

# Chapter 7

## SPIN DYNAMICS

Kinetic spin systems play a crucial role in the development of non-equilibrium statistical physics. The prototypical example is the appealing-simple kinetic Ising model, in which the conventional Ising model of equilibrium statistical mechanics is endowed with physically-motivated transition rates that allows the system to “hop” between different microstates. Just as investigations of the equilibrium Ising model have elucidated the rich phenomenology underlying the transition between the disordered and ferromagnetically-ordered states, studies of the kinetic Ising model have yielded deep insights that have played a starring role in the development of the modern theory of critical phenomena and phase ordering kinetics.

### 7.1 The Voter Model

There is an even simpler kinetic spin system — the voter model — that will be the starting point for our discussion. One reason for focusing on the voter model first is that it is exactly soluble in all spatial dimensions. This solution also provides an instructive introduction for understanding kinetic Ising models. The voter model was introduced in the context of interacting particle systems and has been one of the most extensively examples of such systems. The voter model describes, in an appealing and paradigmatic way, how consensus emerges in a population of spineless individuals. That is, each individual has no firmly fixed opinion and merely takes the opinion of one of its neighbors in an update event. A finite population of such voters eventually achieves consensus in a time that depends on the system size and on the spatial dimension. In this section, we employ techniques inspired from non-equilibrium statistical physics, to solve some of the most basic and striking dynamical properties of the voter model on regular lattices in all dimensions.

In the voter model, an individual is situated at each site of a graph. This graph could be a regular lattice in  $d$  dimensions, or it could be any type of graph—such as the Erdős-Rényi random graph, or a graph with a broad distribution of degrees. Each voter can be in one of two states that, for this presentation, we label as “Democrat” and “Republican”. Mathematically, the state of the voter at  $\mathbf{x}$ ,  $s(\mathbf{x})$ , can take the values  $\pm 1$  only;  $s(\mathbf{x}) = +1$  for a Democrat and  $s(\mathbf{x}) = -1$  for a Republican.

The dynamics of the voter model is simplicity itself. Each voter has no confidence and looks to a neighbor to decide what to do. A single update event in the voter model therefore consists of:

1. Pick a random voter.
2. The selected voter at  $\mathbf{x}$  adopts the state of a randomly-selected neighbor at  $\mathbf{y}$ ; that is,  $s(\mathbf{x}) \rightarrow s(\mathbf{y})$ .
3. Repeat steps 1 & 2 *ad infinitum* or stop when consensus is achieved.

Notice that a voter changes opinion only when its neighbor has the opposite opinion. A typical realization of the voter model on the square lattice is shown in Fig. 7.1, showing how the system tends to organize into single-opinion domains as time increases.

It is expedient to have each update step occur at a fixed rate. The rate at which a voter at  $\mathbf{x}$  changes to

the state  $-s(\mathbf{x})$  may then be written as

$$w(s(\mathbf{x})) = \frac{1}{2} \left( 1 - \frac{s(\mathbf{x})}{z} \sum_{\mathbf{y} \text{ n.n. } \mathbf{x}} s(\mathbf{y}) \right), \quad (7.1)$$

where the sum is over the nearest neighbors of site  $\mathbf{x}$ . Here  $z$  is the coordination number of the graph and we tacitly assume that each site has the same coordination number. The basic feature of this dynamical rule is that the transition rate of a voter at  $\mathbf{x}$  equals the fraction of disagreeing neighbors — when a voter at  $\mathbf{x}$  and all its neighbors agree, the transition rate is zero; conversely, the transition rate equals 1 if all neighbors disagree with the voter at  $\mathbf{x}$ . This linearity is the primary reason why the voter model is soluble. One can generalize the voter model to include opinion changes,  $s(\mathbf{x}) \rightarrow -s(\mathbf{x})$ , whose rate does not depend on the local environment, by simply adding a constant to the flip rate.

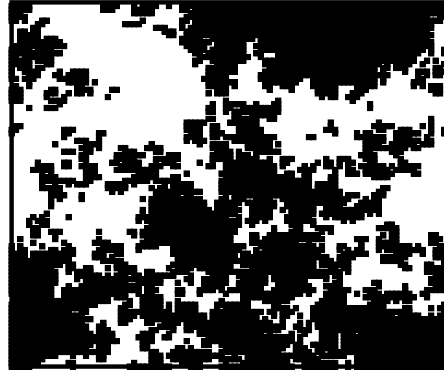


Figure 7.1: The voter model in two dimensions. Shown is a snapshot of a system on a  $100 \times 100$  square lattice at time  $t = 1000$ , obtained by a Monte Carlo simulation. Black and white pixels denote the different opinion states.

To solve the voter model, we need, in principle, the probability distribution  $P(\{\mathbf{s}\}, t)$  that the set of all voters are in configuration  $\{\mathbf{s}\}$  at time  $t$ . This probability distribution satisfies the master equation

$$\frac{dP(\{\mathbf{s}\})}{dt} = - \sum_{\mathbf{x}} w(s(\mathbf{x})) P(\{\mathbf{s}\}) + \sum_{\mathbf{x}} w(-s(\mathbf{x})) P(\{\mathbf{s}\}_{\mathbf{x}}). \quad (7.2)$$

Here  $\{\mathbf{s}\}_{\mathbf{x}}$  denotes the state that is the same as  $\{\mathbf{s}\}$  except that the voter at  $\mathbf{x}$  has changed opinion. In this master equation, the loss term accounts for all possible transitions out of state  $\{\mathbf{s}\}$ , while the gain term accounts for transitions to the state  $\{\mathbf{s}\}$  from states in which one spin differs from the configuration  $\{\mathbf{s}\}$ . In principle, we can use this master equation to derive closed equations for all moments of the probability distribution — namely, all multi-spin correlation functions of the form  $S_{\mathbf{x}, \dots, \mathbf{y}} \equiv \langle s(\mathbf{x}) \cdots s(\mathbf{y}) \rangle$  where the angle brackets denote the average  $\langle f(\{\mathbf{s}\}) \rangle \equiv \sum_{\mathbf{s}} f(\{\mathbf{s}\}) P(\mathbf{s})$ .

Let's begin by considering the simplest such correlation function, namely, the mean spin, or equivalently, the one-point function,  $S(\mathbf{x}) \equiv \langle s(\mathbf{x}) \rangle$ . While it is possible to obtain the evolution of the mean spin and indeed any spin correlation function directly from the master equation (7.2), this approach involves some bookkeeping that is prone to error. We therefore present a simpler alternative method. In a small time interval  $\Delta t$ , the state of a given voter changes as follows:

$$s(\mathbf{x}, t + \Delta t) = \begin{cases} s(\mathbf{x}, t) & \text{with probability } 1 - w(s(\mathbf{x}))\Delta t, \\ -s(\mathbf{x}, t) & \text{with probability } w(s(\mathbf{x}))\Delta t. \end{cases} \quad (7.3)$$

Since the opinion at  $\mathbf{x}$  changes by  $-2s(\mathbf{x})$  with rate  $w(s(\mathbf{x}))$ , the average opinion evolves according to the rate equation

$$\frac{dS(\mathbf{x})}{dt} = -2\langle s(\mathbf{x})w(s(\mathbf{x})) \rangle. \quad (7.4)$$

Substituting in the transition rate from (7.1) and using the fact that  $s(\mathbf{x})^2 = 1$ , we find that for voters that are located on the sites of a  $d$ -dimensional hypercubic lattice, the rate equation has the form

$$\frac{dS(\mathbf{x})}{dt} = -S(\mathbf{x}) + \frac{1}{z} \sum_i S(\mathbf{x} + \mathbf{e}_i) = \Delta S(\mathbf{x}), \quad (7.5)$$

where  $\mathbf{e}_i$  are the unit vectors of the lattice and  $\Delta$  denotes the discrete Laplacian operator

$$\Delta F(\mathbf{x}) \equiv -F(\mathbf{x}) + \frac{1}{z} \sum_i F(\mathbf{x} + \mathbf{e}_i).$$

This rate equation shows that the mean spin undergoes a continuous-time random walk on the lattice. As a result, the mean magnetization,  $m \equiv \sum_{\mathbf{x}} S(\mathbf{x})/N$  is conserved, as follows by summing Eq. (7.5) over all sites. A subtle aspect of this conservation law is that while the magnetization of a specific system *does* change in a single update event by construction, the average over all sites and over all trajectories of the dynamics *is* conserved. The consequence of this conservation law is profound. Consider a finite system with an initial fraction  $\rho$  of Democrats and  $1 - \rho$  of Republicans; equivalently, the initial magnetization  $m_0 = 2\rho - 1$ . Ultimately, this system will reach consensus by voter model dynamics — Democrat consensus with probability  $E(\rho)$  and Republican consensus with probability  $1 - E(\rho)$ . The magnetization of this final state is  $m_\infty = E(\rho) \times 1 + (1 - E(\rho)) \times (-1) = 2E(\rho) - 1$ . Using magnetization conservation, we obtain a basic conclusion about the voter model: because  $m_\infty = m_0$ , the “exit probability” is  $E(\rho) = \rho$ .

### Discrete Diffusion Equation and Bessel Functions

For a continuous-time nearest-neighbor lattice random walk, the master equation for the probability that the particle is at site  $n$  at time  $t$  has the generic form:

$$\dot{P}_n = \frac{\gamma}{2}(P_{n-1} + P_{n+1}) - P_n. \quad (7.6)$$

The random walk corresponds to  $\gamma = 1$  in which the total probability is conserved. Here we consider general values of  $\gamma$  because this case arises in the equations of motion for correlation functions in the kinetic Ising model. For simplicity, suppose that the random walk is initially at site  $n = 0$ . To solve this equation, we introduce the Fourier transform  $P(k, t) = \sum_n P_n(t) e^{ikn}$  and find that the Fourier transform satisfies  $\frac{dP(k, t)}{dt} = [\frac{1}{2}\gamma(e^{ik} + e^{-ik}) - 1]P(k, t)$ . For the initial condition  $P(k, t = 0) = 1$ , the solution is simply  $P(k, t) = \exp[\gamma t \cos k - t]$ . Now we use the generating function representation of the Bessel function,

$$\exp(z \cos k) = \sum_{n=-\infty}^{\infty} e^{ikn} I_n(z).$$

Expanding the generating function in a power series in  $\gamma t$ , we obtain the final result

$$P_n(t) = I_n(\gamma t) e^{-t}. \quad (7.7)$$

In the long-time limit, we use the asymptotics of the Bessel function  $I_n(t) \sim (2\pi t)^{-1/2} e^t$ , to give the asymptotic behavior

$$P_n(t) \sim \frac{1}{\sqrt{2\pi\gamma t}} e^{-(1-\gamma)t}.$$

Let's now solve the rate equation (7.5) explicitly for the mean spin at  $\mathbf{x}$  for the initial condition  $S(x, t = 0) = \delta_{x,0}$ ; that is, a single Democrat in a background population of undecided voters. In one dimension, the rate equation is

$$\frac{dS(x)}{dt} = -S(x) + \frac{1}{2}[S(x-1) + S(x+1)]. \quad (7.8)$$

Using the results from the above highlight on the Bessel function solution to this type of master equation, we simply have

$$S(x, t) = I_x(t) e^{-t} \sim \frac{1}{\sqrt{2\pi t}} \quad \text{as } t \rightarrow \infty. \quad (7.9)$$

Exactly the same approach works in higher dimensions. Now we introduce the multidimensional Fourier transform  $P(k_1, k_2, \dots, t) = \sum_{x_1, x_2, \dots} P_{x_1, x_2, \dots}(t) e^{ik_1 x_1} e^{ik_2 x_2} \dots$  and find that the Fourier transform in each coordinate direction factorizes. For the initial condition of one Democrat at the origin in a sea of undecided voters, the mean spin is then given by

$$S(\mathbf{x}, t) = \prod_{i=1}^d I_{x_i}(t) e^{-dt} \sim \frac{1}{(2\pi t)^{d/2}}. \quad (7.10)$$

Thus the fate of a single voter is to quickly relax to the average opinion of the rest of the population — namely everyone is undecided, on average.

While the above result is exact, it provides no information about how consensus is actually achieved in the voter model. What we need is a quantity that tells us the extent to which two distant voters agree. Such a measure is provided by the two-point correlation function,  $S(\mathbf{x}, \mathbf{y}) \equiv \langle s(\mathbf{x})s(\mathbf{y}) \rangle$ . Proceeding in close analogy with Eq. (7.3) the two-point function evolves as

$$s(\mathbf{x}, t + \Delta t)s(\mathbf{y}, t + \Delta t) = \begin{cases} s(\mathbf{x}, t)s(\mathbf{y}, t) & \text{with probability } 1 - [w(s(\mathbf{x})) + w(s(\mathbf{y}))]\Delta t, \\ -s(\mathbf{x}, t)s(\mathbf{y}, t) & \text{with probability } [w(s(\mathbf{x})) + w(s(\mathbf{y}))]\Delta t. \end{cases} \quad (7.11)$$

Thus  $\langle s(\mathbf{x})s(\mathbf{y}) \rangle$  changes by  $-2\langle s(\mathbf{x})s(\mathbf{y}) \rangle$  if either of the voters at  $\mathbf{x}$  or  $\mathbf{y}$  changes state with respective rates  $w(s(\mathbf{x}))$  and  $w(s(\mathbf{y}))$ , so that  $S(\mathbf{x}, \mathbf{y})$  evolves according to

$$\frac{dS(\mathbf{x}, \mathbf{y})}{dt} = -2 \langle s(\mathbf{x})s(\mathbf{y}) [w(s(\mathbf{x})) + w(s(\mathbf{y}))] \rangle.$$

On a hypercubic lattice, the explicit form of this rate equation is

$$\frac{dS(\mathbf{x}, \mathbf{y})}{dt} = -2S(\mathbf{x}, \mathbf{y}) + \sum_i \frac{1}{z} [S(\mathbf{x} + \mathbf{e}_i, \mathbf{y}) + S(\mathbf{x}, \mathbf{y} + \mathbf{e}_i)]. \quad (7.12)$$

In what follows, we discuss spatially homogeneous and isotropic systems in which the correlation function depends only on the distance  $r = |\mathbf{x} - \mathbf{y}|$  between two voters at  $\mathbf{x}$  and  $\mathbf{y}$ ; thus  $G(r) \equiv S(\mathbf{x}, \mathbf{y})$ . Then the last two terms on the right-hand side of (7.12) are identical and this equation reduces to (7.5) apart from an overall factor of 2. It is now convenient to consider the continuum limit, for which Eq. (7.12) reduces to the diffusion equation

$$\frac{\partial G}{\partial t} = D\nabla^2 G, \quad (7.13)$$

with  $D$  is the diffusion coefficient associated with the continuum limit of (7.12). For the undecided initial state in which each voter is independently a Democrat or a Republican with equal probability, the initial condition is  $G(r, t = 0) = 0$  for  $r > 0$ . On the other hand, each voter is perfectly correlated with itself, that is  $S(\mathbf{x}, \mathbf{x}) = 1$ . In the continuum limit, we must impose a lower cutoff  $a$  in the argument of the correlation function, so that the statement of perfect self correlation becomes  $G(a, t) = 1$ .

To understand physically how the correlation function evolves, it is expedient to work with  $c \equiv 1 - G$ ;  $c$  also satisfies the diffusion equation, but now with the initial condition  $c(r > a, t = 0) = 1$ , and the boundary condition  $c(r = a, t) = 0$ ; that is, the absorbing point at the origin is replaced by a small absorbing sphere of non-zero radius  $a$ . One should think of  $a$  as playing the role of the lattice spacing; a non-zero radius is needed so that a diffusing particle can actually hit the sphere. Physically, then, we study how an initially constant density profile evolves in the presence of a small absorbing sphere at the origin. The exact solution for this concentration profile can be easily obtained in the Laplace domain. Laplace transforming the diffusion equation gives  $sc - 1 = D\nabla^2 c$ ; the inhomogeneous term arises from the constant-density initial condition. A particular solution to the inhomogeneous equation is simply  $c = 1/s$ , and the homogeneous equation

$$c'' + \frac{d-1}{r} c' - \frac{s}{D} c = 0$$

has the general solution  $c = Ar^\nu I_\nu(r\sqrt{s/D}) + Br^\nu K_\nu(r\sqrt{s/D})$ , where  $I_\nu$  and  $K_\nu$  are the modified Bessel functions of order  $\nu$ , with  $\nu = (2 - d)/2$ . Since the concentration is finite as  $r \rightarrow \infty$ , the term with  $I_\nu$  must

be rejected. Then matching to the boundary condition  $c = 0$  at  $r = a$  gives

$$c(r, s) = \frac{1}{s} \left[ 1 - \left( \frac{r}{a} \right)^\nu \frac{K_\nu(r\sqrt{s/D})}{K_\nu(a\sqrt{s/D})} \right]. \quad (7.14)$$

For spatial dimension  $d > 2$ , corresponding to  $\nu < 0$ , we use  $K_\nu = K_{-\nu}$  and the small-argument form  $K_\nu(x) \propto (2/x)^\nu$  to give the leading small- $s$  behavior

$$c(r, s \rightarrow 0) = \frac{1}{s} \left[ 1 - \left( \frac{a}{r} \right)^{d-2} \right].$$

Thus in the time domain, the concentration profile approaches the static electrostatic solution,  $c(r) = 1 - (a/r)^{d-2}$ . A steady state is achieved because there is a non-zero probability that a diffusing particle never hits the absorbing sphere. This is the phenomenon of *transience* that was discussed in Sec. (2.4). The depletion of the concentration near the sphere is sufficiently slow that it is replenished by re-supply from more distant particles. In terms of the voter model, the two-particle correlation function asymptotically becomes  $G(r) \rightarrow (a/r)^{d-2}$  for  $d > 2$ . Thus the influence of one voter on a distant neighbor decays as a power law in their separation.

Now let's study the case  $d \leq 2$  ( $\nu \geq 0$ ). Here a diffusing particle eventually hits the sphere; this is the property of *recurrence* (see again Sec. 2.4) that leads to a growing depletion zone about the sphere. While the time dependence of  $c$  can be obtained by inverting the Laplace transform in Eq. (7.14), it is much simpler to apply the quasi-static approximation as first outlined in Sec. 2.5. From the results given in that section [Eqs. (2.52a) and (2.52b)], the two-spin correlation function for  $r > a$  has the asymptotic behavior for general spatial dimensions:

$$G(r, t) \sim \begin{cases} 1 - \left( \frac{r}{\sqrt{Dt}} \right)^{2-d} & d < 2 \text{ and } 0 < r < \sqrt{Dt}; \\ 1 - \frac{\ln(r/a)}{\ln(\sqrt{Dt}/a)} & d = 2 \text{ and } a < r < \sqrt{Dt}; \\ \left( \frac{a}{r} \right)^{d-2} & d > 2 \text{ and } a < r. \end{cases} \quad (7.15)$$

An important feature for  $d \leq 2$  is that the correlation function at fixed  $r$  approaches 1—distant spins gradually become more strongly correlated. This feature is a manifestation of *coarsening* in which the voters organize into a mosaic of single-opinion enclaves whose characteristic size increases with time. As we shall discuss in more detail in chapter 8, coarsening typifies many types of phase-ordering kinetics. On the other hand, for  $d > 2$  the voter model approaches a steady state and there is no coarsening in the spatial arrangement of the voters if the population is infinite.

There are two important consequences for the voter model that can be deduced from the behavior of the correlation function. The first is that we can immediately determine the time dependence of the density of “interfaces”, namely, the fraction  $n$  of neighboring voters of the opposite opinion. As we shall use extensively later in this chapter, it is helpful to represent an interface as an effective particle that occupies the bond between two neighboring voters of the opposite opinion. This effective particle, or domain wall, provides the right way to characterize the departure of system from consensus. For nearest-neighbor sites  $\mathbf{x}$  and  $\mathbf{y}$ , we relate the correlation function to the domain wall density by

$$\begin{aligned} G(\mathbf{x}, \mathbf{y}) &= \langle s(\mathbf{x})s(\mathbf{y}) \rangle = [\text{prob}(++) + \text{prob}(--)] - [\text{prob}(+-) + \text{prob}(-+)] \\ &= 1 - n \quad n = 1 - 2n. \end{aligned} \quad (7.16)$$

Thus the density of interfaces is related to the near-neighbor correlation function via  $n = (1 - G(\mathbf{x}, \mathbf{y}))/2$ . Using our result (7.15) for the correlation function, the time dependence of the interfacial density is then

$$n(t) \sim \begin{cases} t^{d/2-1} & d < 2, \\ 1/\ln t & d = 2, \\ \mathcal{O}(1) & d > 2. \end{cases} \quad (7.17)$$

When  $d \leq 2$ , the probability of having two voters with opposite opinions asymptotically vanishes and the system develops a coarsening mosaic of single-opinion domains (Fig. 7.1). At the marginal dimension of  $d = 2$  the coarsening process is very slow and the density of interfaces asymptotically vanishes as  $1/\ln t$ . In higher dimensions, an infinite system reaches a dynamic frustrated state where voters of opposite opinion coexist and continually evolve such that the mean density of each type of voter remains fixed.

The second basic consequence that follows from the correlation function is the time  $T_N$  to reach consensus for a finite system of  $N$  voters. For this estimate of the consensus time, we use the fact that the influence of any voter spreads diffusively through the system. Thus starting with some initial state, the influence range of one voter is of the order of  $\sqrt{Dt}$ . We then define consensus to occur when the total amount of correlation within a distance of  $\sqrt{Dt}$  of a particular voter equals the total number of voters  $N$ . The consensus criterion therefore becomes

$$\int^{\sqrt{Dt}} G(r) r^{d-1} dr = N. \quad (7.18)$$

The lower limit can be set to 0 for  $d = 1$  and should be set to  $a$  for  $d > 1$ . Substituting the expressions for the correlation function given in Eq. (7.15) into this integral, the time dependence can be extracted merely by scaling and we find the asymptotic behavior

$$T_N \propto \begin{cases} N^{2/d} & d < 2; \\ N \ln N & d = 2; \\ N & d > 2. \end{cases}$$

Thus as the dimension decreases below 2, consensus takes a progressively longer to achieve. This feature reflects the increasing difficulty in transmitting information when the dimensionality decreases.

**This last part of the section hanging and incomplete.** Let us now derive the exact solution for the correlation function without using the continuum approximation. This solution is nothing more than the lattice Green's function for the diffusion equation. It is convenient to rescale the time variable by 2,  $\tau = 2t$ , so that the correlation function satisfies precisely the same equation of motion as the average magnetization

$$\frac{d}{d\tau} G(\mathbf{x}) = -G(\mathbf{x}) + \frac{1}{z} \sum_i G(\mathbf{x} + \mathbf{e}_i). \quad (7.19)$$

We consider the uncorrelated initial condition  $G(\mathbf{x}, 0) = \delta(\mathbf{x})$  and the boundary condition is  $G(\mathbf{0}) = 1$ . The evolution equation and the initial conditions are as for the autocorrelation function where the solution is  $I_{\mathbf{m}}(\tau)e^{-d\tau}$ . Since the equation is linear, every linear combination of these "building-blocks" is also a solution. Therefore, we consider the linear combination

$$G(\mathbf{x}, \tau) = I_{\mathbf{x}}(\tau)e^{-d\tau} + \int_0^\tau d\tau' J(\tau - \tau') I_{\mathbf{x}}(\tau') e^{-d\tau'}. \quad (7.20)$$

The kernel of the integral is identified as a source with strength  $\delta(\tau) + J(\tau)$ . This source is fixed by the boundary condition:

$$1 = [I_0(\tau)e^{-\tau}]^d + \int_0^\tau d\tau' J(\tau - \tau') [I_0(\tau')e^{-\tau'}]^d. \quad (7.21)$$

We are interested in the asymptotic behavior of the correlation function. This requires the  $\tau \rightarrow \infty$  behavior of the source term. Thus, we introduce the Laplace transform  $\hat{J}(s) = \int_0^\infty d\tau e^{-s\tau} J(\tau)$ . Exploiting the convolution structure of the integral yields

$$\hat{J}(s) = [s\hat{I}(s)]^{-1} - 1 \quad \text{with} \quad \hat{I}(s) = \int_0^\infty d\tau e^{-s\tau} [I_0(\tau)e^{-\tau}]^d. \quad (7.22)$$

Using the integral representation of the Bessel function,  $I_0(\tau) = \int_0^{2\pi} \frac{dq}{2\pi} e^{\tau \cos q}$ , the latter transform is expressed as an integral

$$\hat{I}(s) = \int_0^{2\pi} \frac{d\mathbf{q}}{(2\pi)^d} \frac{1}{s + \sum_{i=1}^d (1 - \cos q_i)}. \quad (7.23)$$

The  $\tau \rightarrow \infty$  asymptotic behavior of the source and the correlation function is ultimately related to the  $s \rightarrow 0$  asymptotic behavior of this integral. The integral diverges,  $\hat{I}(s) \sim s^{d/2-1}$ , when  $d < 2$ , but it remains finite when  $d > 2$ . The leading  $s \rightarrow 0$  behavior of the Laplace transform is therefore

$$\hat{J}(s) \sim \begin{cases} s^{-d/2} & d < 2, \\ s^{-1} \ln s^{-1} & d = 2, \\ s^{-1} & d > 2. \end{cases} \quad (7.24)$$

## 7.2 Glauber Model in One Dimension

In the Ising model, a regular lattice is populated by 2-state spins that may take one of two values:  $s(\mathbf{x}) = \pm 1$ . Pairs of nearest-neighbor spins experience a ferromagnetic interaction that favors their alignment. The Hamiltonian of the system is

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j, \quad (7.25)$$

where the sum is over nearest neighbors  $(i, j)$  on the lattice. Every parallel pair of neighboring spins contributes  $-J$  to the energy and every antiparallel pair contributes  $+J$ . When the coupling constant is positive, the interaction favors ferromagnetic order. The main feature of the Ising model is that ferromagnetism appears spontaneously in the absence of any driving field when the temperature  $T$  is less than a critical temperature  $T_c$  and the spatial dimension  $d > 1$ . Above  $T_c$ , the spatial arrangement of spins is spatially disordered, with equal numbers of spins in the states  $+1$  and  $-1$ . Consequently, the magnetization is zero and spatial correlations between spins decay exponentially with their separation. Below  $T_c$ , the magnetization is non-zero and distant spins are strongly correlated. All thermodynamic properties of the Ising model can be obtained from the partition function  $Z = \sum \exp(-\beta \mathcal{H})$ , where the sum is over all spin configurations of the system, with  $\beta = 1/kT$  and  $k$  is the Boltzmann constant.

While equilibrium properties of the Ising model follow from the partition function, its non-equilibrium properties depend on the nature of the spin dynamics. There is considerable freedom in formulating this dynamics that is dictated by physical considerations. For example, the spins may change one at a time or in correlated blocks. More fundamentally, the dynamics may or may not conserve the magnetization. The role of a conservation law depends on whether the Ising model is being used to describe alloy systems, where the magnetization (related to the composition of the material) is necessarily conserved, or spin systems, where the magnetization does not have to be conserved. This lack of uniqueness of dynamical rules is generic in non-equilibrium statistical physics and it part of the reason why there do not exist universal principles, such as free energy minimization in equilibrium statistical mechanics, that definitively prescribe how a non-equilibrium spin system evolves.

### Spin evolution

We now discuss a simple version of the kinetic Ising model — first introduced by Glauber in 1963 — with non-conservative single-spin-flip dynamics that allows one to extend the Ising model to non-equilibrium processes. We first focus on the exactly-soluble one-dimensional system, and later in this chapter we will study the Ising-Glauber model in higher dimensions, and well as different types of spin dynamics, including conservative Kawasaki spin-exchange dynamics, and cluster dynamics, in which correlated blocks of spins flip simultaneously. In the Glauber model, spins are selected one at a time in random order and each changes at a rate that depends on the change in the energy of the system as a result of this update. Because only single spins can change sign in an update,  $s_j \rightarrow -s_j$ , where  $s_j$  is the spin value at site  $j$ , the magnetization is generally *not* conserved.

There are three types of transitions when a single spin flips: energy raising, energy lowering, and energy neutral transitions (Fig. 7.2). Energy raising events occur when a spin is aligned with a majority of its neighbors and *vice versa* for energy lowering events. Energy conserving events occur when the magnetization of the neighbors is zero. The basic principle to fix the rates of these of events is the *detailed balance condition*. Mathematically, this condition is:

$$P(\{s\})w(s \rightarrow s'_j) = P(\{s'_j\})w(s'_j \rightarrow s). \quad (7.26)$$

Here  $\{s\}$  denotes the state of all the spins in the system,  $\{s'_j\}$  denotes the state derived from  $\{s\}$  in which the spin at  $i$  is flipped, and  $w(s \rightarrow s'_j)$  denotes the transition rate from  $\{s\}$  to  $\{s'_j\}$ .

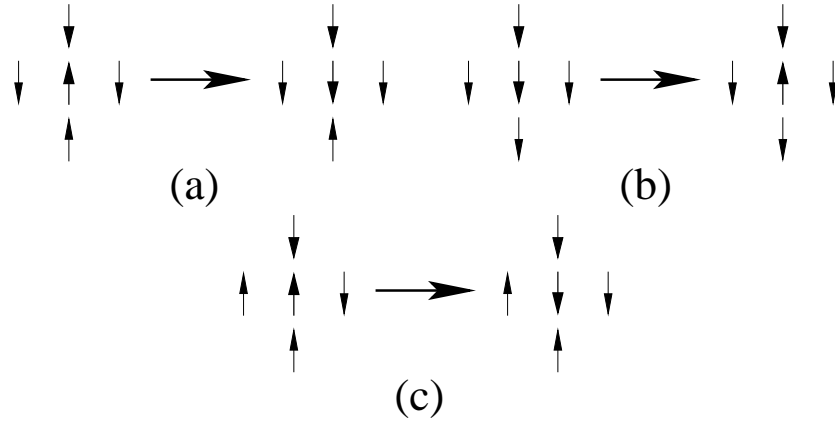


Figure 7.2: (a) Energy lowering, (b) energy raising, and (c) energy conserving spin-flip events on the square lattice.

The detailed balance condition is merely a statement of current conservation. In the abstract space of all  $2^N$  possible spin states of a system of  $N$  spins, Glauber dynamics connects states which differ by the flipping of a single spin. When detailed balance holds, the probability currents from state  $\{s\}$  to  $\{s'_j\}$  and from  $\{s'_j\}$  to  $\{s\}$  (the left and right sides of Eq. (7.26)) are equal so there is no net probability current across any link in this state space. If  $P(\{s\})$  are the equilibrium Boltzmann weights, then the transition rates defined by Eq. (7.26) ensure that any initial spin state will eventually relax to the equilibrium thermodynamic equilibrium state for any non-zero temperature. Thus dynamics that satisfy detailed balance are required if one seeks to understand how equilibrium is approached when a system is prepared in an out-of-equilibrium state.

In one dimension, the detailed balance condition is sufficient to actually fix the flip rates. Following Glauber, we assume that the flip rate of the  $j^{\text{th}}$  spin depends on the neighbors with which there is a direct interaction, namely,  $s_j$  and  $s_{j\pm 1}$ . For an isotropic system, the rate should have left/right symmetry (invariance under the interchange  $i+1 \leftrightarrow i-1$ ) and up/down symmetry (invariance under the reversal of all spins)<sup>1</sup>. For a homogeneous one-dimensional system, these conditions constrain the rate to have the form  $w(s \rightarrow s'_j) = A + Bs_j(s_{j-1} + s_{j+1})$ . This flip rate is simply the energy of the  $i^{\text{th}}$  spin up to an additive constant. We now write this flip rate in the following suggestive form

$$w(s \rightarrow s'_j) = \frac{\alpha}{2} \left[ 1 - \frac{\gamma}{2} s_j (s_{j-1} + s_{j+1}) \right] = \begin{cases} \frac{\alpha}{2}(1 - \gamma) & \text{for spin state } \uparrow\uparrow\uparrow \text{ or } \downarrow\downarrow\downarrow; \\ \frac{\alpha}{2} & \text{for spin state } \uparrow\uparrow\downarrow \text{ or } \downarrow\downarrow\uparrow; \\ \frac{\alpha}{2}(1 + \gamma) & \text{for spin state } \uparrow\downarrow\uparrow \text{ or } \downarrow\uparrow\downarrow. \end{cases} \quad (7.27)$$

When the two neighbors are antiparallel (no local field), the flip rate is simply a constant that we take to be  $1/2$  ( $\alpha = 1$ ) without loss of generality. For  $\gamma > 0$ , the flip rate favors aligning  $s_j$  with its neighbors and *vice versa* for  $\gamma < 0$ .

We now fix  $\gamma$  by applying detailed balance:

$$\frac{w(s \rightarrow s'_j)}{w(s'_j \rightarrow s)} = \frac{1 - \frac{\gamma}{2} s_j (s_{j-1} + s_{j+1})}{1 + \frac{\gamma}{2} s_j (s_{j-1} + s_{j+1})} = \frac{P(\{s'_j\})}{P(\{s\})} = \frac{e^{+\beta J \epsilon_j}}{e^{-\beta J \epsilon_j}}, \quad (7.28)$$

with  $\epsilon_j \equiv -s_j(s_{j-1} + s_{j+1})$ . We simplify the last quantity by exploiting the  $\pm 1$  algebra of Ising spins to write

$$\frac{e^{+\beta J \epsilon_j}}{e^{-\beta J \epsilon_j}} = \frac{\cosh \beta J \epsilon_j + \sinh \beta J \epsilon_j}{\cosh(-\beta J \epsilon_j) + \sinh(-\beta J \epsilon_j)} = \frac{1 + \tanh(2\beta J \frac{\epsilon_j}{2})}{1 - \tanh(2\beta J \frac{\epsilon_j}{2})} = \frac{1 + \frac{1}{2} \epsilon_j \tanh 2\beta J}{1 - \frac{1}{2} \epsilon_j \tanh 2\beta J},$$

<sup>1</sup>Actually the most general rate that satisfies the constraints of locality within the interaction range, symmetry, and isotropy is  $w(s_j) = (1/2)(1 + \delta s_{j-1} s_{j+1}) [1 - (\gamma/2) s_j (s_{j-1} + s_{j+1})]$

where in the last step we use the fact that  $\tanh ax = a \tanh x$  for  $a = 0, \pm 1$ . Comparing with Eq. (7.27), we deduce that  $\gamma = \tanh 2\beta J$ . Thus the flip rate is

$$w(s_j) = \frac{1}{2} \left[ 1 - \frac{1}{2} \tanh 2\beta J s_j (s_{j-1} + s_{j+1}) \right]. \quad (7.29)$$

For  $T \rightarrow \infty$ ,  $\gamma \rightarrow 0$  and all three types of spin-flip events shown in Eq. (7.27) are equiprobable. Conversely, for  $T \rightarrow 0$ ,  $\gamma \rightarrow 1$ , and energy raising spin-flip events are prohibited.

The probability distribution  $P(\{\mathbf{s}\}, t)$  that the system has the microscopic spin configuration  $\mathbf{s}$  at time  $t$  satisfies the same master equation (7.2) as the voter model. Consequently, the equation of motion for the low-order correlation functions are:

$$\frac{dS_j}{dt} = -2 \langle s_j w(s_j) \rangle, \quad (7.30a)$$

$$\frac{dS_{i,j}}{dt} = -2 \langle s_i s_j [w(s_i) + w(s_j)] \rangle, \quad (7.30b)$$

where the subscripts  $i$  and  $j$  denote the  $i^{\text{th}}$  and  $j^{\text{th}}$  site of a one-dimensional lattice.

Using the transition rates given in (7.29) and the identity  $s_j^2 = 1$ , the rate equation for the average spin  $S_j$  is

$$\frac{dS_j}{dt} = -S_j + \frac{\gamma}{2} (S_{j-1} + S_{j+1}). \quad (7.31)$$

With the initial condition  $S_j(0) = \delta_{j,0}$ , the solution is (see the highlight on page 117 on the Bessel function solution to discrete diffusion)

$$S_j(t) = I_j(\gamma t) e^{-t}. \quad (7.32)$$

The new feature compared to the corresponding voter model solution is the presence of the temperature-dependent factor  $\gamma$ . Now the average spin at any site decays as  $S_j(t) \sim (2\pi\gamma t)^{-1/2} e^{-(1-\gamma)t}$ . For  $T > 0$ , the decay is exponential in time,  $S_j \sim e^{-t/\tau}$ , with relaxation time  $\tau = (1-\gamma)^{-1}$ , while for  $T = 0$  the decay is algebraic in time,  $S_j \simeq (2\pi t)^{-1/2}$ . The magnetization  $m = N^{-1} \sum_j S_j$  satisfies  $\frac{dm}{dt} = -(1-\gamma)m$ , so that  $m$  decays exponentially with time at any positive temperature,

$$m(t) = m(0) e^{-(1-\gamma)t}, \quad (7.33)$$

and is conserved only at zero temperature, just as in the voter model. The Ising-Glauber in one dimension model illustrates critical slowing down — slower relaxation at the critical point ( $T = 0$  in one dimension) than for  $T > 0$ .

