Solutions 9

1. a) The transition probabilities are given by

\[
p_{01} = \psi_{01} \min \left( 1, \frac{\psi_{10}}{\psi_{01}} \right) = e^{-\beta/2} \quad p_{21} = \psi_{21} \min \left( 1, \frac{\psi_{12}}{\psi_{21}} \right) = e^{-\beta/2} \\
p_{10} = \psi_{10} \min \left( 1, \frac{\psi_{01}}{\psi_{10}} \right) = \frac{\sqrt{e^{-4\beta} - 2e^{-3\beta} + e^{-2\beta} + 4}}{4} \sqrt{e^{-4\beta} - 2e^{-3\beta} + e^{-2\beta} + 4} \\
p_{02} = p_{20} = p_{11} = 0 \\
p_{00} = 1 - e^{-\beta} \quad p_{22} = 1 - e^{-\beta/2} \quad (1)
\]

b) Let us now check that the detailed balance equation is satisfied:

\[
p_{01} \pi_0 = \frac{1}{2} e^{-2\beta} = p_{10} \pi_1 \\
p_{02} \pi_0 = 0 = p_{20} \pi_2 \\
p_{12} \pi_1 = \frac{1}{2} e^{-2\beta} = p_{21} \pi_2.
\]

c) As usual, there are several methods to compute the eigenvalues. For example, one can find the three solutions \( \lambda_0, \lambda_1, \) and \( \lambda_2 \) to the equation

\[
det(P - \lambda I) = 0, \quad (2)
\]

where \( I \) is the \( 3 \times 3 \) identity matrix and \( P \) the matrix of the transition probabilities computed in (1).

Another (perhaps even simpler method) method is to solve the following system of equations:

\[
\begin{align*}
\lambda_0 &= 1 \\
\lambda_0 + \lambda_1 + \lambda_2 &= \text{tr}(P), \\
\lambda_0 \cdot \lambda_1 \cdot \lambda_2 &= \det(P)
\end{align*}
\]

as we know that the largest eigenvalue is 1, the sum of the eigenvalues equals the trace of \( P \), and their product equals the determinant of \( P \).

Consequently, we obtain

\[
\begin{align*}
\lambda_0 &= 1 \\
\lambda_1 &= -\frac{e^{-2\beta}}{4} - \frac{e^{-\beta}}{4} + \frac{1}{2} + \frac{1}{4} \sqrt{e^{-4\beta} - 2e^{-3\beta} + e^{-2\beta} + 4}, \\
\lambda_2 &= -\frac{e^{-2\beta}}{4} - \frac{e^{-\beta}}{4} + \frac{1}{2} - \frac{1}{4} \sqrt{e^{-4\beta} - 2e^{-3\beta} + e^{-2\beta} + 4}
\end{align*}
\]

d) The spectral gap is given by

\[
\gamma = 1 - \lambda_1 = \frac{1}{2} + \frac{e^{-2\beta}}{4} + \frac{e^{-\beta}}{4} - \frac{1}{4} \sqrt{e^{-4\beta} - 2e^{-3\beta} + e^{-2\beta} + 4}. \quad (3)
\]
Therefore, when $\beta$ is large, we have
\[
\gamma \approx \frac{1}{4} e^{-\beta}.
\]  

(4)

Remark. The value of $\beta$ has to be tuned carefully and there is an inherent trade-off in its choice. If we pick $\beta$ too large, then the spectral gap is small and the convergence to the global minimum occurs very slowly. On the other hand, if we pick $\beta$ too small, we might not be able to visit all the states and, therefore, we might get stuck in the local minimum (=state 2).