Examen

1.1 Probability conservation

$$p_i = \sum_{j=1}^{n} p_j \pi(i \to j)$$

$$= \sum_{j=1}^{n} v(i \to j)$$

1.2 Stationarity

$$-\sum_{j=1}^{n} \pi(i \to j) p_i + \sum_{j=1}^{n} p_j \pi(j \to i) = 0$$

$$-\underbrace{\left[\sum_{j=1}^{n} \pi(i \to j)\right]}_{=1} p_i + \sum_{j=1}^{n} v(j \to i) = 0$$

$$p_i = \sum_{j=1}^{n} v(j \to i)$$

1.3 One sums over all flux of rejection normalized by the total probability

$$R = \frac{\sum_i v(i \to i)}{\sum_i p_i}$$

1.4 In a Metropolis algorithm one put chose among $n-1$ new trials configurations and one applies $\min\left(1, \frac{p_j}{p_i}\right)$

$$w(i \to j) = \frac{1}{n-1} \min\left(1, \frac{p_j}{p_i}\right)$$

$$v(i \to j) = \frac{p_i}{n-1} \min\left(1, \frac{p_j}{p_i}\right)$$

$$= \frac{\min(p_i, p_j)}{n-1}$$

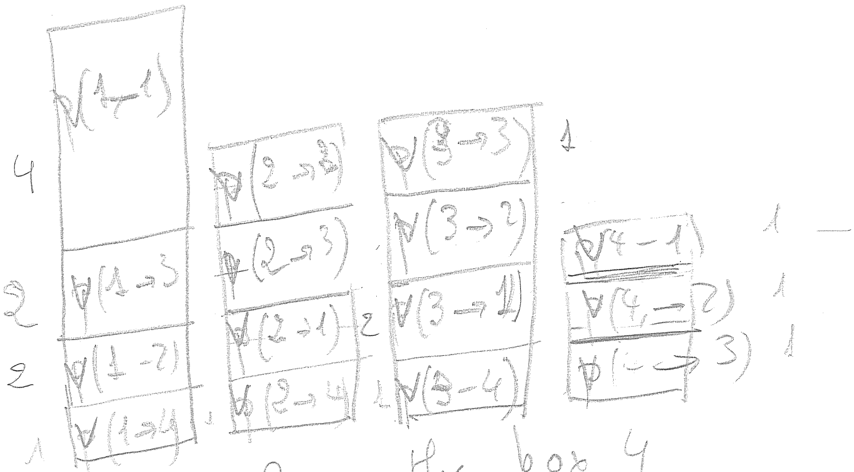
1.5 $p_i W(i \to f) = p_f W(f \to i)$

$\nu(i \to f) = \nu(f \to i)$

1.6 a) Using Eq(1), the area of each box corresponds to the sum of $\nu(i \to f)$

b) $p_3 < p_2$ and $p_3 < p_1$ there is no rejection when a particle tries to exit the state 3

1,7



Starting from the box 4

$\nu(4 \to 4) = 0$ $\quad \nu(4 \to 1) = \nu(4 \to 2) = \nu(4 \to 3) = 1$

and Detailed Balance $\Rightarrow$ $\nu(1 \to 4) = \nu(2 \to 4) = \nu(3 \to 4) = 1$

$\nu(2 \to 3) = \nu(3 \to 2) = 2$

$\nu(2 \to 1) = \nu(1 \to 2) = 2$

$\nu(3 \to 1) = \nu(1 \to 3) = 2$

$\Rightarrow$ $\nu(2 \to 2) = \nu(3 \to 3) = 1$

$\nu(1 \to 1) = 4$

(3)

8 $v(1\to 1) = v(2\to 2) = v(3\to 3) = 0$

No rejection.

9 $v(1\to 2) \neq v(2\to 1)$

$\sum_{f=1} v(f\to i) = p_i$ is satisfied

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2 -

2 - 1 $$W = \int_0^2 dt\, \partial_\lambda V(x,\lambda) \frac{d\lambda}{dt}$$

V depends on x which is a stochastic variable $\Rightarrow$ W is stochastic

$$\langle W\rangle = \int_0^2 dt\, \langle \partial_\lambda V(x,\lambda)\rangle \frac{d\lambda}{dt}$$

