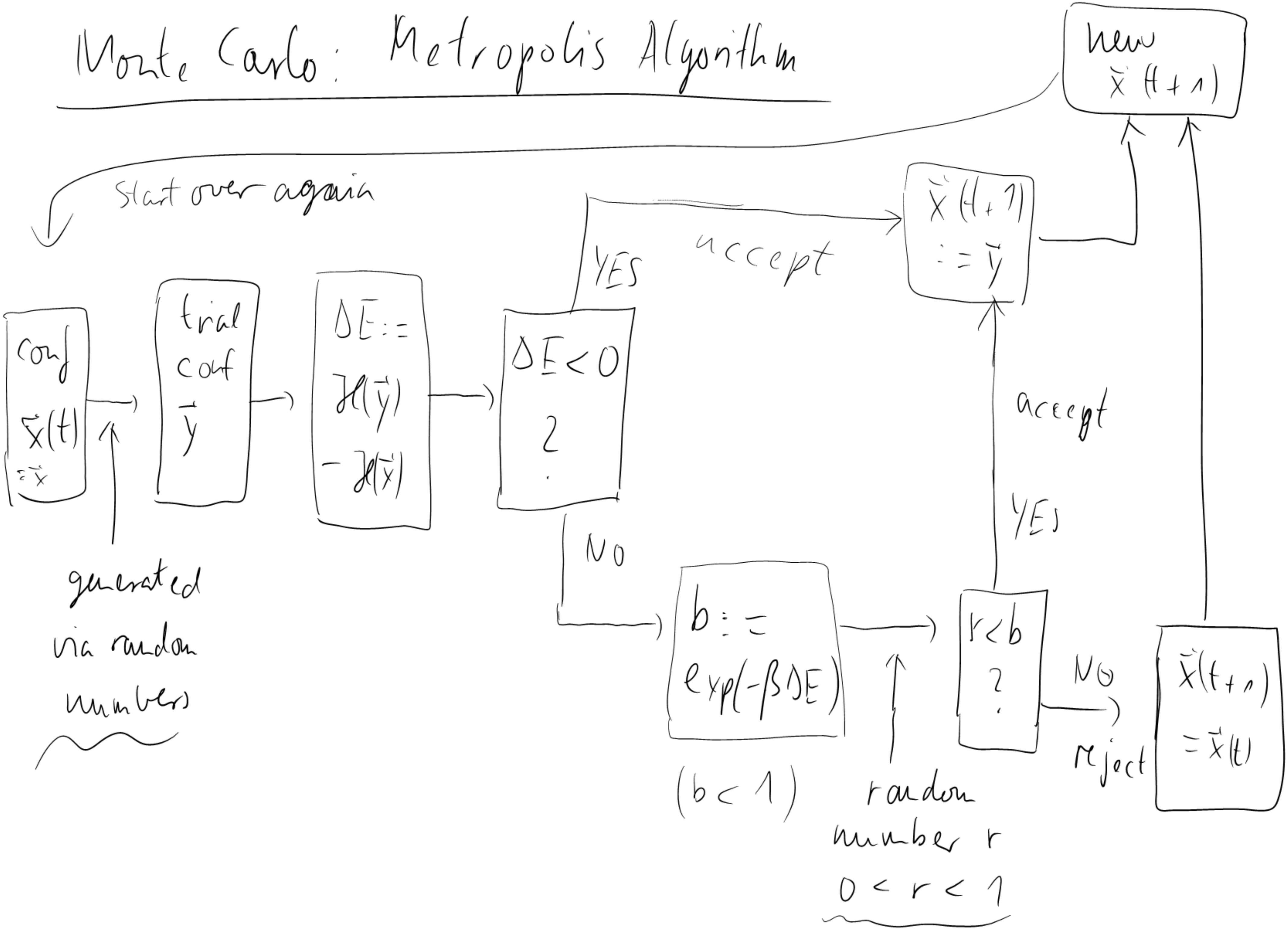
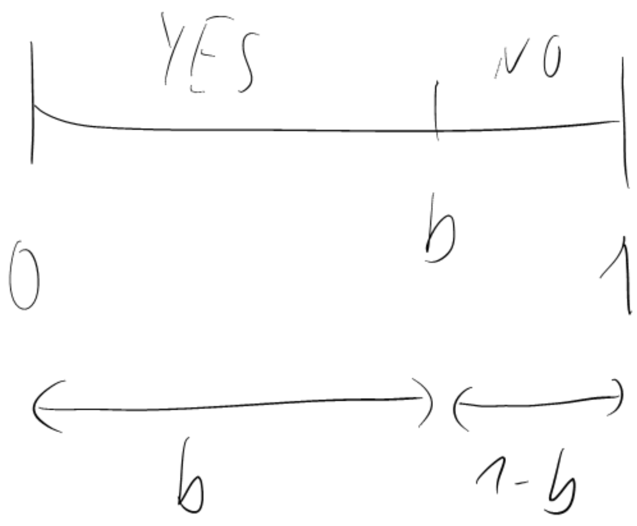
Monte Carlo: Metropolis Algorithm