The mean spin can also be directly solved for a general initial condition,  $S_j(t=0) = \sigma_j$ , with  $\sigma_j$  an arbitrary function between +1 and -1. Then the Fourier transform of the initial condition is  $s_k(t=0) = \sum_n \sigma_n e^{ikn}$ . Using this result, the Fourier transform of the solution to the equation of motion (7.31) is

$$S_k(t) = S_k(t=0) e^{(\gamma \cos k-1)t} = \sum_m e^{ikm} \sigma_m \sum_n I_n(\gamma t) e^{ikn} e^{-t}.$$

Now define  $\ell = m+n$  to recast the exponential factors as a single sum to facilitate taking the inverse Fourier transform:

$$S_k(t) = \sum_{\ell} e^{ik\ell} \sum_m \sigma_m I_{\ell-m}(\gamma t) e^{-t}.$$

From the expression above we may simply read off the solution as the coefficient of  $e^{ik\ell}$ :

$$S_{\ell} = \sum_m \sigma_m I_{\ell-m}(\gamma t) e^{-t}. \quad (7.34)$$

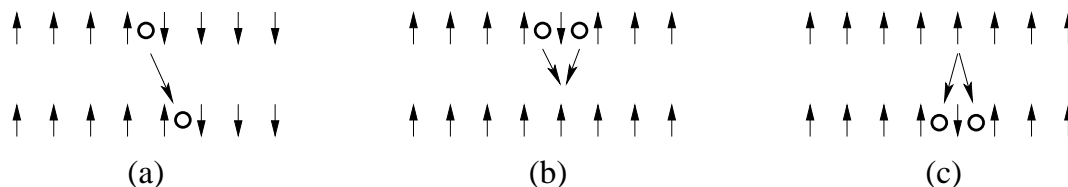


Figure 7.3: Mapping between states of the Ising or the voter models in one dimension and domain wall particles between neighboring pairs of antiparallel spins. Shown are the equivalences between: (a) an energy conserving move and diffusion of a domain wall, (b) energy lowering moves and annihilation of two domain walls, and (c) energy raising moves and creation of a pair of domain walls.

Let's now study the pair correlation function,  $S_{i,j} = \langle s_i s_j \rangle$ . As a preliminary, we highlight a geometrical equivalence between the kinetic Ising model and diffusion-limited reactions. As given by Eq. (7.16), there is a one-to-one mapping between a spin configuration and an arrangement of domain wall quasi particles. Two neighboring antiparallel spins are equivalent to a domain wall that is halfway between the two spins, while two neighboring parallel spins has no intervening domain wall (Fig. 7.3). Energy raising spin flips are equivalent to creating a nearest-neighbor pair of domain walls, while energy lowering moves correspond to annihilation of two neighboring walls. Energy conserving flips correspond to the hopping of a domain wall between neighboring sites. At  $T = 0$ , where domain wall creation is forbidden, Ising-Glauber kinetics is then equivalent to *irreversible diffusion-controlled annihilation*,  $A + A \rightarrow 0$  that we will discuss in more detail in chapter 9.

We focus on translationally invariant systems where the correlation function depends only the separation of the two spins,  $G_k \equiv S_{i,i+k}$ . The master equation (7.30b) becomes

$$\frac{dG_k}{dt} = -2G_k(t) + \gamma(G_{k-1} + G_{k+1}) \quad (7.35)$$

for  $k > 0$ . This equation needs to be supplemented by the boundary condition  $G_0(t) = 1$ . Thus the pair correlation function evolves in nearly the same way as the mean spin. However, because of the existence of the fixed boundary condition at the origin, the master equation also admits an exponential equilibrium solution. This solution is determined by assuming that  $G_k(\infty) \propto \eta^k$  and substituting this form into Eq. (7.35) with the left-hand side set to zero. These steps lead to the following condition for  $\eta$ :  $2 = \gamma(\eta + \eta^{-1})$ , whose solution is  $\eta = [1 - \sqrt{1 - \gamma^2}]/\gamma = \tanh \beta J$ . The equilibrium pair correlation function therefore decays exponentially in the distance between the two spins,

$$G_k(\infty) = e^{-k/\xi}, \quad (7.36)$$

with correlation length  $\xi^{-1} = \ln(\coth \beta J)$ . This result coincides with the correlation function obtained directly from thermodynamics. As expected, the correlation length  $\xi$  diverges as  $T \rightarrow 0$ , indicative of a phase transition, and  $\xi$  vanishes at infinite temperature.

To solve the time dependence of the correlation function with the prescribed initial and boundary conditions, we use the fact that master equation for the correlation function has the same form as that for the mean spin, apart from an overall factor of 2. Thus the general solution will be built from components of the same form as (7.34), with the replacement of  $\gamma \rightarrow 2\gamma$ . We now need to determine the appropriate linear combination of these component solutions that simultaneously satisfy the initial condition  $G_k(t = 0)$  and the boundary condition  $G_0 = 1$ . One piece of the full solution is just the equilibrium correlation function  $G_k(\infty) = \eta^{|k|}$ . To this we add the general homogeneous solution that satisfies the prescribed constraints. Pictorially, the appropriate initial condition for the homogeneous solution consists of an arbitrary odd function plus an antisymmetric piece that cancels the equilibrium solution for  $k > 0$  (Fig. 7.4). The antisymmetry of these pieces ensure that  $G_0 = 1$  and that the prescribed initial condition is satisfied for  $k > 0$ .

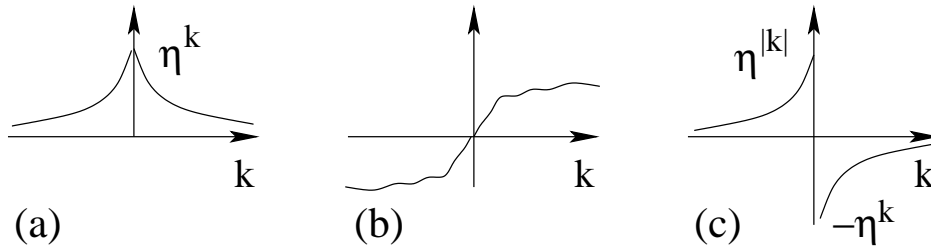


Figure 7.4: (a) Equilibrium correlation function and (b) an arbitrary antisymmetric initial condition. To find  $G_k(t)$  for  $k > 0$ , we superpose the solutions for the three initial conditions shown. The influence of the initial condition (c) cancels that of (a) in the region  $k > 0$  so that only (b) remains—an arbitrary initial condition that vanishes at  $k = 0$ .

The general solution for  $k > 0$  therefore is:

$$\begin{aligned}
 G_k(t) &= \eta^k + e^{-2t} \sum_{\ell=-\infty}^{\infty} G_\ell(0) I_{k-\ell}(2\gamma t) \\
 &= \eta^k + e^{-2t} \sum_{\ell=1}^{\infty} [G_\ell(0) - \eta^\ell] I_{k-\ell}(2\gamma t) + e^{-2t} \sum_{\ell=-1}^{-\infty} [G_\ell(0) + \eta^{|\ell|}] I_{k-\ell}(2\gamma t) \\
 &= \eta^k + e^{-2t} \sum_{\ell=1}^{\infty} [G_\ell(0) - \eta^\ell] [I_{k-\ell}(2\gamma t) - I_{k+\ell}(2\gamma t)]. \tag{7.37}
 \end{aligned}$$

We restrict ourselves to the case of  $T = 0$ , where two special cases lead to nice results:

1. Antiferromagnetic initial state,  $G_k(0) = (-1)^k$ . In this case, every site of the dual lattice is initially occupied by domain wall particle. For this initial state, the nearest-neighbor correlation function in Eq. (7.37) reduces to

$$G_1(t) = 1 - 2e^{-2t} \sum_{j \text{ odd}} [I_{1-j}(2t) - I_{1+j}(2t)] = 1 - 2e^{-2t} I_0(2t),$$

where we have used  $I_n = I_{-n}$ .

2. Random initial state,  $G_k(0) = m_0^2$ , where  $m_0$  is the initial magnetization. Then the nearest-neighbor correlation function is

$$G_1(t) = 1 + e^{-2t} (m_0^2 - 1) \sum_j [I_{1-j}(2t) - I_{1+j}(2t)] = 1 - 2e^{-2t} (m_0^2 - 1) [I_0(2t) + I_1(2t)].$$

From these two solutions, the domain wall densities are

$$\rho(t) = \frac{1 - G_1}{2} = \begin{cases} I_0(2t) e^{-2t} \sim \frac{1}{\sqrt{4\pi t}} & \text{antiferromagnetic,} \\ \frac{1 - m_0^2}{2} [I_0(2t) + I_1(2t)] e^{-2t} \sim \frac{1 - m_0^2}{\sqrt{4\pi t}} & \text{uncorrelated.} \end{cases} \tag{7.38}$$

If the initial magnetization  $m_0 = 0$  for the random initial condition, then the asymptotic domain wall density universally vanishes as

$$\rho(t) \sim (4\pi t)^{-1/2}, \tag{7.39}$$

independent of the initial domain wall density! Because the number of domain walls decrease with time, their separation correspondingly increases. The system therefore coarsens, as domains of parallel spins grow with the diffusive length scale  $t^{1/2}$ . A final important point is that Eq. (7.38) also represents the exact solution for diffusion-limited annihilation  $A + A \rightarrow 0$ ! We will return to this reaction in chapter 9.

## Domain length distribution

In the previous section, we obtained the density of domain walls or alternatively, the average domain length. Now we ask the more fundamental question: what is the distribution of domain lengths in a one-dimensional system of length  $L$ ? Let  $P_k$  be the probability for a domain of length  $k$ , namely, a string of  $k$  consecutive aligned spins that is flanked by oppositely-oriented spins at each end. To have a system-size independent quantity, we define this probability per unit length.

Partial information about this distribution follows from basic physical considerations. For example, the domain wall density  $\rho$ , which scales as  $t^{-1/2}$ , is given by  $\sum_k P_k$ , while the domain length distribution obeys the normalization condition  $\sum_k k P_k = 1$ . Furthermore, from the diffusive nature of the evolution, the only physical length scale grows as  $t^{1/2}$ . These facts suggest that the domain length distribution has the scaling form

$$P_k(t) \simeq t^{-1} \Phi(kt^{-1/2}). \quad (7.40)$$

The prefactor ensures that the mean domain length (per unit length) equals 1, *i.e.*,  $\int x \Phi(x) dx = 1$ , while the asymptotic decay of the total density (7.39) gives the condition  $\int \Phi(x) dx = (4\pi)^{-1/2} \equiv C$ .

We can also infer the short-distance tail of the scaling function  $\Phi(x)$  from the long-time decay of the domain density. Consider the role of the shortest possible domain of length 1 in the rate equation for the domain density  $\rho$ . When a domain that consists of a single spin flips, three domains merge into a single larger domain, as illustrated below:

$$\cdots \downarrow \underbrace{\uparrow \cdots \uparrow \uparrow \downarrow}_{\text{domain 1}} \underbrace{\uparrow \uparrow \cdots \uparrow}_{\text{domain 2}} \downarrow \cdots \xrightarrow{1} \cdots \downarrow \underbrace{\uparrow \cdots \uparrow \downarrow \uparrow \uparrow \cdots \uparrow}_{\text{domain 3}} \downarrow \cdots$$

Since such events, in which two domains disappear, occur with a unit rate, the domain density decays as

$$\frac{d\rho}{dt} = -2P_1, \quad (7.41)$$

and using Eq. (7.39), we obtain  $P_1 \sim \frac{C}{4} t^{-3/2}$ . On the other hand, expanding  $\Phi$  in a Taylor series gives  $P_1 \cong \Phi(0)t^{-1} + \Phi'(0)t^{-3/2} + \cdots$ . Comparing these two results, we deduce that  $\Phi(0) = 0$  and  $\Phi'(0) = \frac{C}{4}$ . Therefore the scaling function vanishes linearly in the small-argument limit:

$$\Phi(x) \sim \frac{C}{4} x, \quad \text{as } x \rightarrow 0. \quad (7.42)$$

This linear decrease in the small-size tail of the probability distribution is a generic feature of many one-dimensional interacting many-body systems.

