In the Metropolis approach the acceptance matrix is

$$A_{xy} = \min(R_{xy}, 1)$$

Algorithm: one Metropolis iteration works as follows.

1. At iteration n the system is in the state point x_n.
2. We generate a new state point y using the proposal matrix $P^{(0)}$.
3. We compute the ratio $R = \pi_y P^{(0)}_{yx} / (\pi_x P^{(0)}_{xy})$.
4. If $R \geq 1$ we accept the proposal and set $x_{n+1} = y$. Otherwise, we generate a number U uniformly distributed in $[0,1]$. If $U \leq R$, the proposal is accepted and $x_{n+1} = y$; in the opposite case a null transition is performed and $x_{n+1} = x_n$.

In many applications $P^{(0)}$ is symmetric and therefore $R_{xy} = \pi_y / \pi_x$.

In statistical mechanics $\pi_x = e^{-\beta E_x}/Z$. In this case, for a symmetric proposal, we have

$$R_{xy} = \frac{\pi_y}{\pi_x} = e^{-\beta(E_y - E_x)}$$

NOTE: The partition function cancels out and R_{xy} depends only on the energy difference. The condition on R_{xy} can be rewritten as a condition on the difference: if $\Delta E = E_y - E_x < 0$ then $R_{xy} > 1$, while if $\Delta E = E_y - E_x > 0$ then $R_{xy} < 1$.

In this case, for a symmetric proposal, the last two steps of the algorithm can be rewritten as follows:

3. Compute $\Delta E = E_y - E_x$;
4. If $\Delta E \leq 0$ accept the proposal and set $x_{n+1} = y$. Otherwise, generate a number U uniformly distributed in $[0, 1]$. If $U \leq \exp(-\beta \Delta E)$, the proposal is accepted and $x_{n+1} = y$; in the opposite case a null transition is performed and $x_{n+1} = x_n$.

Exercise: Metropolis for the Ising model

The ferromagnetic Ising model Hamiltonian is

$$H = -\sum_{\langle ij \rangle} s_i s_j$$

where $s_i = \pm 1$ are defined on the sites of a lattice (for instance a cubic lattice) and the sum is over all nearest-neighbor pairs $\langle ij \rangle$.

Dynamics. It is based on the following (symmetric) proposal: choose a site i and propose a flip of the spin s_i.

The proposal probability is clearly symmetric. For two spins, this is the dynamics we have considered a few lessons ago with $p = 1$ (in the dynamics defined here we always perform the flip). From the explicit expression of the matrix we can verify that the matrix is symmetric.

In the general case $P_{xy}^{(0)}$ is nonvanishing only if x and y are two spin configurations that differ by the direction of one (and only one) spin. If n spins belong to the system, we have $P_{xy}^{(0)} = 1/n$ for such a pair of configurations (we must choose the site among n lattice sites). Therefore, if we go from x to y with probability $1/n$, we also go from y to x with the same probability.

We can express the Metropolis acceptance in terms of energies.
To compute the change in the energy we should only consider the terms in H that involve the spin i: $E_x = -s_i V$, $E_y = -(-s_i)V = s_i V$, $E_y - E_x = 2s_i V = \Delta$.
One iteration of the algorithm works as follows:

1. choose randomly a site i;
2. compute $V = \sum_j s_j$, where the sum runs over all nearest neighbors j of site i, and $\Delta = 2s_i V$.
3. If $\Delta \leq 0$, flip the spin at site i: the new configuration $\{s'_j\}$ is given by $s'_j = s_j$ for $j \neq i$, $s'_i = -s_i$. If $\Delta > 0$, generate a number U uniformly distributed in $[0,1]$. If $U < e^{-\beta\Delta}$, flip the spin as explained before; otherwise perform a null transition