,+,-,-) = \exp(-2K_2+K_3)$, and $z(+,-,-,+) = \exp(-4K_1 + 2K_2 + K_3)$.

(c) There are two configurations equivalent to $(+,+,+,+)$, there are eight equivalent to $(+,+,+,-)$, there are four equivalent to $(+,+,-,-)$, and there are two equivalent to $(+,-,-,+)$. (Notice that $2+8+4+2 = 2^4$, the total number of configurations.) Therefore,

$$Z = 2e^{4K_1+2K_2+K_3} + 8e^{-K_3} + 4e^{-2K_2+K_3} + 2e^{-4K_1+2K_2+K_3} \tag{S9.74}$$

The probability function, $P(\sigma_1,\sigma_2,\sigma_3,\sigma_4) = Z^{-1}z(\sigma_1,\sigma_2,\sigma_3,\sigma_4)$.

(d) Taking the logarithms of the equations given in the answer to (B), and letting $\phi = \log Z$, we can write the following linear equations for the Hamiltonian parameters.

$$\begin{aligned} 4K_1 + 2K_2 + K_3 &= \log P(+,+,+,+) - \phi \\ -K_3 &= \log P(+,+,+,-) - \phi \\ -2K_2 + K_3 &= \log P(+,+,-,-) - \phi \\ -4K_1 + 2K_2 + K_3 &= \log P(+,-,-,+) - \phi \end{aligned} \tag{S9.75}$$

These equations can easily be solved to give

$$\begin{aligned} K_1 &= \log\big[P(+,+,+,+)/P(+,-,-,+)\big]/8 \\ K_2 &= \log\big[P(+,+,+,+)/P(+,+,-,-)\big]/4 + K_1 \\ K_3 &= \log\big[P(+,+,-,-)/P(+,+,+,-)\big]/2 + K_2 \end{aligned} \tag{S9.76}$$

This exercise allows one to convert from the probability distribution on the $2 \times 2$ lattice to the Hamiltonian parameters that will produce that probability distribution. The next exercise shows how to go from the Hamiltonian parameters on a $4 \times 4$ lattice to the probability distribution on the corresponding $2 \times 2$ lattice of block spins. Combining the two transformations, we can then go from the Hamiltonian parameters on a $4 \times 4$ lattice to the Hamiltonian parameters on the $2 \times 2$ lattice of block spins. The two taken together give a complete renormalization transformation on a very small system.

**Exercise 9.10** Consider the $4 \times 4$ lattice shown in Fig. S9.6. For notational simplicity, the spin variables are named $a$, $b, \ldots, p$, rather than $\sigma_a$, $\sigma_b$, etc. The lattice is broken up into four $2 \times 2$ blocks, as shown. For the block having the spins $a$, $b$, $c$, and $d$, the block spin variable $B(a,b,c,d)$ is defined as

$$B(a,b,c,d) = \begin{cases} \text{sgn}(a+b+c+d), & \text{if } a+b+c+d \neq 0 \\ a, & \text{if } a+b+c+d = 0 \end{cases} \tag{S9.77}$$