2 - 2 $$\langle W\rangle = \int_0^2 (\lambda - \langle x\rangle)\frac{d\lambda}{dt}\, dt$$

when $t\to +\infty$ $\langle x\rangle_t = \lambda$ $\langle W\rangle = 0$

$t\to 0$ $\langle W\rangle = \frac{1}{2}(\lambda_f^2 - \lambda_0^2)$

2 - 3 Taking the average of the Langevin equation

$$\dot{u} = -(u - \lambda)$$

2 - 4 $$\langle W\rangle = \int_0^t dz\, \dot{u}\left[\ddot{u} + \dot{u}\right]$$

$$= \left[\frac{\dot{u}^2}{2}\right]_0^t + \int_0^t \dot{u}^2\, dz$$

2.5 $\quad u = at + b$

$t=0 \quad u = \langle x \rangle_0 = b = 0$

$$\dot{u}(0) = \lambda_0 - u(0) = 0$$

$$\dot{u}(t) = \lambda f - u(t) = \lambda f - at$$

Discontinuities at the boundaries

$$\langle W \rangle = a^2 t + \frac{(\lambda f - at)^2}{2}$$

$$= \frac{\lambda^2 f^2}{2} - a\lambda f t + a^2\left(\frac{t^2}{2} + t\right)$$

2.6 $$\frac{\partial \langle W \rangle}{\partial a} = -\lambda f t + 2a\left(\frac{t^2}{2} + t\right) = 0$$

$$\Rightarrow \quad a = \frac{\lambda f}{2+t}$$

Inserting a in $\dot{u} = (\lambda - u)$ yields

$$\frac{\lambda f}{t+2} = \lambda - \frac{\lambda f\, t}{t+2}$$

$$\boxed{\lambda = \lambda f \frac{t+1}{t+2}}$$

2.7 $$\langle W \rangle_{min} = \left(\frac{\lambda f}{2+t}\right)^2 t + \frac{\left(\lambda f - \frac{\lambda f\, t}{2+t}\right)^2}{2}$$

$$\langle W \rangle_{min} = \frac{\lambda f^2}{2+t} + [illegible]$$

[illegible]

2.7 When $t \to +\infty$ $\langle W \rangle \to 0$

When $t \to 0$ $\langle W \rangle = \frac{\lambda f^2}{2}$

Agreement

2.8 The optimal solution has a minimum work of $\frac{\lambda f^2}{(t+2)}$ -

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3 3.1 $H = -\frac{J_0}{2N}\left(N^2 m^2 - N\right)$

$H = -\frac{J_0 N m^2}{2} + \frac{J_0}{2}$

when $N \to +\infty$ $H \sim -\frac{J_0 N m^2}{2}$

Minimizing $H \Leftrightarrow$ maximizing m^2

3.2 $m^2 = 1 \Leftrightarrow \begin{cases} \sigma_i = +1 \\ \sigma_i = -1 \end{cases}$

3.3 $Z = e^{-\frac{\beta J_0}{2}} \sum_{\{\sigma_i\}} e^{+\frac{J_0 \beta N m^2}{2}}$

with $b = \frac{J_0 \beta N}{2}$

$Z = \sum_{\{\sigma_i\}} e^{-\frac{\beta J_0}{2}} \sqrt{\frac{J_0 \beta N}{\pi}} \int_{-\infty}^{+\infty} dx \exp\left[-\frac{J_0 \beta N x^2}{2} + x\beta J_0 N m\right]$

3.4

$$Z = e^{\frac{\beta J_0}{2}} \sqrt{\frac{J_0 \beta N}{2\pi}} \int_{-\infty}^{+\infty} dx \exp\left[-\frac{J_0 \beta N x^2}{2}\right] \underbrace{\sum_{\{\sigma_i\}} e^{x \beta J_0 \sum \sigma_i}}$$ (6)

$$I = \left[2 \operatorname{ch} \beta J_0 x\right]^N = e^{N \ln 2 \operatorname{ch} \beta J_0 x}$$

3.5 By using the saddle point method

$$\beta f(x, \beta) = \frac{J_0 \beta}{2} x^2 - \ln 2 \operatorname{ch}(\beta J_0 x)$$

$$f(x, \beta) = \frac{J_0}{2} x^2 - \frac{1}{\beta} \ln\left[2 \operatorname{ch} \beta J_0 x\right]$$