While scaling provides some glimpses about the nature of the length distribution, we are interested in the distribution itself. The exact solution of the distribution is not yet known, and we present an approximate solution based on the *independent interval approximation*. This approximation is based on assuming that the lengths of neighboring domains are uncorrelated, an assumption makes the calculation of the domain length distribution tractable. This same approximation can be applied to a variety of one-dimensional domain evolution and reaction processes. Under the assumption of uncorrelated domains, their length distribution evolves according to the master equations

$$\frac{dP_k}{dt} = -2P_k + P_{k+1} + P_{k-1} \left(1 - \frac{P_1}{\rho}\right) + \frac{P_1}{\rho^2} \sum_{i+j=k-1} P_i P_j - \frac{P_1}{\rho} P_k. \quad (7.43)$$

The first three terms account for length changes due to a domain wall hopping by  $\pm 1$  and describe the diffusion of a single domain. The factor  $1 - P_1/\rho$  multiplying  $P_{k-1}$  ensures that the neighboring domain has length greater than 1, so that the hopping of a domain wall leads to  $(k-1, j) \rightarrow (k, j-1)$ , and not to  $(k-1, 1, j) \rightarrow (k+j)$ . The remaining terms account for changes in the distribution due to mergings. Because any merger requires a domain of length 1, these terms are proportional to  $P_1$ . The gain term accounts for the merger of three domains of lengths  $i$ ,  $j$ , and 1, with  $i+j+1=k$ , and the loss term accounts for the merger of a domain of length  $k$  with a domain of any length. These master equations apply for any  $k \geq 1$ , subject to the boundary condition  $P_0 = 0$ .

It is easy to check that the total density  $\rho = \sum_k P_k$  satisfies (7.41) and that  $\sum_k k \frac{dP_k}{dt} = 0$ . Since the typical domain length grows indefinitely with time, we replace the integer  $k$  by the continuous variable  $x$ , and substitute the scaling form (7.40), as well as  $\rho \simeq Ct^{-1/2}$  and  $P_1 \simeq \frac{C}{4}t^{-3/2}$  into the master equation to give the integro-differential equation for the scaling function

$$\frac{d^2\Phi}{dx^2} + \frac{1}{2} \frac{d(x\Phi)}{dx} + \frac{1}{4C} \int_0^x \Phi(y)\Phi(x-y) dy = 0. \quad (7.44)$$

We now introduce the Laplace transform,  $\phi(s) = C^{-1} \int_0^\infty \Phi(x)e^{-sx} dx$ , to transform the convolution into a product and reduce this integro-differential equation to the ordinary nonlinear differential equation

$$\frac{d\phi}{ds} = \frac{\phi^2}{2s} + 2s\phi - \frac{1}{2s}, \quad (7.45)$$

with the boundary condition  $\phi(0) = 1$ .

Eq. (7.45) is a Riccati equation and it can be reduced to the second-order linear equation

$$\frac{d^2\psi}{ds^2} + \frac{d\psi}{ds} \left( \frac{1}{s} - 2s \right) - \frac{\psi}{4s^2} = 0.$$

by the standard transformation  $\phi(s) = -2s \frac{d \ln \psi(s)}{ds}$ . We then eliminate the linear term in this equation by writing  $\psi = yv$  and then forcing the term linear in  $\psi'$  to be zero. This requirement gives the condition  $\ln v' = s - 1/(2s)$ , from which we find that the transformation  $\phi(s) = 1 - 2s^2 - 2s \frac{d}{ds} \ln y(s)$  reduces the Riccati equation (7.45) to a linear Schrödinger equation

$$\frac{d^2y}{ds^2} + (2 - s^2)y = 0. \quad (7.46)$$

Eq. (7.46) is the parabolic cylinder equation whose solution is a linear combination of the two linearly independent solutions,  $y(s) = C_+ D_{1/2}(s\sqrt{2}) + C_- D_{1/2}(-s\sqrt{2})$ , with  $D_\nu(x)$  the parabolic cylinder function of order  $\nu$ . From the large- $s$  behavior  $\phi(s) \simeq (4s)^{-2}$ , together with the asymptotics of  $D_\nu(s)$ , it follows that  $C_- = 0$ . Therefore the Laplace transform is

$$\phi(s) = 1 - 2s^2 - 2s \frac{d}{ds} \ln D_{1/2}(s\sqrt{2}). \quad (7.47)$$

The constant  $C_+$  can be evaluated explicitly from the normalization condition  $\phi'(0) = -C_+^{-1}$  and the properties<sup>2</sup> of  $D_\nu(x)$ . Using these facts, we find  $C_+ = \Gamma(3/4)/\Gamma(1/4) = 0.337989\dots$ ; this result should be compared with the exact value  $C = (4\pi)^{-1/2} = 0.28209$ .

The domain length distribution at large length can also be obtained from the small- $s$  limit of the exact solution (7.47). The large- $x$  tail of  $\Phi(x)$  is exponential as follows from the behavior of the Laplace transform near its simple pole at  $s = -\lambda$ ,  $\phi(s) \simeq 2\lambda(s + \lambda)^{-1}$ . The constant  $\lambda$  is given by the first zero of the parabolic cylinder function,  $D_{1/2}(-\lambda\sqrt{2}) = 0$ , located at  $\lambda \approx 0.5409$ . Therefore the domain length distribution asymptotically decays exponentially for large  $x$

$$\Phi(x) \simeq A \exp(-\lambda x), \quad (7.48)$$

with amplitude  $A = 2C\lambda$ . The approximate value for the decay coefficient  $\lambda$  is larger than the exact value  $\zeta(3/2)/\sqrt{16\pi} = 0.368468$ .

While the independent interval approximation is not exact, it is very useful. By invoking the this approximation, we are able to write a closed master equation for the evolution of the domain length distribution. The independent interval approximation then yields the main qualitative behavior of the domain length distribution including: (i) the linear small-length limit of the distribution, (ii) the large-length exponential tail, and (iii) correct integrated properties, such as the  $t^{-1/2}$  decay of the number of domains. As we shall see in later applications, the independent interval approximation applies to a wide range of coarsening processes.

<sup>2</sup>The following properties are needed  $D_\nu(0) = \frac{\sqrt{\pi 2^\nu}}{\Gamma(1/2 - \nu/2)}$ ,  $D'_\nu(0) = \frac{\sqrt{\pi 2^{\nu+1}}}{\Gamma(-\nu/2)}$ , and  $D_\nu(x) \sim x^\nu \exp(-x^2/4)[1 + \mathcal{O}(x^{-2})]$ .

## 7.3 Glauber Model in Higher Dimensions

### Finite spatial dimension

When the spatial dimension  $d$  is greater than one, the Ising-Glauber model is no longer solvable. A variety of approximate continuum theories have been constructed to capture the essence of this model, as will be described in the next chapter. Here we focus on the basic properties of an individual-spin description, there is still much that can be learned.

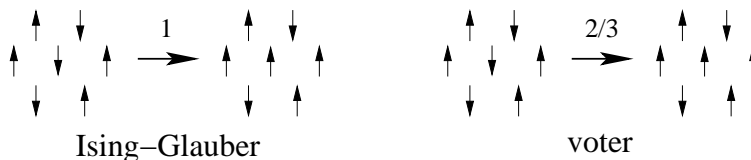


Figure 7.5: Comparison of the rates of an update event in the Ising-Glauber model at zero temperature and in the voter model on the triangular lattice.

First, we address why the voter model is soluble for all  $d$ , while the closely related Ising-Glauber model at zero temperature is not. This dichotomy stems from a simple but profound difference between these two models in  $d > 1$ .<sup>3</sup> Let's determine the transition rates for Glauber dynamics for  $d > 1$  by using detailed balance. Following the same steps that lead to Eq. (7.29), we have

$$\frac{w(s \rightarrow s'_i)}{w(s'_i \rightarrow s)} = \frac{P(\{s'_i\})}{P(\{s\})} = \frac{e^{-\beta J s_i \sum s_j}}{e^{+\beta J s_i \sum s_j}} = \frac{1 - \tanh(\beta J s_i \sum s_j)}{1 + \tanh(\beta J s_i \sum s_j)} = \frac{1 - s_i \tanh \beta J \sum s_j}{1 + s_i \tanh \beta J \sum s_j}, \quad (7.49)$$

where the sum is over the nearest neighbors of  $s_i$ , and in the last step we used  $\tanh(s_i x) = s_i \tanh x$  for  $s_i = \pm 1$ . Thus up to an overall constant that may be set to one, the transition rate for spin  $i$  is

$$w(s_i) = \frac{1}{2} \left[ 1 - s_i \tanh \left( \beta J \sum_j s_j \right) \right]. \quad (7.50)$$

At zero temperature, this rule forbids energy raising updates, while energy lowering updates occur with rate 1 and energy conserving events occur with rate 1/2. This defines a *majority rule* update — a spin flips to agree with the majority of its neighbors (Fig. 7.5). In contrast, the voter model is governed by *proportional rule* — a voter changes to the state of its local majority with a probability equal to the fraction of neighbors in this majority state. This proportionality allows one to factorize the voter model master equation in  $d$  dimensions into a product of soluble one-dimensional master equations. There is no such simplification for the Ising-Glauber model because  $s_j$  appears inside the hyperbolic tangent and the master equation is non-linear. For these reasons, much of our understanding of the Ising-Glauber model in  $d > 1$  is based on simulation results or on continuum theories.

Another important feature of proportional rule is that there is no surface tension between domains of opposite-opinion voters. For example, a straight boundary between two opposite-opinion domains becomes fuzzier in voter model evolution (first line of Fig. 7.6). Additionally, even though the voter model coarsens in two dimensions, the lack of a surface tension means that the interface density disappears very slowly with time, namely, as  $1/\ln t$ . In contrast, for the Ising-Glauber model at zero temperature, there is a surface tension that scales as the inverse curvature for a droplet of one phase that is immersed in a sea of the opposite phase. We will discuss this surface tension in the next chapter; however, let us accept the existence of a surface tension that scales as the inverse curvature. Consequently, a single-phase droplet of radius  $R$

<sup>3</sup>In  $d = 1$ , the two models are identical because the three distinct types of transitions of energy lowering, energy neutral, and energy raising,

$$\downarrow \uparrow \downarrow \rightarrow \downarrow \downarrow \downarrow \quad \uparrow \uparrow \downarrow \rightarrow \uparrow \downarrow \downarrow \quad \uparrow \uparrow \uparrow \rightarrow \uparrow \downarrow \uparrow$$

respectively, occur with the same rates of 1, 1/2, and 0.