Analysis:

generation of $\bar{y}$

$$w(\bar{x} \to \bar{y}) = w_{a\,priori}(\bar{x} \to \bar{y}) \times w_{acc}(\bar{x} \to \bar{y})$$

assume: $w_{a\,priori}(\bar{x} \to \bar{y}) = w_{a\,priori}(\bar{y} \to \bar{x})$

no bias in the generation. **CLAIM:**

$$P_{eq}(\bar{x})\, w(\bar{x} \to \bar{y}) = P_{eq}(\bar{y})\, w(\bar{y} \to \bar{x}) \quad \text{with}$$

$$P_{eq}(\bar{x}) = Z^{-1} \exp(-\beta \mathcal{H}(\bar{x}))$$

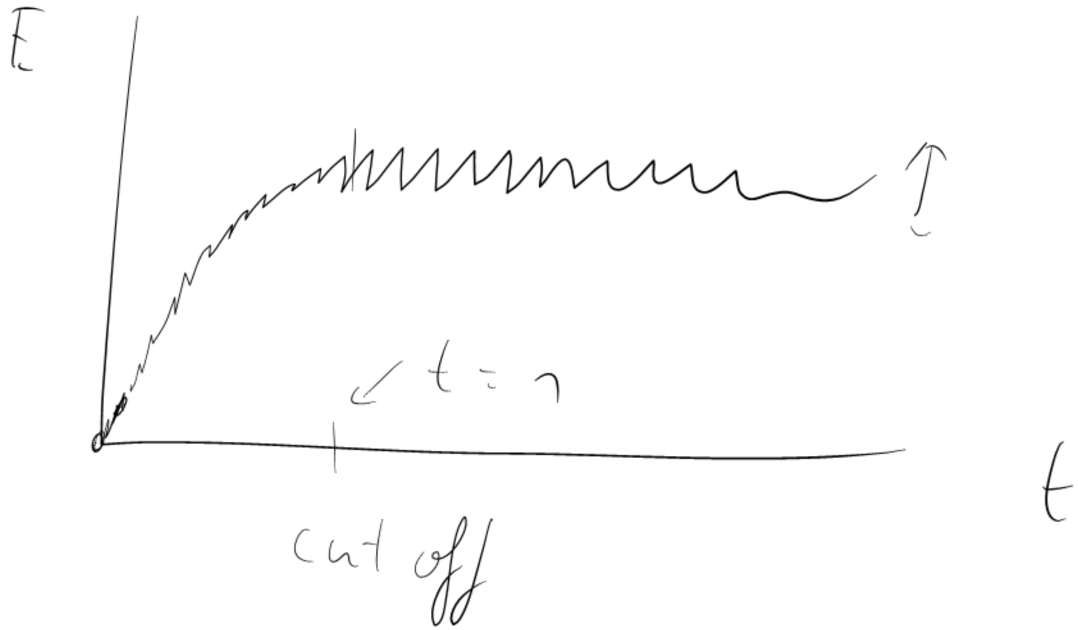
this is equivalent to

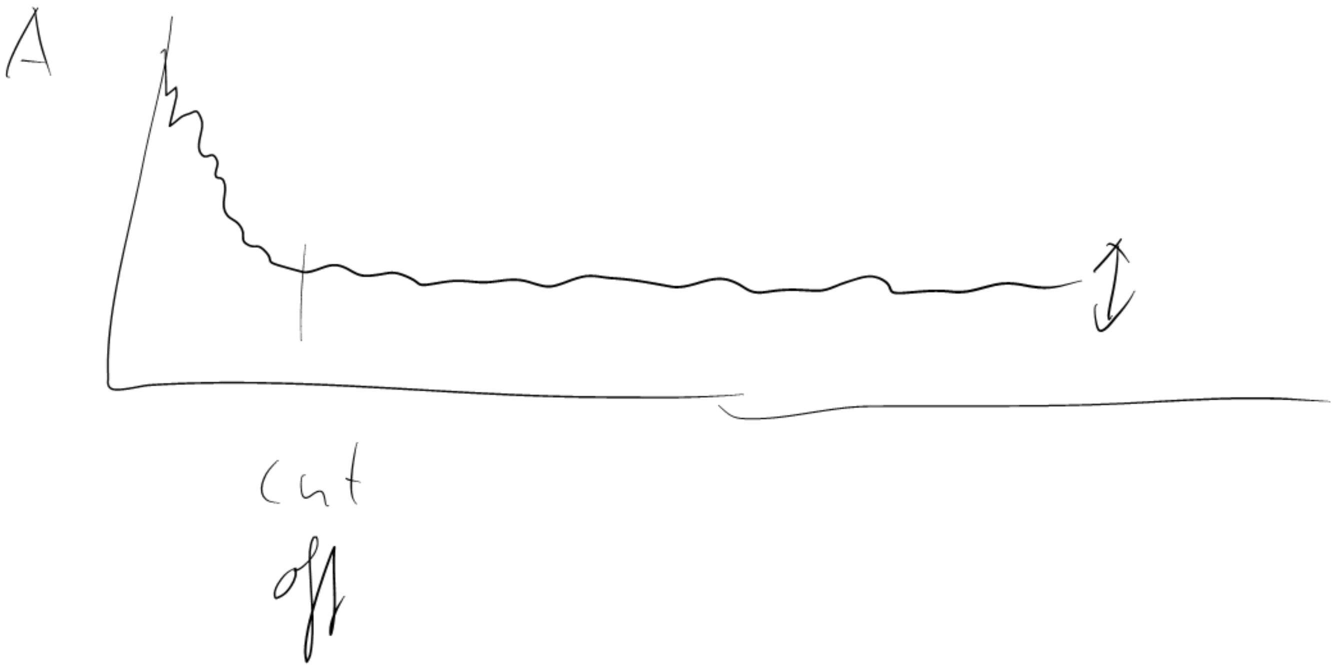
$$\exp(-\beta \mathcal{H}(\vec{x}))\, w_{acc}(\vec{x} \to \vec{y}) = \exp(-\beta \mathcal{H}(\vec{y}))\, w_{acc}(\vec{y} \to \vec{x})$$

<u>or</u> $$\frac{w_{acc}(\vec{x} \to \vec{y})}{w_{acc}(\vec{y} \to \vec{x})} = \exp(-\beta \Delta E) = \frac{\exp(-\beta \mathcal{H}(\vec{y}))}{\exp(-\beta \mathcal{H}(\vec{x}))}$$

<u>case 1:</u> $\Delta E > 0$: $$\left.\begin{aligned} w_{acc}(\vec{x} \to \vec{y}) &= \exp(-\beta \Delta E) \\ w_{acc}(\vec{y} \to \vec{x}) &= 1 \end{aligned}\right\} \text{ok} \checkmark$$

