0 to 9, then the class of a spin that is flipped changes by $+5 \mod 10$, and the class of a neighbor changes by the new spin value equal to $\pm 1$.

(a) Write a program to implement the $n$-fold way algorithm for the Ising model on a square lattice with an applied magnetic field. Check your program by comparing various averages at a few temperatures with the results from your program using the Metropolis algorithm.

(b) Choose the magnetic field $B = -0.5$ at the temperature $T = 1$. Begin with an initial configuration of all spins up and use the $n$-fold way to estimate how long it takes before the majority of the spins flip. Do the same simulation using the Metropolis algorithm. Which algorithm is more efficient?

(c) Repeat part (b) for other temperature and field values. For what conditions is the $n$-fold way algorithm more efficient than the standard Metropolis algorithm?

(d) Repeat part (b) for different values of the magnetic field and plot the number of Monte Carlo steps needed to flip the spins as a function of $1/|B|$ for values of $B$ from 0 to $\approx 3$. Average over at least 10 starting configurations for each field value. ■

**Project 15.37 The Kosterlitz–Thouless transition**

The planar model (also called the $xy$-model) consists of spins of unit magnitude that can point in any direction in the $xy$-plane. The energy or Hamiltonian function of the planar model in zero magnetic field can be written as

$$E = -J \sum_{i,j=nn(i)} [s_{i,x}s_{j,x} + s_{i,y}s_{j,y}], \tag{15.90}$$

where $s_{i,x}$ represents the $x$-component of the spin at the $i$th site, $J$ measures the strength of the interaction, and the sum is over all nearest neighbors. We can rewrite (15.90) in a simpler form by substituting $s_{i,x} = \cos\theta_i$ and $s_{i,y} = \sin\theta_i$. The result is

$$E = -J \sum_{i,j=nn(i)} \cos(\theta_i - \theta_j), \tag{15.91}$$

where $\theta_i$ is the angle that the $i$th spin makes with the $x$-axis. The most studied case is the two-dimensional model on a square lattice. In this case the mean magnetization $\langle \mathbf{M} \rangle = 0$ for all temperatures $T > 0$, but, nevertheless, there is a phase transition at a nonzero temperature $T_{\mathrm{KT}}$, which is known as the Kosterlitz–Thouless (KT) transition. For $T \le T_{\mathrm{KT}}$, the spin-spin correlation function $C(r)$ decreases as a power law; for $T > T_{\mathrm{KT}}$, $C(r)$ decreases exponentially. The power law decay of $C(r)$ for $T \le T_{\mathrm{KT}}$ implies that every temperature below $T_{\mathrm{KT}}$ acts as if it was a critical point. We say that the planar model has a line of critical points. In the following, we explore some of the properties of the planar model and the mechanism that causes the transition.

(a) Write a program that uses the Metropolis algorithm to simulate the planar model on a square lattice using periodic boundary conditions. Because $\theta$ and hence the energy of the system is a continuous variable, it is not possible to store the previously computed values of the Boltzmann factor for each possible value of $\Delta E$. Instead of computing $e^{-\beta\Delta E}$ for each trial change, it is faster to set up an array `w` such that the array element `w(j)` $= e^{-\beta\Delta E}$, where `j` is the integer part of $1000\Delta E$. This procedure leads to an energy resolution of 0.001, which should be sufficient for most purposes.



(b) One way to show that the magnetization $\langle \mathbf{M} \rangle$ vanishes for all $T$ is to compute $\langle \theta^2 \rangle$, where $\theta$ is the angle that a spin makes with the magnetization $\mathbf{M}$ for any given configuration. (Although the mean magnetization vanishes, $\mathbf{M} \neq 0$ at any given instant.) Compute $\langle \theta^2 \rangle$ as a function of the number of spins $N$ at $T = 0.1$ and show that $\langle \theta^2 \rangle$ diverges as $\ln N$. Begin with a $4 \times 4$ lattice and choose the maximum change in $\theta_i$ to be $\Delta\theta_{\max} = 1.0$. If necessary, change $\theta_{\max}$ so that the acceptance probability is about 40%. If $\langle \theta^2 \rangle$ diverges, then the fluctuations in the direction of the spins diverges, which implies that there is no preferred direction for the spins, and hence the mean magnetization vanishes.

(c) Modify your program so that an arrow is drawn at each site to show the orientation of each spin. You can use the `Vector2DFrame` to draw a lattice of arrows. Look at a typical configuration and analyze it visually. Begin with a $32 \times 32$ lattice with spins pointing in random directions and do a temperature quench to $T = 0.5$. (Simply change the value of $\beta$ in the Boltzmann probability.) Such a quench should lock in some long lived but metastable vortices. A vortex is a region of the lattice where the spins rotate by at least $2\pi$ as your eye moves around a closed path (see Figure 15.10). To determine the center of a vortex, choose a group of four spins that are at the corners of a unit square and determine whether the spins rotate by $\pm 2\pi$ as your eye goes from one spin to the next in a counterclockwise direction around the square. Assume that the difference between the direction of two neighboring spins $\delta\theta$ is in the range $-\pi < \delta\theta < \pi$. A total rotation of $+2\pi$ indicates the existence of a positive vortex, and a change of $-2\pi$ indicates a negative vortex. Count the number of positive and negative vortices. Repeat these observations for several configurations. What can you say about the number of vortices of each sign?

(d) Write a method to determine the existence of a vortex for each $1 \times 1$ square of the lattice. Represent the center of the vortices using a different symbol to distinguish between a positive and a negative vortex. Do a Monte Carlo simulation to compute the mean energy, the specific heat, and number of vortices in the range from $T = 0.5$ to $T = 1.5$ in steps of 0.1. Use the last configuration at the previous temperature as the first configuration for the next temperature. Begin at $T = 0.5$ with all $\theta_i = 0$. Draw the vortex locations for the last configuration at each temperature. Use at least 1000 Monte Carlo steps per spin at each temperature to equilibrate and at least 5000 Monte Carlo steps per spin for computing the averages. Use an $8 \times 8$ or $16 \times 16$ lattice if your computer resources are limited and larger lattices if you have sufficient resources. Describe the $T$-dependence of the energy, the specific heat, and the vorticity (equal to the number of vortices per unit area). Plot the logarithm of the vorticity versus $T$ for $T < 1.1$. What can you conclude about the $T$-dependence of the vorticity? Explain why this form is reasonable. Describe the vortex configurations. At what temperature do you find a vortex that appears to be free, that is, a vortex that is not obviously paired with another vortex of opposite sign?