Appendix D

Loop/cluster algorithms: SU(N) model

As mentioned at the beginning of Section 6.2.6, in some cases the loop algorithm (Algorithm 17) for $S = \frac{1}{2}$ is applicable to spin systems with $S > \frac{1}{2}$ without splitting spins. This is always possible if the Hamiltonian decomposes graphically. For example, let us consider the bilinear-biquadratic interaction model with $S = 1$ (Harada and Kawashima, 2001, 2002),

$$H = J \sum_{\langle ij \rangle} [(\cos\theta)\vec{S}_i \cdot \vec{S}_j + (\sin\theta)(\vec{S}_i \cdot \vec{S}_j)^2]. \tag{D.1}$$

The model (D.1) obviously has SU(2) symmetry. At $\theta = \pm\pi/2$ and $\theta = \pm\pi/4$, however, it possesses a higher symmetry. Consider the case of $\theta = -\pi/2$ for which

$$H = -J \sum_{\langle ij \rangle} [(\vec{S}_i \cdot \vec{S}_j)^2 - 1], \tag{D.2}$$

where the constant -1 has been added for convenience. The Hamiltonian (D.2), as well as the Hamiltonian at other special values of θ, has SU(3) symmetry. In the ordinary S^z-basis, $S_i^z|s_i\rangle = s_i|s_i\rangle$, the matrix elements of the pair Hamiltonian are

$$\langle s_i' s_j'| - H_{ij}|s_i s_j\rangle = J\sigma(S_p)\Delta(S_p, g_{\mathrm{H}}). \tag{D.3}$$

The function $\sigma(S_p) = \pm 1$ carries a sign: It is -1 if and only if either the initial state (s_i, s_j) is $(0, 0)$ and the final state (s_i', s_j') is $(\pm 1, \mp 1)$ or vice versa. It is easy to see that this sign is irrelevant since the negative signs always occur an even number of times, leaving the sign of the whole system positive. Therefore, in (D.3) we neglect σ. The function $\Delta(S_p, g_{\mathrm{H}})$ is

$$\Delta(S_p, g_{\mathrm{H}}) \equiv \begin{cases} 1, & \text{if } s_i + s_j = s_i' + s_j' = 0 \\ 0, & \text{otherwise.} \end{cases}$$

This quantity is the horizontal graph operator in Table 6.2, generalized to the present three-state model.

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With the pair Hamiltonian expressed in terms of the graph operators, it is straightforward to apply the general prescription discussed in Section 6.2.2. The only difference between the resulting $S = 1$ algorithm and the $S = \frac{1}{2}$ case is that the density of the graph elements is J, not $J/2$, because of the larger diagonal matrix element and that the variables have three values, $s_i = \{-1, 0, 1\}$, instead of two. Accordingly, loop-flipping is not a coin toss, but proceeds by choosing one of the three values randomly with equal probability.

We can construct a similar algorithm for cases with lower symmetry, for example, SU(2) symmetry, for the parameter region $-3\pi/4 \leq \theta \leq -\pi/2$. The graphical decomposition of the pair Hamiltonian in this case is (Harada and Kawashima, 2001)

$$-H_{ij} = J\left[(-\sin\theta + \cos\theta)D_{ij}(g_{\mathrm{h}}) - (\cos\theta)D_{ij}(g_{\mathrm{d}})\right], \tag{D.4}$$

where an irrelevant sign and an additive constant have been omitted. The symbol $D_{ij}(g_{\mathrm{d}})$ corresponds to the diagonal graph in Fig. 6.2. Its matrix elements are

$$\langle s_i' s_j' | - D_{ij}(g_{\mathrm{d}}) | s_i s_j \rangle = \Delta(S_p, g_{\mathrm{d}}) \equiv \begin{cases} 1, & \text{if } s_i = s_j' \text{ and } s_j = s_i' \\ 0, & \text{otherwise.} \end{cases}$$

The loop construction and the loop flipping are done as before.