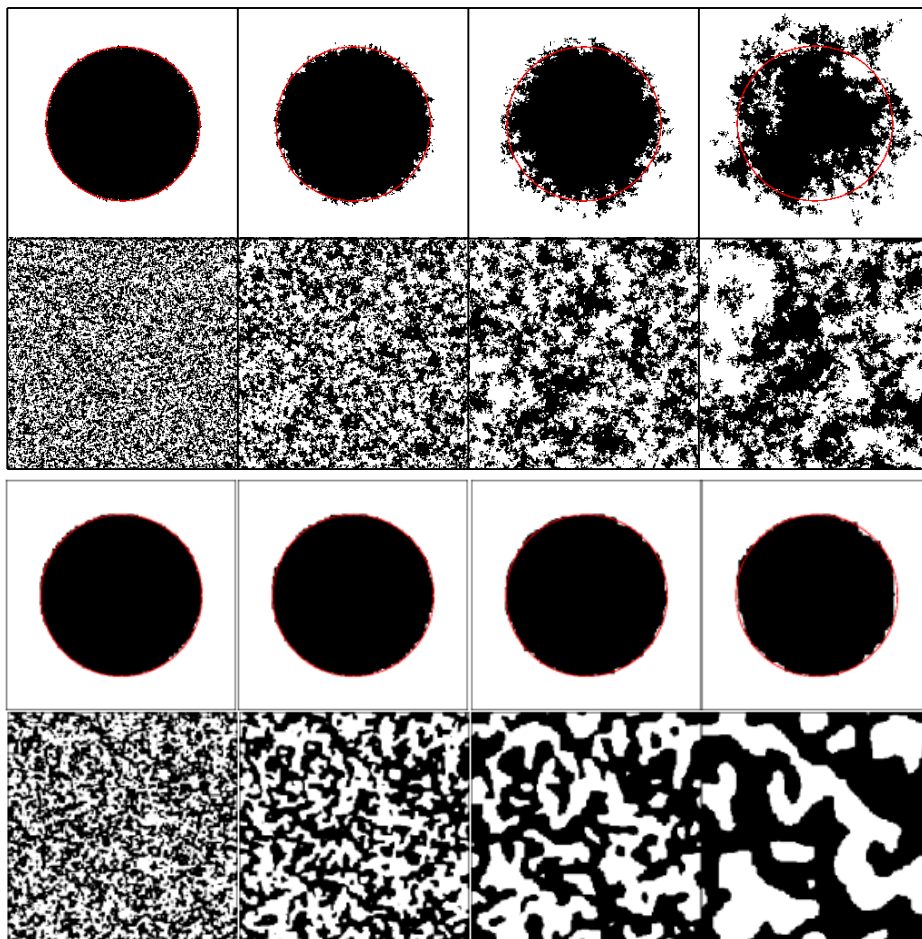


Figure 7.6: Spatial evolution in the voter model (top 2 rows) and the Ising-Glauber model at  $T = 0$  (bottom two rows) on a  $256 \times 256$  square lattice. Lines 1 & 3 shown snapshots at times  $t = 4, 16, 64$ , and  $256$  starting with an initial bubble of radius 180 for the voter model and the Ising-Glauber models, respectively. Lines 2 & 4 show the same evolution starting with a random initial condition with equal density of the two species. The voter model figure is from Dornic et al., Phys. Rev. Lett. **87**, 045701 (2001); courtesy of I. Dornic. The Ising-Glauber model figure is courtesy of V. Spirin.

in a background of the opposite phase will shrink according to  $\dot{R} \propto -1/R$ , or  $R(t)^2 = R(0)^2 - at$  and thus disappear in a finite time (third line of Fig. 7.6). Additionally, the surface tension will quickly eliminate high curvature regions so that the coarsening pattern strongly differs from that of the voter model.

Perhaps the most basic questions about the Ising-Glauber model in  $d > 1$  are concerned with the analog of the domain-size distribution. What is the nature of the coarsening when a system is prepared in a random initial state and then suddenly quenched to a low temperature? What is the final state? How long does it take to reach the final state? For  $d > 1$  and for temperatures below the critical temperature, it has been well established that the system organizes into a coarsening domain mosaic of up and down spins, with the characteristic length scale that grows as  $t^{1/2}$ . For a finite system, this coarsening should stop when the typical domain size reaches the linear dimension  $L$  of the system.

However, when the final temperature  $T$  of the quench is strictly zero, intriguing anomalies occur when the size of the system is finite. At early stages of the relaxation, there is little difference in the dynamics of  $T = 0$  and  $T > 0$  systems. However, when the elapsed time is such that the characteristic time of the coarsening is comparable to the time to diffuse across the system, the two dynamics diverge. Perhaps the most striking feature of the  $T = 0$  dynamics is that a system can get stuck in an infinitely long-lived metastable

state. These metastable states consist of straight stripes in two dimensions, but are more topologically more complex in higher dimension. In two dimensions, the probability of getting stuck in a metastable state is approximately  $\frac{1}{3}$  as  $L \rightarrow \infty$ . In greater than two dimensions, the probability to reach the ground state rapidly vanishes as the system size increases. One obvious reason why the system fails to find the ground state is the rapid increase in the number of metastable states with spatial dimension. This proliferation of metastable states makes it more likely that a typical configuration will eventually reach one of these states rather than the ground state.

## Mean field theory

Mean field theory describes systems in which fluctuations are negligible. One way to construct a mean-field theory for a spin system is to replace the actual environment surrounding each spin by the average environment that is then determined self consistently; this is the Curie-Weiss effective-field theory. Another mean-field description is achieved by embedding the Ising model on a *complete graph* of  $N$  sites, where all the  $N(N-1)/2$  pairs of spin interact with the same strength. The Hamiltonian of the system is now

$$\mathcal{H} = -\frac{J}{N} \sum_{i < j} s_i s_j, \quad (7.51)$$

where the interaction strength scales inversely with the system size so that the energy is extensive, *i.e.*, scales linearly with  $N$ .

From the approach that gave the transition rate on a lattice in greater than one dimension [Eq. (7.50)], the transition rate for Glauber dynamics on the complete graph is simply

$$w(s_i) = \frac{1}{2} \left[ 1 - s_i \tanh \left( \frac{\beta J}{N} \sum_j s_j \right) \right]. \quad (7.52)$$

where the sum  $\sum_j s_j$  is over all other spins in the system, from which the equation of motion for the mean spin is again  $\frac{dS_i}{dt} = -2\langle s_i w_i \rangle$ . We now exploit the fact that there are no fluctuations in the magnetization to write  $\langle f(m) \rangle = f(\langle m \rangle)$ . With this identity we have  $\langle \tanh \frac{\beta}{N} \sum_i s_i \rangle = \tanh \frac{\beta}{N} \sum_i \langle s_i \rangle = \tanh \beta m$ , with  $m = N^{-1} \sum_i \langle s_i \rangle$  the average magnetization. Thus the equation of motion for the mean spin is

$$\frac{dS_i}{dt} = -S_i + \tanh \beta m. \quad (7.53)$$

Summing these rate equations, the average magnetization satisfies

$$\frac{dm}{dt} = -m + \tanh \beta m. \quad (7.54)$$

In contrast to one dimension, the magnetization is generally not conserved. The rate equation has three fixed points, one at  $m = 0$  and two at  $\pm m_{\text{eq}}$ , with the latter determined by the roots of the familiar transcendental equation  $m = \tanh(\beta J m)$ . A linear stability analysis shows that the zero-magnetization state is stable for  $\beta J \leq 1$  but unstable for  $\beta J > 1$ , and vice versa for the states with  $m = \pm m_{\text{eq}}$ . Thus there is a phase transition at  $\beta_c J = 1$ , with  $m_{\text{eq}} \sim (T_c - T)^{1/2}$  for  $T \lesssim T_c$ . The emergence of two equivalent, but symmetry-breaking ground states when the Hamiltonian itself is symmetric is termed *spontaneous symmetry breaking*.

Above the critical temperature, the magnetization decays to zero and we expand  $\tanh \beta m$  in Eq. (7.54) in powers of  $\beta m$  to give

$$\frac{dm}{dt} = -(\beta_c - \beta)m - \frac{1}{3}(\beta m)^3. \quad (7.55)$$

In the high temperature phase, the cubic term is negligible so that the magnetization decays exponentially in time,  $m \sim e^{-t/\tau}$ , with  $\tau = (\beta_c - \beta)^{-1}$ . At the critical point, the relaxation is algebraic,

$$m \sim t^{-1/2}. \quad (7.56)$$

Below the critical temperature, the magnetization also decays exponentially toward its equilibrium value,  $|m - m_{\text{eq}}| \sim e^{-t/\tau}$ , with  $\tau^{-1} = 1 - \beta / \cosh^2(\beta m_{\text{eq}})$  **not explained**. Thus, as the critical point is approached, either from above or from below, the relaxation time scale diverges as

$$\tau \sim |T_c - T|^{-1}. \quad (7.57)$$

The divergence of the relaxation time as  $T \rightarrow T_c$  is a generic sign of critical slowing down as the approach to equilibrium becomes extremely slow.

## 7.4 Kawasaki Spin-Exchange Dynamics

### The transition rate

As mentioned at the outset of Sec. 7.3, there are two fundamental classes of spin dynamics: magnetization conserving and magnetization non-conserving. The former class is appropriate to describe alloy systems, where the two different spin states naturally correspond to the two component atoms that comprise the alloy. In studying the dynamics of phase separation of an alloy into domains of pure metal, a plausible dynamics is that the positions of atoms of different species are exchanged; there is no alchemy where one type of atom can be converted to the other type. In this section, we investigate a simple realization of this order-parameter conserving dynamics — Kawasaki dynamics.

In Kawasaki dynamics, neighboring antiparallel spins simultaneously reverse their states so that

$$\cdots \uparrow \downarrow \cdots \longrightarrow \cdots \downarrow \uparrow \cdots. \quad (7.58)$$

Alternatively, the two spins can be regarded as being exchanged and hence the term *spin-exchange*. Clearly, such moves do not alter the magnetization and so this quantity is *strictly* conserved in every update event. The existence of this strict conservation law has far-reaching consequences that will become clearer when we discuss continuum theories of spin dynamics in the next chapter.

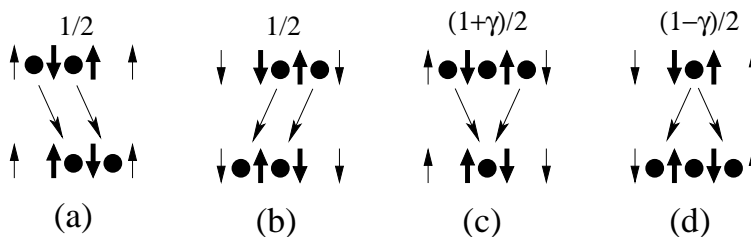


Figure 7.7: Energy neutral update events (a) & (b), energy lowering events (c), and energy raising events (d) for Kawasaki dynamics in one dimension. The spins that flip are shown bold. Also shown are the corresponding domain wall particles ( $\bullet$ ) and the transition rates for these four events.

Again, there are three types of update events: energy raising, energy lowering, and energy neutral. As illustrated in Fig. 7.7, the energy neutral update is equivalent to the simultaneous hopping of two nearest-neighbor domain walls, or to the hopping of an impurity down spin in a sea of up spins. As long as the domain-wall pair remains isolated from all other domain walls, the pair hops freely between neighboring lattice sites. This pair can be viewed as an elementary excitation of the spin system. The hopping rate of a domain wall pair merely sets the time scale, so there is no loss of generality in setting this rate to  $1/2$ , as in Glauber dynamics. Because such diffusive moves do not alter the energy, they automatically satisfy the detailed balance condition. The rates of the remaining two update events are then set by detailed balance. Since spin exchange involves the interactions among four spins—the two spins that flip and their two neighbors—the rates depend on the total energy of the three bonds connecting these four spins. The detailed balance condition is then

$$\frac{w_3}{w_{-1}} = \frac{p_{-1}}{p_3} = \exp(4\beta J), \quad (7.59)$$

where  $w_q$  is the transition rate out of a state with energy  $qJ$  and  $p_q$  its equilibrium probability. Using the convenient Glauber notations of  $w_3 = (1 + \gamma)/2$  and  $w_{-1} = (1 - \gamma)/2$  for energy raising and energy lowering transitions, the detailed balance condition has the same form as in Glauber dynamics,  $\frac{1+\gamma}{1-\gamma} = \exp(4\beta J)$ , or  $\gamma = \tanh 2\beta J$ .

To determine the transition rates, we first must guarantee that spins  $i$  and  $i + 1$  are antiparallel. This constraint can be achieved by the factor  $(1 - s_i s_{i+1})/2$  that equals  $+1$  if the two spins are antiparallel and equals zero otherwise. The form of the flip rate then depends on the interaction energy between the pairs  $s_{i-1}$  and  $s_i$ , and between  $s_{i+1}$  and  $s_{i+2}$ . The flip rate should be a symmetric function of these two bond energies and the rate should be proportional to  $(1 + \gamma)/2$ ,  $1/2$ , and  $(1 - \gamma)/2$  respectively, when the signs of these bond energies are  $--$ ,  $+-$ , and  $++$ . These constraints leads to the transition rate

$$w_i(s_i, s_{i+1}) = \frac{1}{2} \left[ 1 - \frac{\gamma}{2} (s_{i-1} s_i + s_{i+1} s_{i+2}) \right] \times \frac{1}{2} (1 - s_i s_{i+1}). \quad (7.60)$$

An important feature of this rate is that the evolution of spin correlation functions are no longer closed. One-spin averages are coupled to three-spin averages, two-spin averages are coupled to four-spin averages, *etc.* Thus the equation of motion for a particular correlation function generates an infinite hierarchy of equations for high-order correlations. This coupling to higher-order correlation functions arises in a wide range of many-body problems and it is a matter of considerable technical effort and artistry to find a tractable and accurate scheme to truncate this infinite hierarchy.

