Chapter 8

ΔH computations

When computing ΔH for the swap-only, swap-and-reverse, or worm algorithms, it is inefficient to find $H(\pi')$ and $H(\pi)$ separately, then compute their difference: swap and worm moves are local, and most of the energy terms are unchanged from π to π'. Instead (this is true for Metropolis simulations in general), one discovers a formula for the energy change in a proposed Metropolis move. Even though these minimal energy-change formulas are a software-optimization detail, they need to be considered carefully lest errors intrude.

We write the energy of equation (7.2.3) as

$$H = D + V + W \tag{8.0.1}$$

where H is total energy, D is the distance-related single-jump terms, V is the jump-pair-interaction terms, and W is the worm-dependent terms. (Note that V is identically zero if there are no interactions, and W is identically zero for the SO, SAR, and band-update algorithms.)

8.1 Swap and worm with no interactions

Recall that the wormhole point is non-spatial and thus does not participate in distance computations. As is clear from figures 5.1 and 7.2 (on pages 50 and 68, respectively), the change in distance-related terms is

$$\begin{aligned}
\Delta D &= \|\mathbf{x} - \pi(\mathbf{y})\|_\Lambda^2 + \|\mathbf{y} - \pi(\mathbf{x})\|_\Lambda^2 - \|\mathbf{x} - \pi(\mathbf{x})\|_\Lambda^2 - \|\mathbf{y} - \pi(\mathbf{y})\|_\Lambda^2 && \text{(swap-only)}\\
\Delta D &= -\|\mathbf{x} - \pi(\mathbf{x})\|_\Lambda^2 && \text{(worm open)}\\
\Delta D &= \|\pi^{-1}(w) - \pi(w)\|_\Lambda^2 && \text{(worm close)}\\
\Delta D &= \|\pi^{-1}(w) - \pi(\mathbf{x})\|_\Lambda^2 - \|\mathbf{x} - \pi(\mathbf{x})\|_\Lambda^2 && \text{(worm head swap)}\\
\Delta D &= \|\mathbf{x} - \pi(w)\|_\Lambda^2 - \|\mathbf{x} - \pi(\mathbf{x})\|_\Lambda^2 && \text{(worm tail swap).}
\end{aligned}$$

8.2 Swap and worm with two-cycle interactions

The non-spatiality of the wormhole point plays no role in the algebraic notion of cycle lengths. Thus, the same Δr_2 formulas apply to both algorithms. The ΔD is the same as in section 8.1; he we describe only the ΔV.

Recall the definition of a swap from section 5.1. The simplicity of figure 8.1 masks a bit of detail: namely, the four points may not all be distinct. Thus, there are several cases. (See figure 8.2.)

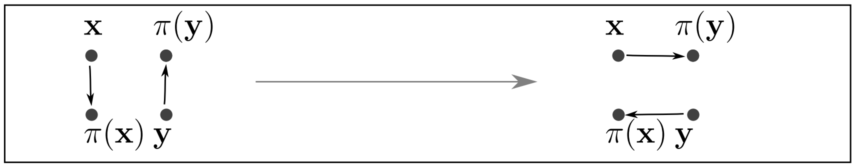

FIGURE 8.1. A swap.

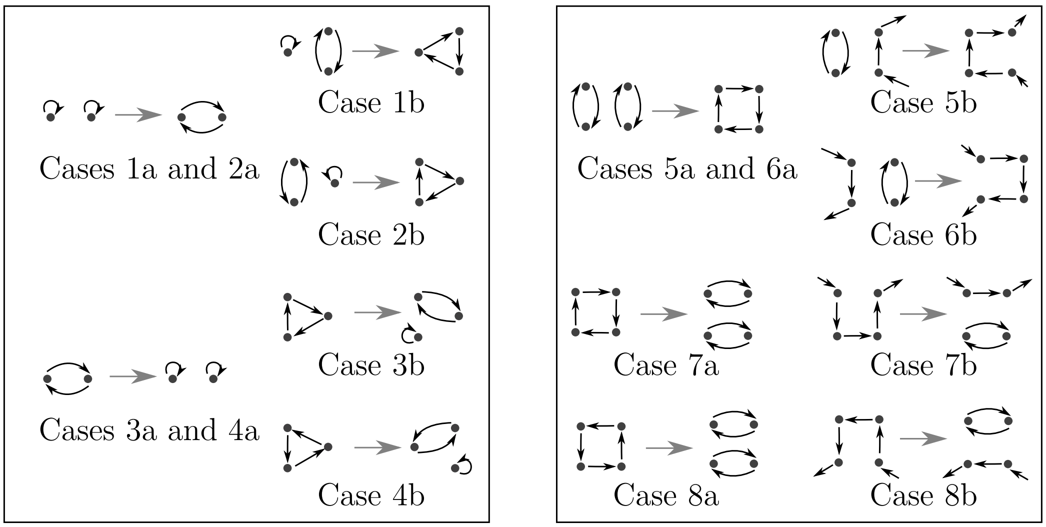

FIGURE 8.2. Cases for Δr_2.