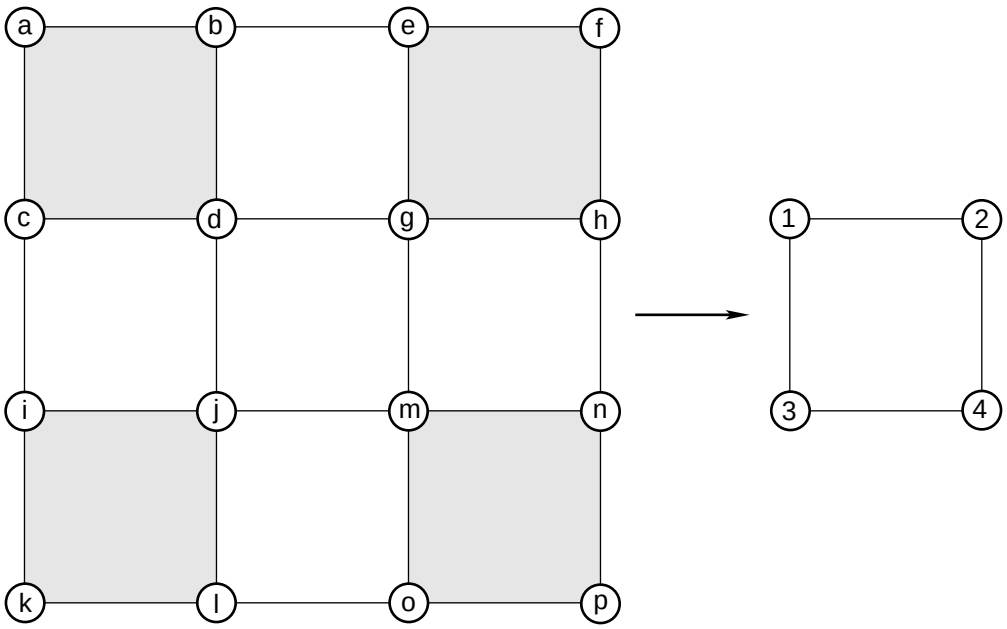


**Fig. S9.6** The single spins on the $2 \times 2$ lattice on the right represent the block spins for the shaded squares on the $4 \times 4$ lattice on the left.

This assigns the block spin $+1$ to the patterns 1, 2, and 3 in Fig. 9.16 and the value $-1$ to the patterns 4, 5, and 6. (a) Assuming that the Hamiltonian on the $4 \times 4$ lattice is of the form given in Eq. (S9.69), write a formula for the probability distribution on the $2 \times 2$ lattice of block spins. (b) Write a Fortran computer program to carry out the complete renormalization transformation from the parameters $K_1$, $K_2$, and $K_3$ on the $4 \times 4$ lattice to the parameters $\tilde{K}_1$, $\tilde{K}_2$, and $\tilde{K}_3$ on the $2 \times 2$ lattice.

**Solution** (a) The canonical probability density on the $4 \times 4$ lattice is

$$P(a, b, \ldots, p) = Z^{-1} \exp\bigl[H(a, b, \ldots, p)\bigr] \tag{S9.78}$$

The Kronecker delta function, $\delta\bigl(B(a, b, c, d) - s_1\bigr)$, is equal to one if the block spin of the upper left block has the value $s_1$, otherwise it is equal to zero. Therefore, if we let $P(s_1, s_2, s_3, s_4)$ be the probability that the four block spins have the values $s_1$, $s_2$, $s_3$, and $s_4$, then, by Eq. (1.51),

$$\begin{aligned} ZP(s_1, s_2, s_3, s_4) = \sum_a \cdots \sum_p & \delta\bigl(B(a, b, c, d) - s_1\bigr)\delta\bigl(B(e, f, g, h) - s_2\bigr) \\ & \times \delta\bigl(B(i, j, k, l) - s_3\bigr)\delta\bigl(B(m, n, o, p) - s_4\bigr) \\ & \times \exp\bigl[H(a, \ldots, p)\bigr] \end{aligned} \tag{S9.79}$$

Since the formulas that were given in the last exercise require only the ratios of probabilities, there will be no need to calculate the partition function $Z$.

(b) The Fortran program, called Renorm_1 in the Program Listing, and included on the program disk, carries out a single renormalization transformation. The user gives the values of $K_1$, $K_2$, and $K_3$, which are called $X_1$, $X_2$, and $X_3$ so that, by Fortran conventions, they will be real numbers. The array $z(s_1, s_2, s_3, s_4)$ will contain the unnormalized block spin probabilities. Their initial values are first set to zero. The unnormalized probability of a configuration of the $4 \times 4$ lattice, called the *Boltzmann weight* of the configuration, is

$$W = e^{X_1 \cdot nn + X_2 \cdot nnn + X_3 \cdot nsq} \tag{S9.80}$$

where $nn$ is the sum over all products of nearest-neighbor spins, $nnn$ is the sum over all products of next-nearest-neighbor spins, and $nsq$ is the sum over all products of the corner spins for each square.