The special case of the SU(N) bilinear-biquadratic model that possesses SU(3) symmetry generalizes to a SU(N) symmetric model. The local spin variable of the SU(N) Heisenberg model takes N possible values, that is, $\sigma_i = \{1, 2, \ldots, N\}$. Expressed in terms of the generators of the SU(N) algebra,

$$H \equiv \frac{J}{N} \sum_{\langle ij \rangle} \sum_{\mu=1}^{N} \sum_{\nu=1}^{N} S_i^{\mu\nu} \bar{S}_i^{\nu\mu}. \tag{D.5}$$

Here, $S_i^{\mu\nu}$, $\bar{S}_j^{\nu\mu}$ satisfy

$$[S_i^{\mu\nu}, S_j^{\sigma\tau}] = \delta_{ij}(\delta_{\mu\tau} S_i^{\sigma\nu} - \delta_{\sigma\nu} S_j^{\mu\tau}) \quad (\mu, \nu, \sigma, \tau = 1, 2, \ldots, N).$$

The operators $\bar{S}_j^{\mu\nu}$ satisfy analogous conditions. We consider the model defined on a bipartite lattice. On one sublattice (say, the sublattice A) we adopt the fundamental representation that corresponds to the Young tableau with a single box. On the other sublattice (B), we adopt the conjugate representation. The bar on the operator $\bar{S}_i^{\mu\nu}$ is a reminder that we are using different representations for the spins on sublattices A and B.

More explicitly, the matrix element of $S_i^{\mu\nu}$ on the sublattice A is $\left\langle \alpha \left| S_i^{\mu\nu} \right| \beta \right\rangle = \delta_{\alpha\mu}\delta_{\beta\nu} - \frac{1}{N}\delta_{\alpha\beta}$, while on B $\langle \alpha | \bar{S}_j^{\mu\nu} | \beta \rangle = -\delta_{\alpha\nu}\delta_{\beta\mu} + \frac{1}{N}\delta_{\alpha\beta}$. Therefore, we are able to rewrite (D.5) as

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$$H = -J \sum_{\langle ij \rangle} \frac{1}{N} \sum_{\mu\nu} S_i^{\mu\nu} S_j^{\mu\nu}.$$

If we define the operator P_{ij} by its matrix element as

$$\left\langle \alpha', \beta' \left| P_{ij} \right| \alpha, \beta \right\rangle \equiv \frac{1}{N} \delta_{\alpha'\beta'} \delta_{\alpha\beta},$$

it is the projection operator to the color singlet-state on the bond $\langle i, j \rangle$,

$$|\text{singlet on } (ij)\rangle \equiv \frac{1}{\sqrt{N}} \sum_{\alpha} |\alpha, \alpha\rangle \,.$$

To convince ourselves that this is indeed a singlet state, we have to recall that we are using the conjugate representation to the fundamental one for one of the two sublattices. In other words, one of the two αs in $|\alpha, \alpha\rangle$ does not represent the same state as the other α, but it is the product of all the states but α. (It is easy to confirm that this state is invariant under P_{ij}.) Using the SU(N) generators, we express the projection operator as

$$P_{ij} = \frac{1}{N} \sum_{\mu\nu} S_i^{\mu\nu} S_j^{\mu\nu} + \frac{1}{N^2}.$$

Therefore, apart from an additive constant,

$$H = -J \sum_{\langle ij \rangle} P_{ij}.$$

Note also that the matrix elements of the projection operator are the product of Kronecker deltas, so they can be represented by a graph element, g_{h}, that is,

$$P_{ij} = \frac{1}{N} D_{ij}(g_{\mathrm{h}}).$$

The two spins bound by this graph element have the same value, whereas they were antiparallel previously. But this difference is removable by a gauge transformation and is not essential. Thus, we have the graphical decomposition of the SU(N) Heisenberg model Hamiltonian, from which a loop algorithm follows. The algorithm is almost identical to the one discussed in Section 6.2.3 for the $S = \frac{1}{2}$ antiferromagnet. The only difference is that each local variable takes N values instead of 2.

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