- Case 0: $\pi(\mathbf{x}) = \pi(\mathbf{y})$ (and so also $\mathbf{x} = \mathbf{y}$): this is a trivial move; $\pi' = \pi$. $\Delta r_2 = 0$.
- Case 1: $\mathbf{x} = \pi(\mathbf{x})$.
  - Case 1a: $\mathbf{y} = \pi(\mathbf{y})$. $\Delta r_2 = +1$.
  - Case 1b: $\mathbf{y} \neq \pi(\mathbf{y})$ but $\mathbf{y} = \pi^2(\mathbf{y})$. $\Delta r_2 = -1$.
  - Case 1c: $\mathbf{y} \neq \pi(\mathbf{y}), \pi^2(\mathbf{y})$. $\Delta r_2 = 0$.
- Case 2: $\mathbf{y} = \pi(\mathbf{y})$.
  - Case 2a: $\mathbf{x} = \pi(\mathbf{x})$. Same as case 1a. $\Delta r_2 = +1$.
  - Case 2b: $\mathbf{x} \neq \pi(\mathbf{x})$ but $\mathbf{x} = \pi^2(\mathbf{x})$. $\Delta r_2 = -1$.
  - Case 2c: $\mathbf{x} \neq \pi(\mathbf{x}), \pi^2(\mathbf{x})$. $\Delta r_2 = 0$.
- Case 3: $\mathbf{x} = \pi(\mathbf{y})$.

  - Case 3a: $\pi(\mathbf{x}) = \mathbf{y}$. $\Delta r_2 = -1$.
  - Case 3b: $\pi^2(\mathbf{x}) = \mathbf{y}$. $\Delta r_2 = +1$.
  - Case 3c: $\mathbf{y} \neq \pi(\mathbf{x}), \pi^2(\mathbf{x})$. $\Delta r_2 = 0$.

- Case 4: $\pi(\mathbf{x}) = \mathbf{y}$.
  - Case 4a: $\pi(\mathbf{y}) = \mathbf{x}$. Same as case 3a. $\Delta r_2 = -1$.
  - Case 4b: $\pi^2(\mathbf{y}) = \mathbf{x}$. $\Delta r_2 = +1$.
  - Case 4c: $\mathbf{x} \neq \pi(\mathbf{y}), \pi^2(\mathbf{y})$. $\Delta r_2 = 0$.

- Case 5: $\pi^2(\mathbf{x}) = \mathbf{x}$.
  - Case 5a: $\pi^2(\mathbf{y}) = \mathbf{y}$. $\Delta r_2 = -2$.
  - Case 5b: $\pi^2(\mathbf{y}) \neq \mathbf{y}$. $\Delta r_2 = -1$.

- Case 6: $\pi^2(\mathbf{y}) = \mathbf{y}$.
  - Case 6a: $\pi^2(\mathbf{x}) = \mathbf{x}$. Same as 5a. $\Delta r_2 = -2$.
  - Case 6b: $\pi^2(\mathbf{x}) \neq \mathbf{x}$. $\Delta r_2 = -1$.

- Case 7: $\pi^2(\mathbf{x}) = \mathbf{y}$.
  - Case 7a: $\pi^2(\mathbf{y}) = \mathbf{x}$. $\Delta r_2 = +2$.
  - Case 7b: $\pi^2(\mathbf{y}) \neq \mathbf{x}$. $\Delta r_2 = +1$.

- Case 8: $\pi^2(\mathbf{y}) = \mathbf{x}$.
  - Case 8a: $\pi^2(\mathbf{x}) = \mathbf{y}$. $\Delta r_2 = +2$.
  - Case 8b: $\pi^2(\mathbf{x}) \neq \mathbf{y}$. $\Delta r_2 = +1$.

- All other cases: $\Delta r_2 = 0$.

8.3 Swap and worm with r_ℓ interactions

The non-spatiality of the wormhole point plays no role in the algebraic notion of cycle lengths. Thus, the same Δr_2 formulas apply to both algorithms.