| $K_1$ | $K_2$ | $K_3$ |
|---|---|---|
| 0.30000 | 0.00000 | 0.00000 |
| 0.18117 | 0.02484 | 0.01156 |
| 0.09911 | 0.01569 | 0.00878 |
| 0.04202 | 0.00505 | 0.00305 |
| 0.01386 | 0.00102 | 0.00063 |
| 0.00393 | 0.00016 | 0.00010 |
| 0.00104 | 0.00002 | 0.00001 |
| 0.00027 | 0.00000 | 0.00000 |
| 0.00007 | 0.00000 | 0.00000 |
| 0.40000 | 0.00000 | 0.00000 |
| 0.29986 | 0.05380 | 0.02588 |
| 0.25176 | 0.06172 | 0.03313 |
| 0.20543 | 0.05221 | 0.02950 |
| 0.14567 | 0.03378 | 0.01969 |
| 0.08039 | 0.01466 | 0.00878 |
| 0.03265 | 0.00390 | 0.00238 |
| 0.01039 | 0.00072 | 0.00044 |
| 0.00289 | 0.00011 | 0.00006 |
| 0.42160 | 0.00000 | 0.00000 |
| 0.32937 | 0.06159 | 0.03007 |
| 0.30275 | 0.07898 | 0.04224 |
| 0.29500 | 0.08392 | 0.04653 |
| 0.29276 | 0.08534 | 0.04796 |
| 0.29217 | 0.08576 | 0.04844 |
| 0.29212 | 0.08593 | 0.04861 |
| 0.29235 | 0.08606 | 0.04871 |
| 0.29288 | 0.08628 | 0.04884 |
| 0.50000 | 0.00000 | 0.00000 |
| 0.44621 | 0.09342 | 0.04872 |
| 0.54526 | 0.16326 | 0.08818 |
| 0.87410 | 0.29197 | 0.15899 |
| 1.73588 | 0.60966 | 0.34877 |
| 0.60000 | 0.00000 | 0.00000 |
| 0.61224 | 0.13954 | 0.08008 |
| 0.94781 | 0.29900 | 0.17416 |
| 1.88057 | 0.65228 | 0.40050 |

**Table S9.1** The result of iterating the renormalization transformation described in Exercise 9.10.

For a given configuration, the Boltzmann weight and the values of the four block spins are calculated, and then, in accordance with Eq. (S9.80), the value of the Boltzmann weight is added to the appropriate array element in $z(s_1, s_2, s_3, s_4)$.

When $z(s_1, s_2, s_3, s_4)$ is calculated, the renormalized interaction parameters, called $Y_1$, $Y_2$, and $Y_3$, are computed using Eq. (S9.76).

We now make the somewhat wild assumption that the renormalization transformation,

$$(K_1, K_2, K_3) \to (\tilde{K}_1, \tilde{K}_2, \tilde{K}_3) \tag{S9.81}$$

is so insensitive to the size of the lattice that one can use the result obtained from a $4 \times 4$ lattice to predict the properties of very large lattices. It would then make sense to iterate the transformation, using the output values of one run as input values for the next, and to search for fixed points.

We begin with a simple Ising model; that is, one with only nearest-neighbor interactions. Such a model has parameters $(K_1, 0, 0)$, where $K_1 = \beta V$. If the value of $K_1$ were exactly equal to the critical value $(\beta V)_c = 0.4407\ldots$ (known from Onsager's exact solution) and if the renormalization transformation were also exact, then, under repeated renormalizations,

$$(K_1, 0, 0) \to (K_1', K_2', K_3') \to (K_1'', K_2'', K_3'') \to \cdots \tag{S9.82}$$

the Hamiltonian parameters would approach a fixed point $(K_1^*, K_2^*, K_3^*)$.

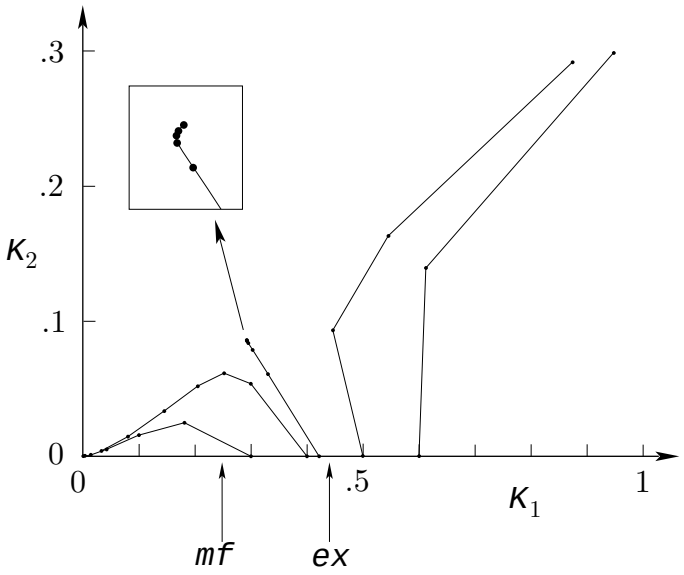


**Fig. S9.7** The renormalization flow diagram for the parameters $K_1$ and $K_2$. The predicted critical value for $K_1 = V/\tau$ is the point that flows into the fixed point. The exact critical value and the mean-field predictions are both indicated by arrows under the $K_1$ axis. In the box is shown a magnification of the flow near the fixed point.

