Exercises

8.8 Wolff.¹ (Mathematics, Computation) (3)

Near the critical point T_c where the system develops a magnetization, any single-spin-flip dynamics becomes very slow (the *correlation time* diverges). Wolff [146], improving on ideas of Swendsen and Wang [135], came up with a clever method to flip whole clusters of spins.

Wolff cluster flips

- (1) Pick a spin at random, remember its direction $D = \pm 1$, and flip it.
- (2) For each of the four neighboring spins, if it is in the direction D, flip it with probability p.
- (3) For each of the new flipped spins, recursively flip their neighbors as in (2).

Because with finite probability you can flip any spin, the Wolff algorithm is ergodic. As a cluster flip it is Markovian. Let us see that it satisfies detailed balance, when we pick the right value of p for the given temperature.

(a) Show for the two configurations in Figs 8.9 and 8.10 that $E_B - E_A = 2(n_{\uparrow} - n_{\downarrow})J$. Argue that this will be true for flipping any cluster of up-spins to down-spins.



Fig. 8.9 Cluster flip: before. The region inside the dotted line is flipped in one Wolff move. Let this configuration be A.

The cluster flip can start at any site α in the cluster C. The ratio of rates $\Gamma_{A \to B}/\Gamma_{B \to A}$ depends upon the number of times the cluster chose *not* to grow

¹From Statistical Mechanics: Entropy, Order Parameters, and Complexity by James P. Sethna, copyright Oxford University Press, 2007, page 177. A pdf of the text is available at pages.physics.cornell.edu/sethna/StatMech/ (select the picture of the text). Hyperlinks from this exercise into the text will work if the latter PDF is downloaded into the same directory/folder as this PDF.

on the boundary. Let P_{α}^{C} be the probability that the cluster grows internally from site α to the cluster C (ignoring the moves which try to grow outside the boundary). Then

$$\Gamma_{A \to B} = \sum_{\alpha} P_{\alpha}^{C} (1-p)^{n_{\uparrow}}, \qquad (1)$$

$$\Gamma_{B \to A} = \sum_{\alpha} P_{\alpha}^{C} (1-p)^{n_{\downarrow}}, \qquad (2)$$

since the cluster must refuse to grow n_{\uparrow} times when starting from the up-state A, and n_{\downarrow} times when starting from B.

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Fig. 8.10 Cluster flip: after. Let this configuration be B. Let the cluster flipped be C. Notice that the boundary of C has $n \uparrow = 2$, $n \downarrow = 6$.

(b) What value of p lets the Wolff algorithm satisfy detailed balance at temperature T?

Unless you plan to implement the Wolff algorithm yourself (Exercise 8.9, download the Wolff simulation from the computer exercises section of the text web site [129]. Run at T = 2.3, using the heat-bath algorithm for a 500×500 system or larger; watch the slow growth of the characteristic cluster sizes. Now change to the Wolff algorithm, and see how much faster the equilibration is. Also notice that many sweeps almost completely rearrange the pattern; the correlation time is much smaller for the Wolff algorithm than for single-spin-flip methods like heat bath and Metropolis. (See [98, sections 4.2–3] for more details on the Wolff algorithm.)