### Frustration at zero temperature

Because Kawasaki dynamics is more constrained than Glauber dynamics, a system will almost always get stuck forever at zero temperature in one of the very large number of metastable states — one whose energy is above the ground state and for which the only possible transitions by Kawasaki dynamics would raise the energy (see Fig. 7.7(d)). The metastable states are characterized by each domain wall particle being separated by more than a nearest-neighbor distance from any other domain wall. Equivalently the lengths of all spin domains are two or longer. The number of such configurations in a system of length  $L$  asymptotically grows as  $g^L$ , where  $g = (1 + \sqrt{5})/2$  is the golden ratio. It is striking how often this beautiful number appears in statistical physics problems. At zero temperature these metastable states prevent the system from reaching the ground state. At non-zero temperature, these states merely slow the approach toward equilibrium.

To study how the system evolves to a metastable state, let's study the case where energy lowering transitions only are allowed, as illustrated in Fig. 7.7(c). The resulting behavior differs only slightly from the situation where diffusive moves are also allowed, but the former is simpler to treat analytically. The dynamics is perhaps best visualized in terms of the domain walls that occupy the sites of the dual lattice. According to Fig. 7.7(c), an update step consists of picking three contiguous domain wall particles at random and then removing the two outside particles. Since pairs of domain walls are removed sequentially from triplets of consecutive domain walls, the process is equivalent to the random sequential adsorption of a  $\bullet \circ \bullet$  “fork” on top of a string of three consecutive domain wall particles. Because of this equivalence, we can use the tools of random sequential adsorption (Chapter 6) to solve the problem.

Let  $E_k$  be the probability that a string of  $k$  sites (in the dual lattice) are all occupied by domain walls. This probability evolves by the master equation

$$\frac{dE_k}{dt} = -(k - 2)E_k - 2E_{k+1} - 2E_{k+2} \quad (7.61)$$

for  $k \geq 3$ . This equation reflects the different ways that the transition  $\circ \circ \circ \rightarrow \bullet \circ \bullet$  can occur and alter the number of empty strings of length  $k$ . There are  $k - 2$  ways that this transition can occur in the interior of a  $k$ -string. There are also 2 ways that this transition can occur with two sites at the edge of the  $k$ -string and one site outside, and also 2 ways with one site at the edge of the  $k$ -string and two sites outside.

We solve this rate equation by introducing the exponential ansatz  $E_k = \Phi(t) e^{-(k-2)t}$  [see the discussion accompanying Eq. (6.4)]. For the initial condition of an antiferromagnetic spin state, the dual lattice is completely occupied. Thus  $E_k = 1$  initially, so that  $\Phi(0) = 1$ . Substituting this ansatz into the rate equation (7.61) leads to the ordinary differential equation for  $\Phi$ :

$$\frac{d\phi}{dt} = -2\phi(e^{-t} + e^{-2t}). \quad (7.62)$$

Integrating this equation gives the string probabilities for  $k \geq 2$ ,

$$E_k(t) = \exp [-(k-2)t + e^{-2t} + 2e^{-t} - 3]. \quad (7.63)$$

Since two domain walls are lost in each update event and these events occur with rate  $E_3$ , the domain wall density  $\rho \equiv E_1$  satisfies  $\frac{d\rho}{dt} = -2E_3$ . Using Eq. (7.63) for  $E_3$  and integrating then yields the domain wall density

$$\rho(t) = 1 - 2 \int_0^t ds \exp [-s + e^{-2s} + 2e^{-s} - 3]. \quad (7.64)$$

The final ‘‘jamming’’ density is finite,  $\rho_{\text{jam}} \equiv \rho(\infty) = 0.450898\dots$ . Thus there is not very much relaxation as almost half of the domain walls still remain in the final jammed state. Moreover, the relaxation to the jamming density is exponential in time,

$$\rho(t) - \rho_{\text{jam}} \simeq e^{-3}e^{-t}. \quad (7.65)$$

We see that the system neither reaches the lowest energy state, nor does it exhibit critical slowing down. The underlying reason for both of these behaviors is that the dynamics samples only a very restricted portion of the phase space.

### Coarsening at infinitesimal temperature

While the one-dimensional chain with Kawasaki dynamics quickly reaches a jammed state at zero temperature, the equilibrium state will be reached for any non-zero temperature, no matter how small. Because the correlation length diverges as the temperature approaches zero, one can set the temperature sufficiently small so that the correlation length is much larger than the length of the system. Then the equilibrium state consists of a single domain and we are interested in the approach to this final state.

The large separation of time scales between energy raising updates and all other update events leads to an appealing description of the domain evolution within the framework of an extremal dynamics. Since the rate of an energy raising update equals  $e^{-4\beta J}$ , the typical time for such an event is  $\tau \equiv e^{4\beta J}$ . We define the time unit to be  $e^{4\beta J}$ . Energy neutral and energy lowering events then occur instantaneously in this time unit. Starting from an initial state, the system instantly reaches a frustrated state in which no further energy neutral or energy lowering moves are possible. After a time  $\tau$  has elapsed (on average) an energy raising event occurs that is then followed by a burst of energy neutral and energy lowering events until the system reaches another frustrated state. This pattern of an energy raising event followed by a burst of complementary events continues until a finite system reaches the ground state. As we will show, this dynamics leads to the typical domain size growing in time as  $t^{1/3}$  and is a general feature of order-parameter conserving dynamics. One of the appealing features of Kawasaki dynamics in one dimension is that this  $t^{1/3}$  coarsening emerges in a direct way. In contrast, we will see in the next chapter that it is much more subtle to deduce the  $t^{1/3}$  coarsening from continuum approaches.

At long times, the system evolves to a low-energy state that consists of alternating domains of typical length  $\ell$ . The subsequent evolution at low temperature is controlled by rare, energy raising updates where a pair of domain walls nucleates around an existing isolated domain wall. Once this triplet of domain walls forms, a bound pair of these domain walls can diffuse freely with no energy cost until another isolated domain wall is encountered. When such a collision occurs, two of the domain walls annihilate so that a static single domain wall remains. As illustrated in Fig. 7.8, the creation of a mobile bound domain wall pair is equivalent to an isolated spin splitting off from a domain and then diffusing freely within a neighboring domain of length  $\ell$  of the opposite orientation. If this diffusing spin returns to its starting point, the net effect is no change in the domain configuration. However, if the spin manages to traverse to the other side of the domain, then one domain has increased its size by one and another has shrunk by one. This effective diffusion of domain lengths is the mechanism that drives the coarsening.

What is the probability that the spin can actually traverse to the other side of the domain? This is given by the classic ‘‘gambler’s ruin’’ problem as discussed in the highlight on page 23. Once the spin has split off, it is a distance 1 from its initial domain and a distance  $\ell - 1$  from the domain on the other side. Since the spin diffuses freely, it eventually reaches the other side with probability  $1/\ell$ , while the spin returns to its

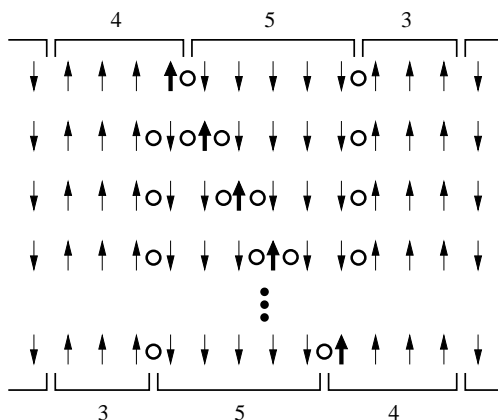


Figure 7.8: Illustration of the effective domain diffusion from Kawasaki dynamics at infinitesimal temperature. The second line shows an energy raising event where a spin (shown bold) splits off from a domain. Eventually this spin joins the next domain to the right. Also shown is the evolution of the domain walls. The net result of the diffusion of the spin across the middle domain is that this moves one step to the left.

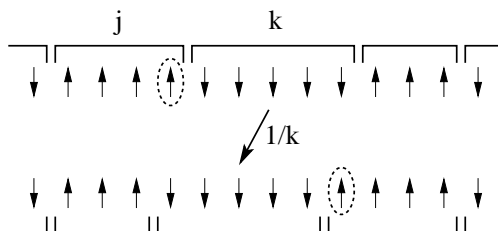


Figure 7.9: Effective domain diffusion by Kawasaki dynamics at infinitesimal temperature. A  $\downarrow$  spin from the  $j$  domain (dashed oval) splits off and eventually reaches the right edge of the  $k$  domain. The  $k$  domain has moved rigidly to the left by one lattice spacing.

starting position with probability  $1 - 1/\ell$ . Thus the probability that the  $\ell$ -domain hops by one step equals  $1/\ell$ . That is, the diffusion coefficient of a domain equals the inverse of its length:  $D(\ell) = \ell^{-1}$ .

Thus in the low-temperature limit, the spin dynamics maps to an effective isotropic hopping of entire domains by one step to the left or the right<sup>4</sup> (Fig. 7.9). Domains of length 1 disappear whenever one of their neighboring domain hops toward them. Concomitantly, the lengths of the neighboring domains are rearranged so that four domains merge into two (Fig. 7.10). The net effect of these processes is coarsening because domains of length 1 disappear. We can determine the typical domain length by a heuristic argument. Because each domain performs a random walk, coalescence occurs whenever a domain diffuses of the order of its own length. In such a coalescence, a domain typically grows by an amount  $\Delta\ell$  that is also of the order of  $\ell$ , while the time between coalescences is  $\Delta t \sim \ell^2/D(\ell)$ . Thus

$$\frac{\Delta\ell}{\Delta t} \sim \frac{\ell}{\ell^2/D(\ell)} \sim \frac{1}{\ell^2},$$

so that domains grow as

$$\ell \sim t^{1/3}. \quad (7.66)$$

It is conventional to define the *dynamical exponent*  $z$  in terms of the growth of the typical length scale in a coarsening process via  $\ell \sim t^z$ . For the non-conserved Glauber and the conserved Kawasaki dynamics,

<sup>4</sup>There is an anomaly involving domains of length 2 that can be ignored for the purposes of this discussion.

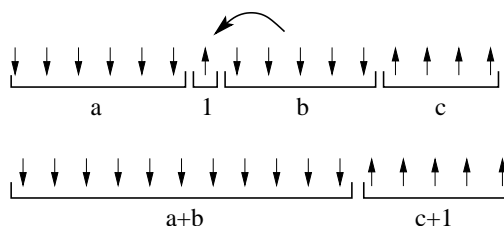


Figure 7.10: The outcome after domain merging.

the dynamical exponent is:

$$z = \begin{cases} 1/2 & \text{nonconservative dynamics,} \\ 1/3 & \text{conservative dynamics.} \end{cases} \quad (7.67)$$

While we have derived these results in one dimension, they are generic for all spatial dimensions. Conservation laws are a crucially important ingredient in determining the nature of non-equilibrium dynamics.

## 7.5 Cluster Dynamics

Glauber single-spin flip dynamics and the Kawasaki spin-exchange dynamics are local in that they involve flipping a single spin or a pair of spins. In spite of their idealized natures, these rules were the basis of many simulational studies of coarsening and dynamic critical phenomena because of their connection to the evolution of real systems. However, a dynamics that is based on flipping single spins is computationally inefficient. Compounding this inefficiency, the dynamics significantly slows down close to criticality. To mitigate these drawbacks, Swendsen and Wang developed a dynamical update rule in which an entire suitably-defined cluster of spins is flipped simultaneously. Because of their efficiency, cluster algorithms have been used extensively to simulate the equilibrium behavior of many-body statistical mechanical and lattice field theory models. The Swendsen-Wang and the Wolff algorithms are two of the earliest and most prominent such examples of cluster dynamics. Remarkably, both of these algorithms are analytically soluble by the master equation approach.