**Exercise 9.11** Starting at points $(K_1, 0, 0)$ for various values of $K_1$, iterate the renormalization transformation derived in the previous exercises and plot the projection of the renormalization flow diagram onto the $(K_1, K_2)$ plane. Table S9.1 gives the result of iterating the renormalization transformation, starting with the values $(K_1, 0, 0)$, where $K_1 = 0.3$, 0.4, 0.4216, 0.5, and 0.6. (Naturally, the middle value was arrived at by trial and error.) For all values of $K_1$ less than the value $K_1^o = 0.4216$ the points flow to the trivial noninteracting $(T = \infty)$ fixed point at $(0, 0, 0)$. For values of $K_1$ larger than $K_1^o$, the points flow to infinity, which is just the other $(T = 0)$ trivial fixed point. The point $(K_1^o, 0, 0)$ flows into a nontrivial, unstable fixed point at $(K_1^*, K_2^*, K_3^*) \approx (0.292, 0.086, -0.048)$. Thus this calculation predicts that the value of $K_1 = V/\tau$ at the critical point is $K_1 = 0.4216$. This is much closer to the true critcal value $K_1 \approx 0.4407$ than is the mean-field prediction of $K_1 = 0.25$. The flow diagram is given in Fig. S9.7. Although this is a very crude calculation, a couple of things should be noted about the results, because they also hold for more accurate (and more complicated) calculations of this type.

1. As we proceed from nearest-neighbor to next-nearest-neighbor and to four-spin and still more complicated interaction terms, the Hamiltonian parameters at the fixed point steadily diminish. That is, $K_1^* > K_2^* > K_3^*$. It is only this fortunate accident that allows one to simplify the calculation by cutting off the proliferating set of Hamiltonian parameters at some fairly small number of terms.
2. Because the nontrivial fixed point is unstable, the sequence of points obtained by any numerical renormalization scheme eventually will diverge from it. Trying to find a sequence that truly converges to the fixed point is like trying to balance a needle on its point. This effect creates serious difficulties when one attemps to do renormalization calculations on larger systems (where one cannot carry out a complete

sum over all configurations) by using the Monte Carlo method to evaluate the probability distribution for the block spins. The Monte Carlo method introduces unavoidable statistical fluctuations into each renormalization step. One is then trying to balance a needle on its point with a trembling hand.

The most unsatisfactory aspect of this calculation, aside from the very small size of the system, is the rather arbitrary treatment of the block spin ambiguity problem. A better method of calculating the block spin probability function $z(s_1, s_2, s_3, s_4)$ is the following.

1. We temporarily allow the block spins to have the values, $\pm 1$ *and* 0. There is then no block spin ambiguity at all.

2. Suppose, in the sum over states on the $4 \times 4$ lattice, we generate a state with a Boltzmann weight $W$ and a block spin configuration $(0, s_2, s_3, s_4)$, where $s_2$, $s_3$, and $s_4$ are nonzero. In the previous method, we would have assigned the weight $W$ either to $z(-1, s_2, s_3, s_4)$ or to $z(+1, s_2, s_3, s_4)$, depending upon the details of the four site spins that make up $s_1$. Clearly, it would be more reasonable to assign half the weight $W$ to each of the two block spin configurations. In a similar way, the Boltzmann weight for a block spin state of the form $(0, 0, s_3, s_4)$ should be evenly redistributed among the four states $(\pm 1, \pm 1, s_3, s_4)$ and so forth for all block spin states involving any number of zeros.

**Exercise 9.12** (a) Modify the program used in the previous exercise to handle the zero block spin values in the way suggested. (b) Iterate the renormalization transformation so obtained and plot the renormalization flow diagram in the $(K_1, K_2)$ plane.

**Solution** (a) In the program Renorm_1, there are storage locations in z$(s_1, s_2, s_3, s_4)$ for the variables $s_1$, $s_2$, $s_3$, and $s_4$ to take the three values, $-1$, 0, and $+1$, although the storage locations associated with the zero values are never actually used. In the modified program, Renorm_2 (see the Program Listings), the unnormalized block spin probability function $z(s_1, s_2, s_3, s_4)$ is first calculated by allowing the block spins to have the values $\pm 1$ and 0. This has been accomplished by a small modification of the function Iblock(K). When that calculation has been completed, the unnormalized probabilities associated with any zero block spin values are redistributed, according to the method described, by the subroutine Redistribute.

