Chapter 6

Band updates

Winding cycles are a global phenomenon, while the SO swaps of section 5.1 are local. The Swendsen-Wang algorithm for the planar Ising model addresses a global/local problem not unlike our winding-number problem, which was presented in detail in section 5.4. Motivated by Swendsen-Wang for the Ising model, we attempt to define a Metropolis step for our random-cycle model which changes one of the winding-number components W_x, W_y, or W_z by ± 1. This attempt at non-local updates has an unreasonably low acceptance rate, namely, on the order of e^{-L} where L is the box length. Nonetheless, this concept may provide fodder for better, future ideas.

6.1 The algorithm

As discussed in section 5.3, a Metropolis transition from π to π' may be thought of as composition with another permutation τ, i.e. $\pi' = \tau\pi$. We replace the swap operator $\tau = G_{\mathbf{a},\mathbf{b}}$ of section 5.3, which was a two-cycle, with a permutation τ which has a winding L-cycle. Without loss of generality, it suffices to discuss a permutation τ which sends every lattice point to itself except for one line of points with y and z coordinates equal to zero (figure 6.1). This τ will have winding number $(W_x, W_y, W_z) = (+1, 0, 0)$. If we can do that, then by reflection and rotation symmetries we can construct similar τ's with W_x, W_y, or W_z equal to ± 1.

Figure 6.1 displays the idea. The permutation τ is an L-cycle; we put $\pi' = \tau\pi$. It seems clear from the picture that the winding number is modified in the desired manner, and moreover it seems plausible to conjecture that winding numbers are additive with respect to permutation composition, i.e. that $\mathbf{W}(\pi') = \mathbf{W}(\tau) + \mathbf{W}(\pi)$. Proving either of these statements rigorously would be worthwhile if band updates were worth pursuing. However, as shown in the next section, they are not.

6.2 Acceptance rate

We examine the acceptance rate of the band-update algorithm using a semi-empirical method. Recall from section 3.3 that we define the random variable $j_{\mathbf{x}}(\pi)$ to be $\|\pi(\mathbf{x}) - \mathbf{x}\|_\Lambda$. By examination of histograms acquired over MCMC simulations, we see that this parameter is noncritical; its values change smoothly with T near T_c. For $T = 6$ and 7, respectively, we find[1] distributions for $j_{\mathbf{x}}$, as shown in table 6.1.

[1] We use the statistics convention wherein $\hat{P}_{\text{Gibbs}}$ is an experimental estimator for the exact (but unknown) value P_{Gibbs}.

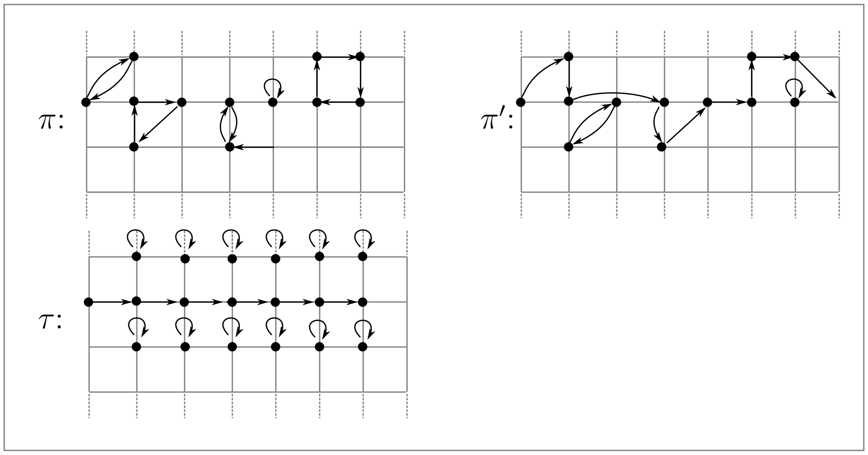

FIGURE 6.1. Example of band update as composition with an L-cycle: $\pi' = \tau\pi$. The winding number W_x increases by $+1$.