Recall proposition 5.3.9 and remark 5.3.10: if $\mathbf{x}$ and $\mathbf{y}$ are in separate cycles before the swap, they are in the same cycle afterward, and vice versa. In the former case, the new common cycle length is the sum of the old separate cycle lengths; in the latter case, the new cycle lengths are taken from the number of permutation jumps from one site to the other. (Throughout this section, please consult figure 8.3 for illumination.) Given that general pair of facts, we split out subcases which are convenient as a software-optimization detail:

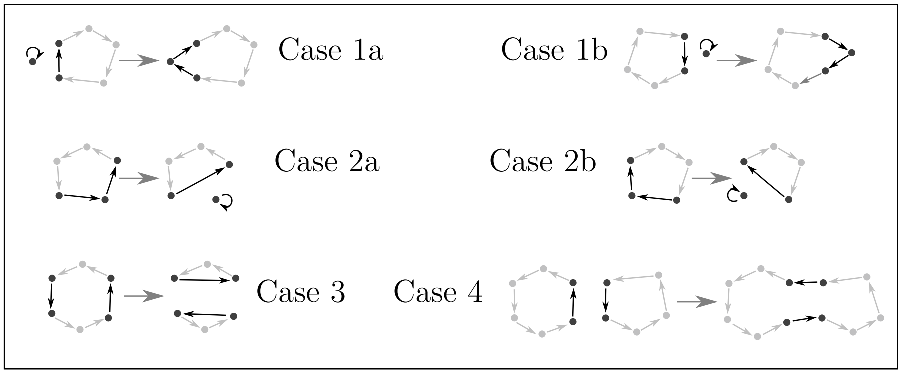

FIGURE 8.3. Cases for Δr_ℓ. Sites and arrows not participating in changes are shown in grey.

- Case 0: $\pi(\mathbf{x}) = \pi(\mathbf{y})$ (and so also $\mathbf{x} = \mathbf{y}$): this is a trivial move; $\pi' = \pi$. $\Delta r_\ell = 0$ for all $\ell = 1, \ldots, N$.
- Case 1: $\mathbf{x}$ and $\mathbf{y}$ are in different cycles, but one of them is in a one-cycle.
  - Case 1a: $\mathbf{x} = \pi(\mathbf{x})$: $\Delta r_1 = -1$, $\Delta r_{\ell_{\mathbf{y}}(\pi)} = -1$, $\Delta r_{\ell_{\mathbf{y}}(\pi)+1} = +1$.
  - Case 1b: $\mathbf{y} = \pi(\mathbf{y})$: $\Delta r_1 = -1$, $\Delta r_{\ell_{\mathbf{x}}(\pi)} = -1$, $\Delta r_{\ell_{\mathbf{x}}(\pi)+1} = +1$.
- Case 2: $\mathbf{x}$ and $\mathbf{y}$ are in the same cycle, but one is the jump target of the other.
  - Case 2a: $\mathbf{y} = \pi(\mathbf{x})$. $\Delta r_{\ell_{\mathbf{x}}(\pi)} = -1$, $\Delta r_{\ell_{\mathbf{x}}(\pi)-1} = +1$, $\Delta r_1 = +1$.
  - Case 2a: $\mathbf{x} = \pi(\mathbf{y})$. $\Delta r_{\ell_{\mathbf{y}}(\pi)} = -1$, $\Delta r_{\ell_{\mathbf{y}}(\pi)-1} = +1$, $\Delta r_1 = +1$.
- Case 3: $\mathbf{x}$ and $\mathbf{y}$ are in the same cycle, and neither is the jump target of the other. Let $a = \ell_{\mathbf{x},\mathbf{y}}(\pi)$ and $b = \ell_{\mathbf{y},\mathbf{x}}(\pi)$. Then $\Delta r_{a+b} = -1$, $\Delta r_a = +1$, $\Delta r_b = +1$.
- Case 4: $\mathbf{x}$ and $\mathbf{y}$ are in separate cycles. $\Delta r_{\ell_{\mathbf{x}}(\pi)} = -1$, $\Delta r_{\ell_{\mathbf{y}}(\pi)} = -1$, $\Delta r_{\ell_{\mathbf{x}}(\pi)+\ell_{\mathbf{y}}(\pi)} = +1$.

8.4 Swap with V interactions

Recall from proposition 7.3.1 that as long as the extended energy function H' agrees with the energy function H on closed cycles, P'_{Gibbs} has the correct marginal distribution on closed cycles. Thus, when writing energy terms for open cycles, we can choose how to define the energy. For r_2 and r_ℓ (the previous two sections), it is simplest to say that the non-spatial point w can participate in permutation cycles. For other interactions that depend on the spatiality of points, it is simplest to say that w does not participate. Thus, here we split out swap and worm cases.