$\Rightarrow$ the canonical partition function given

$$\beta f(\beta) = -\frac{\ln Z}{N}$$

therefore $f(\beta) = \min_x f(\beta, x)$

3.6

$$\langle m \rangle = \frac{\sum_{i=1}^{N} \sum_{\{\sigma_i\}} \sigma_i e^{-\beta H}}{\sum_{\{\sigma_i\}} e^{-\beta H}}$$

$$\frac{\partial f}{\partial x} = J_0 x - J_0 \operatorname{th} \beta J_0 x = 0$$

$$x = \operatorname{th} \beta J_0 x$$

If $\beta J_0 < 1$ 1 solution $x = 0$

$\beta J_0 > 1$ 3 solution $x = 0$

$x_{1,2} = \operatorname{th} \beta J_0 x_{1,2}$

$x_1 = -x_2$ $f(x_1, \beta) = f(x_2, \beta) < f(0, \beta)$

3,7 $$\frac{\Pi(\sigma \to -\sigma_i)}{\Pi(-\sigma_i \to \sigma_i)} = \frac{1 - \sigma_i \tanh \beta h_i}{1 + \sigma_i \tanh \beta h_i}$$

$$= \frac{(1 - \sigma_i \tanh \beta h_i)^2}{1 - \tanh^2 \beta h_i}$$

$$= ch^2 \beta h_i \left[1 - 2\sigma_i \tanh \beta h_i + \tanh^2 \beta h_i\right]$$

$$= ch^2 \beta h_i - 2\sigma_i \, sh \beta h_i \, ch \beta h_i + sh^2 \beta h_i$$

$$= ch\, 2\beta h_i - \sigma_i \, sh\, 2\beta h_i$$

$$= \begin{cases} e^{-2\beta h_i} & \text{if } \sigma_i = +1 \\ e^{2\beta h_i} & \text{if } \sigma_i = -1 \end{cases}$$

$$= e^{-2\beta \sigma_i h_i}$$

$$\frac{P(\sigma_i \to \sigma_i)}{P(\sigma_i \to \sigma_i)} = e^{-\Delta E} = e^{-2\beta \sigma_i h_i}$$

3.8 $$C_g(t,t) = \frac{1}{N} \sum_{i \neq j} C_{ij}(t,t) + \sum_i C_{ii}(t,t)$$

$$C_g(t,t) = \frac{N(N-1)}{N} \frac{C_{loc}}{N} + \frac{1}{N} NC + O\left(\frac{1}{N}\right)$$

$$C_g(t,t) = C_{loc} + C_{inf}$$

3.9 $C_{loc} = \frac{1}{N}\sum_i \left[\langle \sigma_i(t)\sigma_i(t)\rangle - \langle \sigma_i(t)\rangle\langle\sigma_i(t)\rangle\right]$ (8)

$$C_{loc} = \frac{1}{N}\sum_i \langle 1\rangle - \frac{N^2}{N} m^2$$

$$C_{loc}(t,t) = 1 - m^2(t)$$

3.10 $\frac{\partial m}{\partial t} = -m - \langle t_i \rangle = -m + \tanh(\beta J m)$

3.11 $\langle \Delta h_i \Delta\sigma_j\rangle = \frac{1}{N}\langle \sum_{k\neq i} \Delta\sigma_k \Delta\sigma_j\rangle$

$$= \frac{1}{N} C_{loc}(t,t) + O(N^{-2})$$

$$+ \frac{N-2}{N}\frac{C_{\cancel{loc}}(t,t)}{N} = C_g(t,t) + O\left(\frac{1}{N^2}\right)$$

3.12 $\frac{\partial C_{\cancel{loc}\,g}(t,t)}{\partial t} = -2m\frac{\partial m}{\partial t}$

$$\frac{1}{N}\frac{\partial C_{nl}}{\partial t}(t,t) = -\frac{2}{N} C_{nl}(t,t) + \left(\frac{\beta J}{ch^2 \beta J m}\right)\left[\langle \Delta h_i \Delta\sigma_j\rangle + \langle\Delta\sigma_i\Delta h_j\rangle\right]$$

$$= -\frac{2}{N} C_{nl}(t,t) + \frac{2}{N}\frac{\beta J}{ch^2 \beta J m} C_g(t,t)$$

$$\frac{\partial m}{\partial t} = m + th\,\beta m$$

$$\frac{\partial C_{loc}}{\partial t} = \cancel{+}\,2(m^2 + m\, th\,\beta J m) = -2 C_{loc} + 2(m\, th\,\beta J m - 1)$$

Combining ~~with~~ C_{nl} and C_{loc} give the equation (18)

3.13 Standard integration