### Swendsen-Wang dynamics

In one dimension, an Ising spin chain consists of alternating spin-up and spin-down domains. In the Swendsen-Wang algorithm, an entire domain of aligned spins is chosen at random and all its spins are flipped simultaneously, as illustrated below:

$$\cdots \uparrow \underbrace{\downarrow\downarrow\downarrow\downarrow}_{\text{domain}} \uparrow \cdots \longrightarrow \cdots \uparrow \underbrace{\uparrow\uparrow\uparrow\uparrow}_{\text{domain}} \uparrow \cdots .$$

By construction, all such updates decrease the energy. In each update event, there is a net loss of two domains. Consequently, the number density of domains  $\rho$  decreases according to  $\frac{d\rho}{dt} = -2\rho$ , where we take the flip rate to be 1, without loss of generality. The density of domains then decreases exponentially with time, and for the antiferromagnetic initial condition in which  $\rho(0) = 1$ , the domain density is  $\rho(t) = e^{-2t}$ . Since the average domain length  $\langle k \rangle$  is the inverse of the domain density,  $\langle k \rangle = e^{2t}$ . When this average length reaches the system length  $L$  the dynamics is complete. This criterion yields the time to reach the ground state  $T_L \propto \ln L$ .

Now consider the domain length distribution. We define  $c_\ell$  as the density of domains of length  $\ell$ . When a domain is flipped, it merges with its two neighbors, so that the length of the resulting domain equals the length of these three domains. As a result of this three-body aggregation process,  $c_\ell$  evolves according to

$$\frac{dc_\ell}{dt} = -3c_\ell + \frac{1}{\rho^2} \sum_{i+j+k=\ell} c_i c_j c_k. \quad (7.68)$$

The factor of  $-3c_\ell$  accounts for the loss of a domain that occurs when a domain of length  $\ell$  or either of its neighboring domains is flipped. The last term accounts for the gain in  $c_\ell$  due to the flipping of a domain of length  $j$  that then merges with its two neighboring domains of lengths  $i$  and  $k$ , with  $\ell = i + j + k$ . The simplest way to deduce the prefactor  $\rho^{-2}$  is to ensure this master equation consistent with the rate equation for the domain density  $\dot{\rho} = -2\rho$ . Notice that newly-created domains do not affect their neighbors, nor are they affected by their neighbors. Thus if the domains are initially uncorrelated, they remain uncorrelated. Because no spatial correlations are generated, the rate equations are exact!

We can obtain a cleaner-looking master equation by introducing  $P_\ell \equiv c_\ell/\rho$ , namely, the probability for a domain of length  $\ell$  (with the normalization  $\sum_\ell P_\ell = 1$ ). Using  $\dot{\rho} = -2\rho$  in Eq (7.68),  $P_\ell$  evolves as

$$\frac{dP_\ell}{dt} = -P_\ell + \sum_{i+j+k=\ell} P_i P_j P_k. \quad (7.69)$$

As we have seen in many previous examples, the convolution form of the gain term cries out for applying the generating function method. Thus we introduce the generating function  $F(z) = \sum_\ell P_\ell z^\ell$  into (7.69) and find that it satisfies  $\frac{\partial F}{\partial t} = -F + F^3$ . Writing  $1/(F^3 - F)$  in a partial fraction expansion, the equation can be integrated by elementary methods and the solution is

$$F(z, t) = \frac{F_0(z)e^{-t}}{\sqrt{1 - F_0(z)^2(1 - e^{-2t})}}, \quad (7.70)$$

where  $F_0(z)$  is the initial generating function.

For the antiferromagnetic initial condition, the initial condition is  $F_0(z) = z$ . Expanding the generating function in powers of  $z$  then yields the domain number distribution

$$P_{2\ell+1} = \binom{2\ell}{\ell} \left(\frac{1 - e^{-2t}}{4}\right)^\ell e^{-t} \quad (7.71)$$

in which domains have odd lengths only. Since the average domain length grows exponentially with time,  $\langle \ell \rangle = e^{2t}$ , we expect that this scale characterizes the entire length distribution. Employing Stirling's approximation, we find that asymptotically the length distribution approaches the scaling form  $P_\ell \rightarrow e^{-2t} \Phi(\ell e^{-2t})$  with the scaling function

$$\Phi(x) = \frac{1}{\sqrt{2\pi x}} e^{-x/2}. \quad (7.72)$$

Because the scaling function diverges  $\Phi(x) \sim x^{-1/2}$  for  $x \ll 1$ , there is a large number of very small domains.

## Wolff dynamics

In the Wolff cluster algorithm, a spin is selected at random and the domain it belongs to is flipped. This protocol further accelerates the dynamics compared to the Swendsen-Wang algorithm because the larger the domain, the more likely it is updated. Schematically, the Wolff dynamics is

$$\cdots \uparrow \underbrace{\downarrow \downarrow \cdots \downarrow \downarrow}_k \uparrow \cdots \xrightarrow{k} \cdots \uparrow \underbrace{\uparrow \uparrow \cdots \uparrow \uparrow}_k \cdots, \quad (7.73)$$

so that a flipped domain again simply merges with its neighbors. Since each spin is selected randomly, the time increment associated with any update is identical. The domain density therefore decreases with constant rate  $\dot{\rho} = -2$ , so that  $\rho(t) = 1 - 2t$  and the entire system is transformed into a single domain in a finite time,  $t_c = 1/2$ . Correspondingly, the average domain length,  $\langle k \rangle = (1 - 2t)^{-1}$ , diverges as  $t \rightarrow t_c$ .

The evolution of the domain length distribution is governed by the natural generalization of (7.69)

$$\frac{dP_\ell}{dt} = -\ell P_\ell + \sum_{i+j+k=\ell} j P_i P_j P_k. \quad (7.74)$$

The generating function  $F(z, t) = \sum_{\ell} P_{\ell} z^{\ell}$  satisfies

$$\frac{\partial F}{\partial t} = z(F^2 - 1) \frac{\partial F}{\partial z}. \quad (7.75)$$

To solve this equation, we first transform from the variables  $(t, z)$  to  $(\tau, y) \equiv (t, t - \ln z)$  to absorb the negative term on the right-hand side. This transformation gives

$$\frac{\partial F}{\partial \tau} = -F^2 \frac{\partial F}{\partial y}. \quad (7.76)$$

We now employ the same procedure as that used in the solution of aggregation with the product kernel (see the discussion leading up to Eq. (4.37) in chapter 4) to transform among the variables  $(\tau, y, F)$  and reduce (7.76) into the linear differential equation  $\frac{\partial y}{\partial \tau} = F^2$ . The solution to this equation is  $y = G(F) + F^2 \tau$ , with  $G(F)$  determined by the initial conditions, or, equivalently,

$$t - \ln z = G(F) + F^2 t. \quad (7.77)$$

For the antiferromagnetic initial condition  $F_0(z) = z$ , so that  $G(F) = -\ln F$ . Substituting  $G(F) = -\ln F$  into (7.77) and exponentiating yields the following implicit equation for the generating function

$$z = F e^{t - F^2 t}. \quad (7.78)$$

The length distribution  $P_k$  is just the  $k^{\text{th}}$  term in the power series expansion of  $F(z)$ . Formally, this term may be extracted by writing  $P_k$  in terms of the contour integral

$$P_k = \frac{1}{2\pi i} \oint \frac{F(z)}{z^{k+1}} dz,$$

then transforming the integration variable from  $z$  to  $F$ , and using the Lagrange inversion formula (see the discussion on page 51 in Chapter 4). These steps give

$$\begin{aligned} P_k &= \frac{1}{2\pi i} \oint \frac{F(z)}{z^{k+1}} dz = \frac{1}{2\pi i} \oint \frac{F}{z(F)^{k+1}} \frac{dz}{dF} dF, \\ &= \frac{e^{-kt}}{2\pi i} \oint e^{kF^2 t} \left[ \frac{1}{F^k} - \frac{2t}{F^{k-2}} \right] dF, \end{aligned} \quad (7.79)$$

where we use the fact that  $\frac{dz}{dF} = e^{t - F^2 t} (1 - 2F^2 t)$  in the above integral. Now we find the residues simply by expanding  $e^{kF^2 t}$  in a power series and keeping only the coefficient of  $\frac{1}{F}$  in the integrand. Because the power series is even in  $F$ , only  $P_k$  for odd values of  $k$  is non zero and we find

$$P_k = e^{-kt} \left[ \frac{(kt)^{(k-1)/2}}{\left(\frac{k-1}{2}\right)!} - 2t \frac{(kt)^{(k-3)/2}}{\left(\frac{k-3}{2}\right)!} \right].$$

After some simple algebra, the domain length distribution is

$$P_{2k+1}(t) = \frac{(2k+1)^{k-1}}{k!} t^k e^{-(2k+1)t}. \quad (7.80)$$

Near the critical time ( $t \rightarrow 1/2$ ), Stirling's approximation gives, for the leading behavior of domain length distribution,

$$P_k(t) \simeq \frac{1}{\pi^{1/2} k^{3/2}} e^{-k\rho^2/4}, \quad (7.81)$$

with  $\rho = 1 - 2t$ . While this distribution has a characteristic length scale  $k^* = 4/\rho^2 = (1/2 - t)^{-2}$ , this length does not fully characterize the distribution. Since the domain length distribution has a power-law  $k^{-3/2}$  tail that is cut off at  $k^* \propto \rho^{-2}$ , the average domain length  $\langle k \rangle = \sum_k k P_k \sim \int^{k^*} k k^{-3/2} dk$ . This last integral then gives the expected behavior  $\langle k \rangle \sim \rho^{-1}$ .

## Problems

### 7.1 The Voter Model

1. Evaluate the average opinion for a Democrat in a sea of uncommitted voters:  $S(\mathbf{x}, 0) = \delta(\mathbf{x})$ .

### 7.2 & 7.3 Glauber Spin-Flip Dynamics

1. Solve for the domain number distribution in the Potts model with Glauber dynamics. Hint:  $P_1$  is replaced by  $P_1/(q-1)$  in Eq. (7.43).
2. Verify that for the Hamiltonian  $\mathcal{H} = -\sum_{i<j} J_{i,j} s_i s_j$  the spin flip rate is  $w_i = \frac{1}{2}(1 - \tanh \beta s_i \sum_j J_{i,j} s_j)$ .
3. Obtain the entropy in the mean-field model.
4. Determine  $P_M(t)$ , the probability to have  $M$  up spins and  $N - M$  down spins,<sup>5</sup> for zero-temperature dynamics.
5. Examine  $P_M(t)$  for the critical dynamics.
6. In the low temperature regime ( $\infty > \beta > \beta_c$ ), the distribution  $P_M(t)$  is bimodal with peaks of width  $\propto \sqrt{N}$  around  $M_{\pm} = \frac{1}{2} N (1 \pm m_{\infty})$ . The system spends almost all time in the proximity of the peaks yet occasionally it leaves one peak and reaches the other. Estimate the transition time.

### 7.4 Glauber Spin-Exchange Dynamics

1. Show that the correlation functions obey an infinite hierarchy of equations. Write the evolution equation for  $S_i$ .
2. Obtain the number of frozen configurations in the zero-temperature limit for Kawasaki dynamics.
3. Solve for the domain wall density at zero-temperature for random initial conditions.

### 7.5 Cluster Dynamics

1. Consider the zero-temperature Swendsen-Wang dynamics, with energy lowering moves only, for the  $q = \infty$  Potts model. In this case a domain merges with only one of its neighbors. Determine the domain density and the domain length distribution.

*Solution:* Since there is a net loss of one domain in a single update, the number density obeys  $d\rho/dt = -\rho$ . Therefore  $\rho(t) = e^{-t}$  while the average domain length again grows exponentially with time. The domain length size distribution now evolves by two-body aggregation, so that this distribution satisfies

$$\frac{dP_k}{dt} = -P_k + \sum_{i+j=k} P_i P_j. \quad (7.82)$$

To solve this equation, we again introduce the generating function into this equation to give  $\frac{\partial F}{\partial t} = -F + F^2$ , whose solution is simply

$$F(z, t) = \frac{F_0(z)e^{-t}}{1 - (1 - e^{-t})F_0(z)}. \quad (7.83)$$

Expanding this generating function in a power series we immediately obtain

$$P_k(t) = e^{-t}(1 - e^{-t})^{k-1}. \quad (7.84)$$

Asymptotically, the distribution attains the scaling form  $P_k(t) \sim e^{-t}\Phi(ke^{-t})$  with the purely exponential scaling function  $\Phi(x) = \exp(-x)$ . The enhancement of smaller than average domains disappears in the  $q \rightarrow \infty$  limit.

2. Analyze a domain coarsening process where the smallest domain merges with one of its neighbors.

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<sup>5</sup>In all problems in this paragraph the system is *finite*.