<u>case 2:</u> $\Delta E < 0$ $$\left.\begin{aligned} w_{acc}(\vec{x} \to \vec{y}) &= 1 \\ w_{acc}(\vec{y} \to \vec{x}) &= \exp(+\beta \Delta E) \end{aligned}\right\} \text{ok} \checkmark$$


E
t = 1
t
cut off

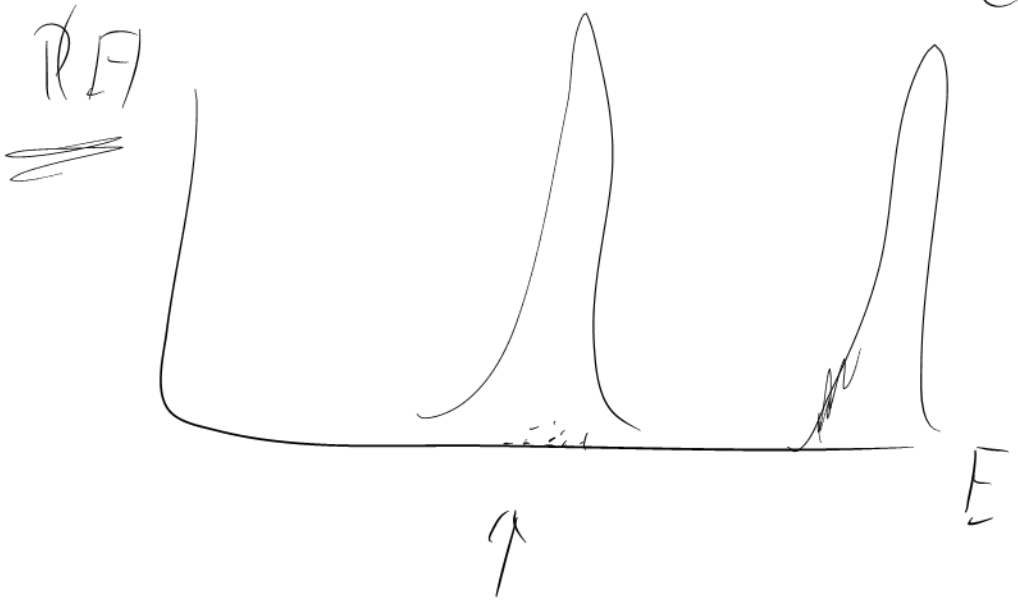

A
cut off

$$\langle A \rangle = \frac{1}{T} \sum_{t=1}^{T} A(\vec{x}(t))$$

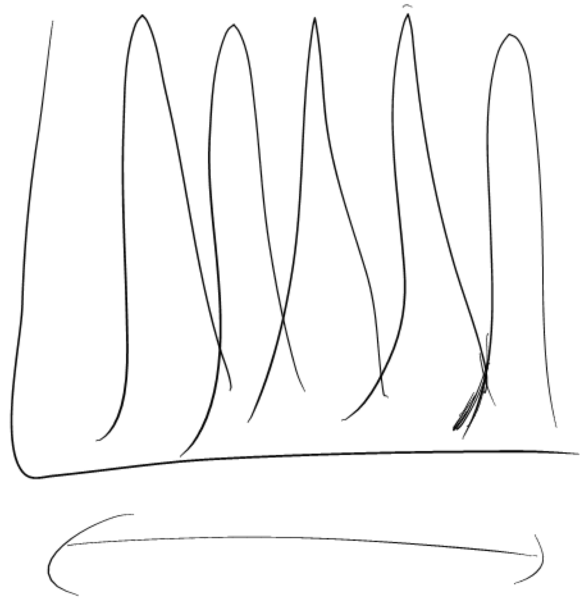
example $A = E$

simple sampling

$\beta = 0$



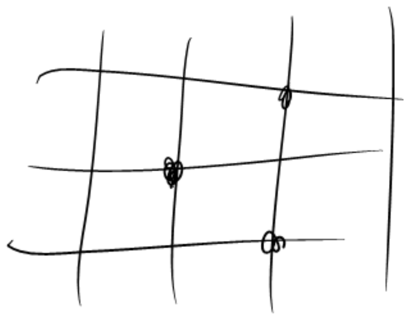
IMPORTANCE SAMPLING



1 MCS (Monte Carlo Step) "time unit" for MC simulations:

Each degree of freedom has been touched once (on average)

<u>Example</u>: <u>Hard-Sphere Lattice Gas</u>



$L \times L$ square lattice (periodic b.c.)

