[nex85] Detailed balance condition and thermal equilibrium

Consider a statistical mechanical system specified by a Hamiltonian $H(\mathbf{x})$. Here the *random field* $\mathbf{x} = (x_1, x_2, \ldots)$ specifies the microstate. At thermal equilibrium, the macrostate is specified by the probability distribution $\rho(\mathbf{x}) = Z^{-1} \exp[-\beta H(\mathbf{x})]$. Now consider a Markov process specified by the master equation

$$\frac{\partial}{\partial t} P(\mathbf{x}, t) = \sum_{\mathbf{x}'} \left[W(\mathbf{x}|\mathbf{x}') P(\mathbf{x}', t) - W(\mathbf{x}'|\mathbf{x}) P(\mathbf{x}, t) \right].$$

Show that the equilibrium distribution $\rho(\mathbf{x})$ satisfies the detailed balance condition $W(\mathbf{x}'|\mathbf{x})\rho(\mathbf{x}) = W(\mathbf{x}|\mathbf{x}')\rho(\mathbf{x}')$ for the *Metropolis algorithm* and the *heat bath algorithm*, which are specified, respectively by the transition rates $[\Delta H \equiv H(\mathbf{x}') - H(\mathbf{x})]$:

$$W(\mathbf{x}'|\mathbf{x})dt = \begin{cases} e^{-\beta \Delta H} & \text{if } \Delta H \geq 0 \\ 1 & \text{if } \Delta H \leq 0 \end{cases}, \qquad W(\mathbf{x}'|\mathbf{x})dt = \frac{e^{-\beta \Delta H}}{1 + e^{-\beta \Delta H}}.$$

Solution: