Exercise 3:

(a) Metropolis criterion: $\overset{w_{ij}}{\cancel{p_{ij}}} = \min\left(1, \exp\left(-\frac{\Delta E}{kT}\right)\right)$, $\Delta E = E_j - E_i$

$\rightsquigarrow$ $\underline{\Delta E < 0} \Leftrightarrow E_j < E_i \Leftrightarrow \exp\left(-\frac{E_j - E_i}{k_B T}\right) > 1$

$\Rightarrow w_{ij} = 1$, $w_{ji} = \exp\left(-\frac{E_i - E_j}{k_B T}\right)$

$p_i = \exp\left(-\frac{E_i}{k_B T}\right)$, $p_j = \exp\left(-\frac{E_j}{k_B T}\right)$

$$\frac{w_{ij}}{w_{ji}} = \frac{1}{\exp\left(\frac{E_j - E_i}{k_B T}\right)} = \exp\left(\frac{E_i - E_j}{k_B T}\right)$$

$$\frac{p_j}{p_i} = \frac{\exp\left(-\frac{E_j}{k_B T}\right)}{\exp\left(-\frac{E_i}{k_B T}\right)} = \exp\left(\frac{-E_j + E_i}{k_B T}\right) = \frac{w_{ij}}{w_{ji}} \quad \checkmark$$

$\underline{\Delta E > 0} \Leftrightarrow E_i < E_j \Leftrightarrow \exp\left(-\frac{E_j - E_i}{k_B T}\right) < 1$

$\Rightarrow w_{ij} = \exp\left(-\frac{E_j - E_i}{k_B T}\right)$, $w_{ji} = 1$

$$\frac{w_{ij}}{w_{ji}} = \exp\left(\frac{E_i - E_j}{k_B T}\right) = \frac{p_j}{p_i} \quad \checkmark$$

(b) $w_{ij} = \dfrac{\exp(-\beta \Delta E)}{\exp(-\beta\Delta E)+1}$, $\Delta E = E_j - E_i$

$$w_{ji} = \frac{\exp(\beta\Delta E)}{\exp(\beta\Delta E)+1}$$

$$\rightsquigarrow \frac{w_{ij}}{w_{ji}} = \frac{\exp(-\beta\Delta E)}{\exp(-\beta\Delta E)+1} \frac{\exp(\beta\Delta E)+1}{\exp(\beta\Delta E)}$$

$$= \exp(-\beta\Delta E - \beta\Delta E) \frac{\exp(\beta\Delta E)+1}{\exp(-\beta\Delta E)+1}$$

$$= \exp(-2\beta\Delta E) \frac{\exp(\beta\Delta E)+1}{\frac{1}{\exp(\beta\Delta E)} + \frac{\exp(\beta\Delta E)}{\exp(\beta\Delta E)}}$$

$$= \exp(-2\beta\Delta E)\exp(\beta\Delta E) \frac{\exp(\beta\Delta E)+1}{\exp(\beta\Delta E)+1}$$

$$= \exp(-\beta\Delta E)$$

$\frac{p_j}{p_i} = \exp(-\beta\Delta E)$ ~~in (a) geze~~ shown in (a)

(c) $V(\vec{r}_1,\vec{r}_2) = \begin{cases} 0 & , |\vec{r}_1-\vec{r}_2| \geq \sigma \\ \infty & , |\vec{r}_1 - \vec{r}_2| < 0 \end{cases}$

the total energy E_i of system i is

$$E_i = \begin{cases} E_{kin,i} & \text{if } V(\vec{r}_{l,i},\vec{r}_{m,i})=0 \text{ for every hard disk } l \text{ and } m \text{ in system } i \\ \infty & \text{if there exist two hard disks } l \text{ and } m \text{ in system } i \text{ s.t. } V(\vec{r}_{l,i},\vec{r}_{m,i})=\infty \end{cases}$$

with $E_{kin,i} = \sum_{l=0}^{n} \frac{1}{2} m_{l,i} \dot{\vec{r}}_{l,i}^{\,2}$ ~~for every~~ , n: number of hard disks in system i
$m_{l,i}$: mass of hard disk l

the probability of being in a system i where $E_i = \infty$ is 0:

$$p_i = \lim_{E_i \to \infty} \exp(-\beta E_i) = 0$$

so we can only be in systems where $E_i = E_{kin,i}$

Metropolis criterion:

$E_j = E_{kin,j}$: $\Delta E = E_{kin,j} - E_{kin,i}$, $w_{ij} = \min(1, \exp(-\frac{\Delta E}{kT}))$

$E_j = \infty$: $w_{ij} = 0$

heat bath criterion:

$E_j = E_{kin,j}$: $\Delta E = E_{kin,j} - E_{kin,i}$, $w_{ij} = \frac{e^{-\beta \Delta E}}{e^{-\beta \Delta E} + 1}$

$E_j = \infty$: $w_{ij} = 0$

Exercise 4:

low temperature: particles barely move around, build clusters like a solid state

high temperature: particles move around very quick and chaotic, no pattern visible, like a gas state

critical temperature is around 2,3

the Wolff-algorithm is useful at temperatures around the critical temperature or at high temperatures

the metropolis algorithm is stable at all temperatures but it is very harder to see the state change at the critical temperature

(b) Metropolis:

```
possible_states [S_i]
~~init~~
current state S
sim_time T

for j in 1:T
   S_j = #random state drawn out of [S_i]
     r = #random number between 0 and 1
   w_ij = min (1, exp(-(E_Sj - E_S)/(k_B T))
   if r ≤ w_ij
      S = S_j
   end if
end
```

in 1D the ~~ba~~ Hamiltonian is given only by the interaction strength ~~of two~~ corresponds to neighbours for one particle:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \cdot \sigma_j$$

with spin-states ~~ing~~ σ_i and the sum goes over all pairs (neighbors) in the chain. J is the coupling strength

in 2D each particle has 4 neighbors ~~so the Hamiltonian changes~~ so the coupling strength may be different for vertical or horizontal coupling

$$\cancel{\mathcal{H} = -J \sum_{\langle ij \rangle} \sigma_i \cdot \sigma_j \; \text{null}}$$