(b) With this new method of handling block spin ambiguity, the renormalization tranformation was iterated to produce the flow diagram shown in Fig. S9.8. The predicted critical value of $K_1$ is now $K_1^o = 0.438$ in comparison with the exact value of 0.4407. The error, which is about 0.6%, is not readily discernible on the scale of the diagram.

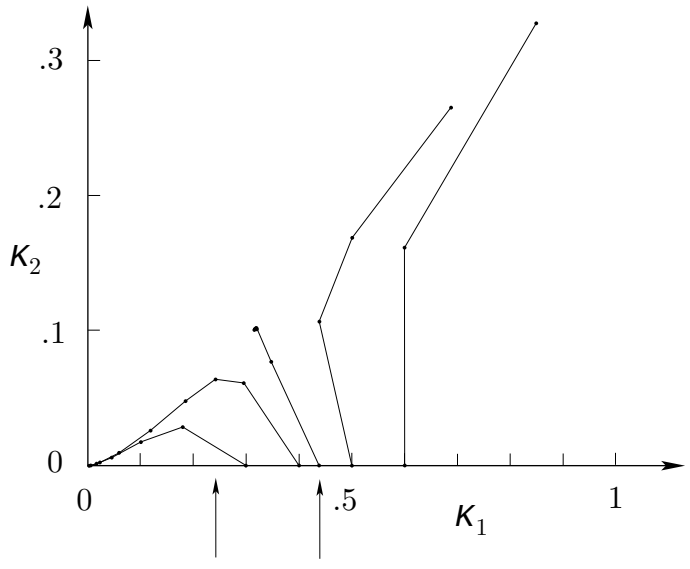


**Fig. S9.8** The renormalization flow diagram produced by the program Renorm_2.

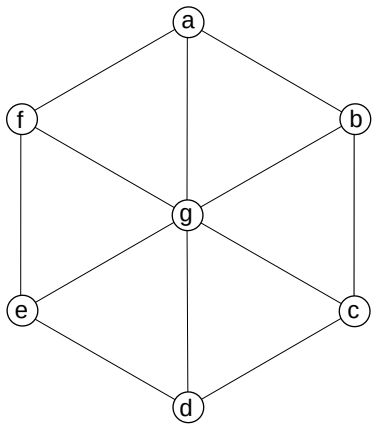


**Fig. S9.9** A set of seven spins, arranged in a hexagon. The underlying lattice is triangular.

**Exercise 9.13** Consider the set of seven spins shown in Fig. S9.9. For simplicity, we call them $a$, $b, \ldots, g$. We define $S_1$ as the sum of the products of all pairs of nearest-neighbor spins, $S_2$ as the sum of the products of all pairs of next-nearest-neighbor spins, and $S_3$ as the sum, over all four-spin parallelograms, of the product of the four vertex spins.* That is,

$$S_1 = (a+b+c+d+e+f)g + ab + bc + cd + de + ef + fa \tag{S9.83}$$

$$S_2 = ac + bd + ce + df + ea + fb \tag{S9.84}$$

and

$$S_3 = (abc + bcd + cde + def + efa + fab)g \tag{S9.85}$$

Assume that the Hamiltonian of the system has the form

$$-\beta E = H = K_1 S_1 + K_2 S_2 + K_3 S_3 \tag{S9.86}$$

We define the three correlation functions

$$C_n(K_1, K_2, K_3) \equiv \frac{\sum S_n e^{K_1 S_1 + K_2 S_2 + K_3 S_3}}{\sum e^{K_1 S_1 + K_2 S_2 + K_3 S_3}} \tag{S9.87}$$

where the sum is over the $2^7$ configurations of the system. Show how one may calculate the value of the Hamiltonian parameters that will give some specified set of correlation functions, $C_1^o$, $C_2^o$, and $C_3^o$. That is, give a practical method of solving the equations

$$C_n(K_1^o, K_2^o, K_3^o) = C_n^o \tag{S9.88}$$

for $K_1^o$, $K_2^o$, and $K_3^o$, with some preassigned accuracy, given $C_1^o$, $C_2^o$, and $C_3^o$.