The change in energy is simply the contributions from the old arrows $\mathbf{x} \mapsto \pi(\mathbf{x})$ and $\mathbf{y} \mapsto \pi(\mathbf{y})$ to all other arrows, along with their mutual interaction, subtracted from the contributions from the new arrows $\mathbf{x} \mapsto \pi(\mathbf{y})$ and $\mathbf{y} \mapsto \pi(\mathbf{x})$ to all other arrows, along with their mutual interaction:

$$\begin{aligned}\Delta V = &\sum_{\mathbf{v}\neq\mathbf{x},\mathbf{y}} V(\mathbf{x},\pi(\mathbf{y}),\mathbf{v},\pi(\mathbf{v})) + \sum_{\mathbf{v}\neq\mathbf{x},\mathbf{y}} V(\mathbf{y},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})) + V(\mathbf{x},\pi(\mathbf{y}),\mathbf{y},\pi(\mathbf{x})) \\ &- \sum_{\mathbf{v}\neq\mathbf{x},\mathbf{y}} V(\mathbf{x},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})) - \sum_{\mathbf{v}\neq\mathbf{x},\mathbf{y}} V(\mathbf{y},\pi(\mathbf{y}),\mathbf{v},\pi(\mathbf{v})) - V(\mathbf{x},\pi(\mathbf{x}),\mathbf{y},\pi(\mathbf{y})).\end{aligned}$$

8.5 Worm with V interactions

The non-spatial point has no interactions, so we simply track the creation and destruction of spatial-to-spatial arrows for the four types of worm move. (See figure 8.4.)

Open:

$$-\sum_{\mathbf{v}\neq\mathbf{x},w} V(\mathbf{x},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})).$$

Close:

$$\sum_{\mathbf{v}\neq\pi^{-1}(w),w} V(\pi^{-1}(w),\pi(w),\mathbf{v},\pi(\mathbf{v})).$$

Head swap:

$$\sum_{\mathbf{v}\neq\mathbf{x},\pi^{-1}(w)} V(\pi^{-1}(w),\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})) - \sum_{\mathbf{v}\neq\mathbf{x},\pi^{-1}(w)} V(\mathbf{x},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})).$$

Tail swap:

$$\sum_{\mathbf{v}\neq\mathbf{x},w,\pi^{-1}(w)} V(\mathbf{x},\pi(w),\mathbf{v},\pi(\mathbf{v})) - \sum_{\mathbf{v}\neq\mathbf{x},w,\pi^{-1}(w)} V(\mathbf{x},\pi(\mathbf{x}),\mathbf{v},\pi(\mathbf{v})).$$

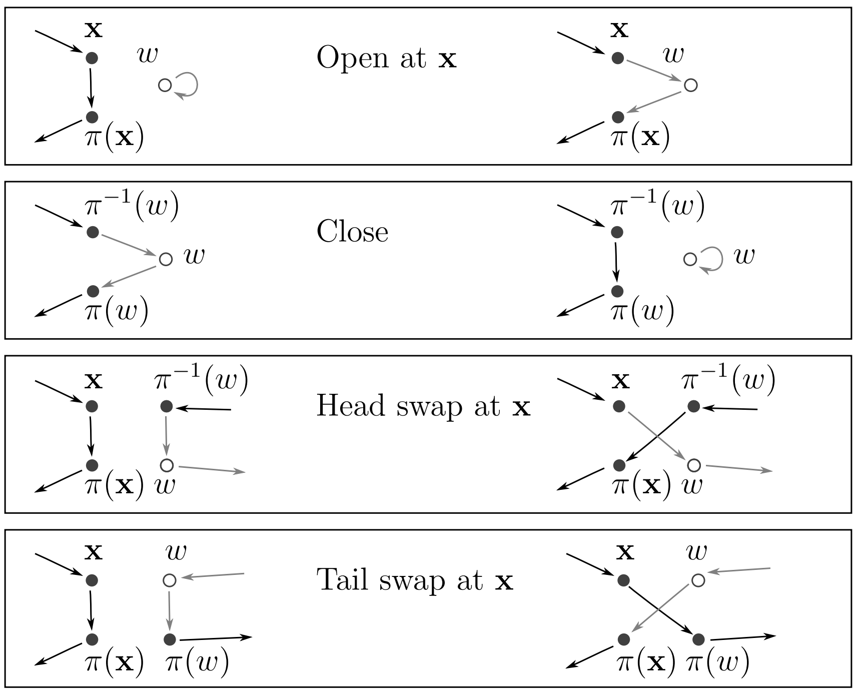

FIGURE 8.4. Cases for worm ΔV. Non-spatial arrows (i.e. those starting or ending at w) are shown in grey.