Thus for $T = 6, 7$, respectively, mean jump lengths are 0.608 and 0.245, while mean

j	$\hat{P}_{\text{Gibbs}}(J = j), T = 6$	j	$\hat{P}_{\text{Gibbs}}(J = j), T = 7$
0	0.4801	0.0000000	0.7745
1	0.3361	1.0000000	0.1822
$\sqrt{2}$	0.1545	1.4142136	0.0378
$\sqrt{3}$	0.0216	1.7320508	0.0042
4	0.0036	2.0000000	0.0012
$\sqrt{5}$	0.0032	2.2360680	0.0001
$\sqrt{6}$	0.0009		

TABLE 6.1. Empirical jump-length distribution for $T = 6, 7$.

squared jump lengths are 0.746 and 0.276. Roughly, the latter is of order 0.5. Recall in particular that it is the squared jump length which provides the main contribution to the system energy (equation (2.1.3)).

The left-hand side of figure 6.2 shows (in two dimensions only) various possibilities for a permutation arrow from a point $\mathbf{x}$. The right-hand side of the figure shows what happens to the jump lengths at $\mathbf{x}$ on a right shift. (All L points in the L-cycle will be affected similarly.) An up arrow of length 1 becomes a diagonal up-left arrow of length $\sqrt{2}$, a right arrow of length 1 becomes a right arrow of length 2, and so on. Given an attempted band update $\pi \to \pi'$, the typical value of the energy change ΔH at a single point (remembering that cycle-weight corrections are low-order perturbations,

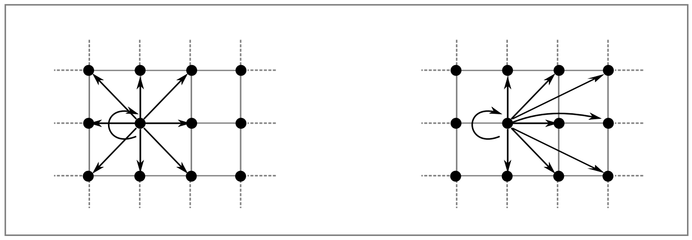

FIGURE 6.2. Change in jump lengths for a point affected by a band update.

since α is small) is

$$\frac{T}{4}\left(\mathbb{E}[j_{\mathbf{x}}(\pi')^2] - \mathbb{E}[j_{\mathbf{x}}(\pi)^2]\right).$$

From the table just above, we can compute the expected values of $j_{\mathbf{x}}(\pi)^2$ and $j_{\mathbf{x}}(\pi')^2$. We find the energy difference per point to be on the order of $+0.8 \cdot T/4 \approx +1.2$. Since L points are involved in a band update, this means $\mathbb{E}[\Delta H] \approx 1.2L \approx L$. Transitions are accepted with probability $\min\{1, e^{-\Delta H}\}$ (section 4.5) which is approximately e^{-L}. We need to consider L from approximately 30 and upward to get past the most severe finite-size effects; $e^{-30} \approx 10^{-14}$ is effectively zero, and thus proposed band updates are effectively never accepted. This calculation matches with simulation tests performed in software.

6.3 Band updates with compensation

At the 2010 Workshop of David Landau's Center for Simulational Physics at the University of Georgia, Friederike Schmid of the University of Mainz suggested a solution to the acceptance-rate problem with the band-update algorithm. This idea comes too late to include in the large-scale computational runs done for this dissertation; however, it should work, and might be used in subsequent computational work on this problem.

Specifically, the problem with the band update is that the change in energy is of order L. To counteract this, in the same Metropolis step in which one proposes a band update as described above, one should also find another cycle of π, not intersecting the band, with cycle length approximately L. The proposed change will do the band shift, while also replacing this second cycle with one-cycles at each of its points — the latter reducing the energy by L or so. The total energy change will be approximately zero, and thus the acceptance rate should be usably high.