Problem 1: Spin density matrix

Sethna: problem 7.6. $\bar{\bar{H}} = -\frac{\hbar}{2}\vec{B}\cdot\bar{\bar{\sigma}}$

$$\bar{\bar{\rho}} = \frac{1}{2}\left(\bar{\bar{I}} + \vec{p}\cdot\bar{\bar{\sigma}}\right) = \frac{1}{2}\begin{pmatrix} 1+p_z & p_x - ip_y \\ p_x + ip_y & 1-p_z \end{pmatrix}$$

$\mathrm{Tr}\,\bar{\bar{\rho}} = 1$ $\qquad \bar{\bar{\rho}}^* = \bar{\bar{\rho}}^T$

$$\hookrightarrow \frac{1}{2}\begin{pmatrix} 1+p_z & p_x + ip_y \\ p_x - ip_y & 1-p_z \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+p_z & p_x + ip_y \\ p_x - ip_y & 1-p_z \end{pmatrix}$$

$$i\hbar\frac{\partial\bar{\bar{\rho}}}{\partial t} = [\bar{\bar{H}}, \bar{\bar{\rho}}] \to -\frac{\hbar}{4}\left[B_x\bar{\bar{\sigma}}_x + B_y\bar{\bar{\sigma}}_y + B_z\bar{\bar{\sigma}}_z, p_x\bar{\bar{\sigma}}_x + p_y\bar{\bar{\sigma}}_y + p_z\bar{\bar{\sigma}}_z\right]$$

$$= -\frac{\hbar}{4}\Big[B_x p_y[\bar{\bar{\sigma}}_x, \bar{\bar{\sigma}}_y] + B_x p_z[\bar{\bar{\sigma}}_x, \bar{\bar{\sigma}}_z] + B_y p_x[\bar{\bar{\sigma}}_y, \bar{\bar{\sigma}}_x] + B_y p_z[\bar{\bar{\sigma}}_y, \bar{\bar{\sigma}}_z] + B_z p_x[\bar{\bar{\sigma}}_z, \bar{\bar{\sigma}}_x] + B_z p_y[\bar{\bar{\sigma}}_z, \bar{\bar{\sigma}}_y]\Big]$$

$$= -\frac{2\hbar}{4} i\Big[(B_x p_y - B_y p_x)\sigma_z - (B_x p_z - B_z p_x)\sigma_y + (B_y p_z - B_z p_y)\bar{\bar{\sigma}}_x\Big]$$

$$\frac{i\hbar}{2}\frac{\partial\vec{p}}{\partial t}\cdot\bar{\bar{\sigma}} = -\frac{i\hbar 2}{4}(\vec{B}\times\vec{p})\cdot\bar{\bar{\sigma}}$$

$$\hookrightarrow \frac{\partial\vec{p}}{\partial t} = -(\vec{B}\times\vec{p})$$

Problem 2: Monte Carlo (detailed balance)

Let $P(x)$ be a probability distribution.

a. Show that if a Markov chain described by transition matrix $T(x|x')$ obeys detailed balance, then it holds that

$$P(x) = \sum_{x'} T(x|x')\, P(x').$$

In a Monte Carlo algorithm the transition matrix can be written

$$T(x|x') = M(x|x')A(x|x'),$$

where $M(x|x')$ denotes the matrix associated with the random proposed move, and $A(x|x')$ denotes the acceptance probability.

Suppose you want to sample the unnormalized probability distribution $P(x) = exp(-x^2/2)$.

b. Construct an algorithm to sample $P(x)$ using a *uniform* random number generator. In other words give the expression for the matrices $M(x|x')$ and $A(x|x')$.

c. Construct an algorithm to sample $P(x)$ using a Gaussian random number generator which generates random numbers according to the distribution $exp(-x^2/2)$.

a.) deteiled balance: $T(x|x')P(x') = T(x'|x)P(x)$

$$\Downarrow$$

$$\sum_{x'} T(x|x')\, P(x') = \sum_{x'} T(x'|x) P(x) = P(x) \checkmark$$

b.) uniform random number generator:

$M(x|x') = c \quad \text{if } |x-x'| < \Delta$

$T(x|x') = \exp(-\frac{1}{2}(x^2 - x'^2))$

c.) in this case no acceptance or rejection criterion is needed

Problem 3 More detailed balance

a. Sethna Problem 8.5(a).

b. Sethna Problem 8.6

a.) $P_{\alpha\leftarrow\beta}\rho_\beta = P_{\beta\leftarrow\alpha}\rho_\alpha$

$P_{\gamma\leftarrow\alpha}P_{\alpha\leftarrow\beta}\rho_\beta = P_{\gamma\leftarrow\alpha}P_{\beta\leftarrow\alpha}\rho_\alpha = P_{\beta\leftarrow\alpha}P_{\gamma\leftarrow\alpha}\rho_\alpha$
$= P_{\beta\leftarrow\alpha}P_{\alpha\leftarrow\gamma}\rho_\gamma$

$P_{\beta\leftarrow\gamma}P_{\gamma\leftarrow\alpha}P_{\alpha\leftarrow\beta}\rho_\beta = P_{\beta\leftarrow\gamma}P_{\beta\leftarrow\alpha}P_{\alpha\leftarrow\gamma}\rho_\gamma$
$= P_{\beta\leftarrow\alpha}P_{\alpha\leftarrow\gamma}P_{\beta\leftarrow\gamma}\rho_\gamma$
$= P_{\beta\leftarrow\alpha}P_{\alpha\leftarrow\gamma}P_{\gamma\leftarrow\beta}\rho_\beta$

$$\Downarrow \qquad \Downarrow$$

$$\boxed{P_{\beta\leftarrow\gamma}P_{\gamma\leftarrow\alpha}P_{\alpha\leftarrow\beta} = P_{\beta\leftarrow\alpha}P_{\alpha\leftarrow\gamma}P_{\gamma\leftarrow\beta}}$$

b.) detailed balance:

pick spin at random $\Rightarrow$ $M(x\to x') = M(x'\to x)$

so only acceptance needs to satisfy detailed balance

$$e^{-\beta E_i} A(i\to j) = e^{-\beta E_j} A(j\to i)$$

if $A(i\to j) = \min\{1, e^{-\beta(E_j - E_i)}\}$

detailed balance is satisfied

$\to$ ~~less~~ as efficient ~~than~~ as <u>heat bath</u>

~~one ra~~ needs <u>two random numbers</u> for each move