**Solution** The calculational method is based on the observation that, according to Eq. (S9.87),

$$\begin{aligned} \frac{\partial C_m}{\partial K_n} &= \frac{\sum S_m S_n e^H}{\sum e^H} - \frac{(\sum S_m e^H)(\sum S_n e^H)}{(\sum e^H)^2} \\ &= \langle S_m S_n \rangle - \langle S_m \rangle \langle S_n \rangle \\ &\equiv M_{mn}(K_1, K_2, K_3) \end{aligned} \tag{S9.89}$$

* It might seem more natural that the term following the next-nearest-neighbor spins would be the products of the three vertex spins over all triangles. In the absence of an external magnetic field, because the initial Hamiltonian has up–down spin symmetry, the expectation value of any product of three spins is exactly zero. The three spin terms become important when an external magnetic field is introduced.

Using this formula, it is relatively easy to calculate $M_{mn}$ for given values of $K_1$, $K_2$, and $K_3$. The calulational procedure for solving Eq. (S9.88) is as follows.
1. Begin with some starting values of $K_1$, $K_2$, and $K_3$. Define $\delta K_n$ by

$$\delta K_n = K_n^o - K_n \tag{S9.90}$$

where $(K_1^o, K_2^o, K_3^o)$ is the, as yet unknown, solution of Eq. (S9.88). Then

$$\begin{aligned} C_m^o &= C_m(K_1 + \delta K_1, K_2 + \delta K_2, K_3 + \delta K_3) \\ &\approx C_m(K_1, K_2, K_3) + \sum_n \frac{\partial C_m}{\partial K_n} \delta K_n \\ &= \langle S_m \rangle + \sum_n M_{mn}\, \delta K_n \end{aligned} \tag{S9.91}$$

The equations

$$\sum_n M_{mn}\, \delta K_n = C_m^o - \langle S_m \rangle \tag{S9.92}$$

are three linear equations for the unknowns, $\delta K_1$, $\delta K_2$, and $\delta K_3$.
2. Replace the original values of $K_1$, $K_2$, and $K_3$ with $K_1 + \delta K_1$, $K_2 + \delta K_2$, and $K_3 + \delta K_3$. Calculate $|\delta K| = (\sum \delta K_n^2)^{1/2}$. If $|\delta K|$ is less then the desired accuracy we are finished; if not, go back to (1).

This algorithm is implemented in the subroutine FindHamPars, which is part of the program Renorm_3 in the Program Listings (and the Program Disk). The Subroutine Solve(A,B,X), called by FindHamPars, is simply a linear equation solver for three variables.

This calculation should be compared with part (d) of Exercise 9.9, where the Hamiltonian parameters were computed from the probability function $P(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ for a $2 \times 2$ lattice. In that case there were just enough independent probabilities to determine uniquely the values of the three Hamiltonian parameters. For the system of seven spins being considered here, the number of independent probability values would be much larger than the number of Hamiltonian parameters to be determined unless one allowed the number of parameters to increase beyond three. One cannot exactly match an arbitrary probability distribution on a lattice of seven spins with only three Hamiltonian parameters. That is exactly why the proliferation of interactions takes place in an exact calculation. If one demands that the system have only three parameters, then they must be determined from only three relations, as they were in this exercise. One cannot expect to reproduce exactly the detailed probability distribution on a lattice of more than four spins.

**Exercise 9.14** In Fig. S9.10, the shaded triangles are associated with the block spins $A$, $B, \ldots, G$. The site spins associated with block spin $A$ are called $a_1$, $a_2$, and $a_3$, counting clockwise from the top of the triangle. There is no block spin ambiguity for a triangular lattice. For example,

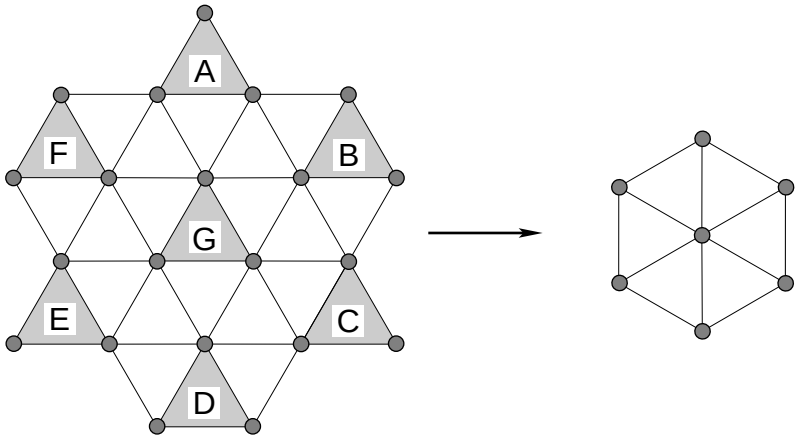


**Fig. S9.10** The renormalization transformation of a small system on a triangular lattice.

$$A = \mathrm{sgn}(a_1 + a_2 + a_3) \tag{S9.93}$$

always gives a unique value for $A$ of plus or minus one. The Hamiltonian of the system of 21 spins is of the same form as that in the system considered in the previous exercise.

$$-\beta E = H = K_1 \sum_{\mathrm{NN}} \sigma_i\sigma_j + K_2 \sum_{\mathrm{NNN}} \sigma_i\sigma_j + K_3 \sum_{\mathrm{four.}} \sigma_i\sigma_j\sigma_k\sigma_\ell \tag{S9.94}$$

We define block spin correlation functions, $C_1$, $C_2$, and $C_3$, as the expectation value in the 21-spin system of the observables [compare with Eqs. (S9.83–85)],

$$S_1 = (A + B + C + D + E + F)G + AB + BC + CD + DE + EF + FA \tag{S9.95}$$

$$S_2 = AC + BD + CE + DF + EA + FB \tag{S9.96}$$

and

$$S_3 = (ABC + BCD + CDE + DEF + EFA + FAB)G \tag{S9.97}$$

Write a Fortran program to compute $C_1$, $C_2$, and $C_3$, given $K_1$, $K_2$, and $K_3$.

**Solution** The program is part of Renorm_3, in the form of a subroutine (called FindCorrFtns) whose input is the set of three Hamiltonian parameters, here called $X_1$, $X_2$, and $X_3$, and whose output is the set of correlation functions $C_1$, $C_2$, and $C_3$ (called $Y_1$, $Y_2$, and $Y_3$ in the program). The peculiar business in the middle of the subroutine that involves the function Ibits is a trick that allows the needed 21 levels of Do Loop nesting in spite of the fact that most Fortran compilers do not permit such deep nesting.

**Exercise 9.15** (a) Using the subroutines FindCorrFtns and FindHamPars write a program to carry out a renormalization transformation $(K_1, K_2, K_3) \rightarrow (\tilde{K}_1, \tilde{K}_2, \tilde{K}_3)$, on the system shown in Fig. S9.10. (b) Iterate the transformation, plot the flow diagram for the parameters $K_1$ and $K_2$, and compare the value of $(K_1^o, 0, 0)$ that flows to a fixed point with the exact critical value for the triangular lattice, namely $K_c = 0.27465\ldots$.

**Solution** (a) The program, called Renorm_3, is in the Program Listings. Each iteration involves converting the Hamiltonian parameters into correlation functions and then converting the correlation functions back into Hamiltonian parameters. The progrm has not been written to run interactively because it is much too slow. Each iteration requires a sum over the $2^{21} \approx 2 \times 10^6$ states of the 21-spin system. The values of $K_1$, $K_2$, and $K_3$ for each iteration are printed in the file Renorm_3.out.

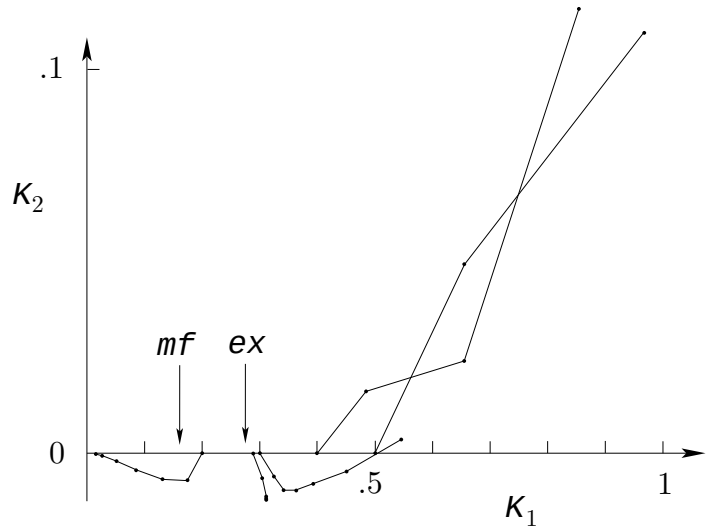


**Fig. S9.11** The renormalization flow diagram produced by Renorm_3. The exact critical value of $K_1$ and the mean-field prediction are shown by arrows.

(b) The flow diagram produced by Renorm_3 is shown in Fig. S9.11. The value of $(K_1^o, 0, 0)$ that flows to the fixed point is about 0.288, which is reasonably close to the exact value of $V/\tau_c \approx 0.275$. The error is larger than that obtained for the square lattice by Renorm_2, but much smaller than the error that would be given by mean-field theory, which predicts a critical value of $K_c = 1/6$.

**Exercise 9.16** Write a Fortran program to carry out the renormalization transformation indicated in Fig. S9.12.

**Solution** The system considered in the previous exercise was clearly close to the maximum size that could be analyzed by summing over all of its configurations. For the system shown in Fig. S9.12, the number of configurations is $2^{36} \approx 7 \times 10^{10}$—too large to be completely summed over. Some approximation method is necessary. The large sum would occur only in calculating the block spin correlation functions on the $6 \times 6$ system. Since they are canonical expectation values of observables, the obvious thing to do is to calculate them by the Monte Carlo method. In the second step,

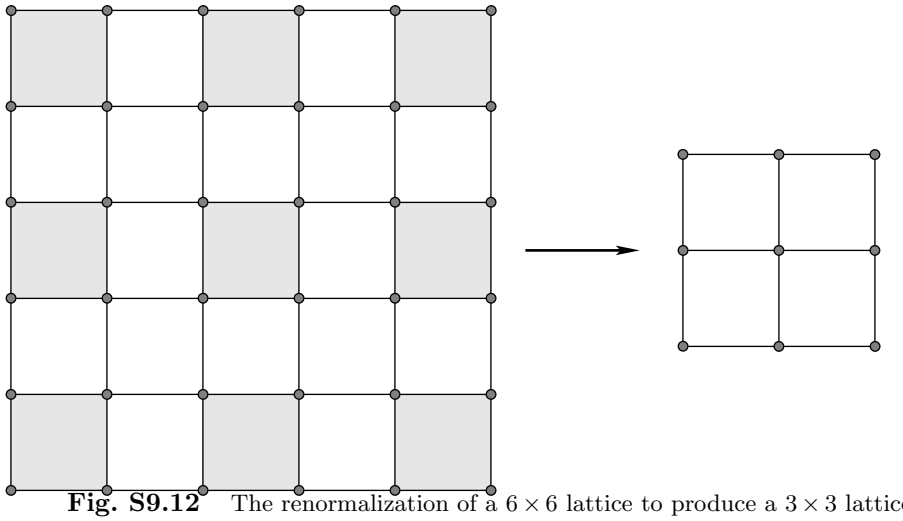

**Fig. S9.12** The renormalization of a $6 \times 6$ lattice to produce a $3 \times 3$ lattice.

namely finding the Hamiltonian parameters from the given correlation functions, we are working on the $3 \times 3$ lattice, which is small enough to be treated exactly. Therefore, it is only the subroutine FindCorrFtns that must be significantly revised. The subroutine FindHamPars must be changed in order to make it applicable to a square, rather than a triangular lattice, but that is completely straightforward. The revised subroutine FindCorrFtns is part of the program Renorm_4 in the Program Listings. A number of comments are necessary to explain certain details of the program.

1. $I_s$ and $I_b$ are the arrays of site spins and block spins, respectively. The free boundary conditions on the site spin system are taken care of by extending the $6 \times 6$ lattice to an $8 \times 8$ lattice and setting all of the outer edge spins equal to zero. Those spins are never changed. When making Monte Carlo moves on the spins of the internal $6 \times 6$ lattice, it is not necessary to check whether a spin is an edge or a corner spin. All spins now have neighbors in all directions. (The outer spins are actually set to zero in the subroutine Initialize, which is not listed here.)
2. The block spin ambiguity problem is treated here in still another new way. If the sum of the site spins is zero, then the block spin is randomly set to plus or minus one. In a long enough Monte Carlo run, this will have the same effect as the redistribution program that is used in Renorm_2. Half of the zero block spin contributions will be assigned to $+1$ and half to $-1$.

When the full program, Renorm_4, is used to construct a flow diagram, the result is not visually distinguishable from the diagram produced by Renorm_2. This seems to support the assumption, made in that calculation, that the renormalization flow pattern is quite insensitive to the size of the system, which has been increased by a factor of 1.5 in going from Renorm_2 to Renorm_4.