N particles on L^2 sites

$$\text{occupancy} = \begin{cases} 0 & \text{or} \\ 1 & \end{cases}$$

Alg. 1: - pick a particle at random
- pick a direction at random

$$\left.\begin{array}{l}\text{pick a particle at random}\\ \text{pick a direction at random}\end{array}\right\} w_{apriori} = \frac{1}{N} \cdot \frac{1}{4}$$

- if free, go there
- if not, stay where you are

$$w_{acc} = \begin{cases} 1 & \text{free} \\ 0 & \text{occupied} \end{cases}$$

$$P_{eq}(\vec{x})\, w(\vec{x} \to \vec{y}) \stackrel{??}{=} P_{eq}(\vec{y})\, w(\vec{y} \to \vec{x}) \quad \Big| : w_{apriori}$$

$$P_{eq}(\vec{x})\, w_{acc}(\vec{x} \to \vec{y}) \stackrel{?}{=} P_{eq}(\vec{y})\, w_{acc}(\vec{x} \to \vec{y})$$

Case 1: Move is possible

$$P_{eq}(\vec{x}) > 0 \,, \quad P_{eq}(\vec{y}) > 0 \,, \quad P_{eq}(\vec{x}) = P_{eq}(\vec{y})$$

$$W_{acc}(\vec{x} \to \vec{y}) = 1 \qquad W_{acc}(\vec{y} \to \vec{x}) = 1 \qquad \text{OK}$$

case 2: Move is impossible

$$P_{eq}(\vec{x}) > 0 \qquad\qquad P_{eq}(\vec{y}) = 0$$

$$\underbrace{W_{acc}(\vec{x} \to \vec{y}) = 0}_{\text{l.h.s.} = 0} \qquad \underbrace{W_{acc}(\vec{y} \to \vec{x}) \text{ is not interesting}}_{\text{r.h.s.} = 0} \qquad \text{OK}$$

Alg. 2: Replace particles by holes !

Alg. 3: Something "really smart"

- Make a list of all possible moves
- pick one of these moves at random
- do this move
- update the list

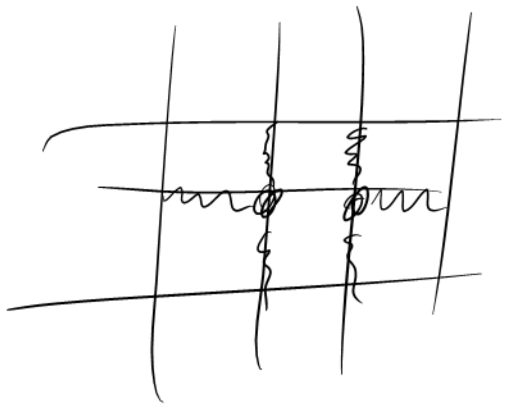
THIS VIOLATES DETAILED BALANCE !

$W_{acc} = 1$

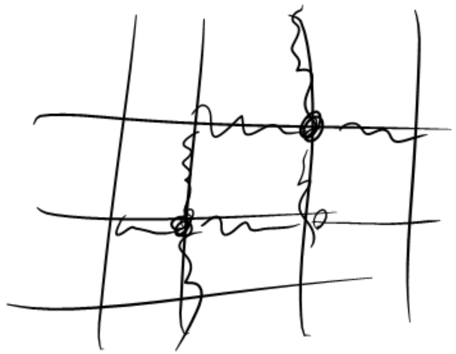
$W_{apriori} = [\text{length of the list}]^{-1}$

is NOT CONSTANT!

example:



6 possibilities

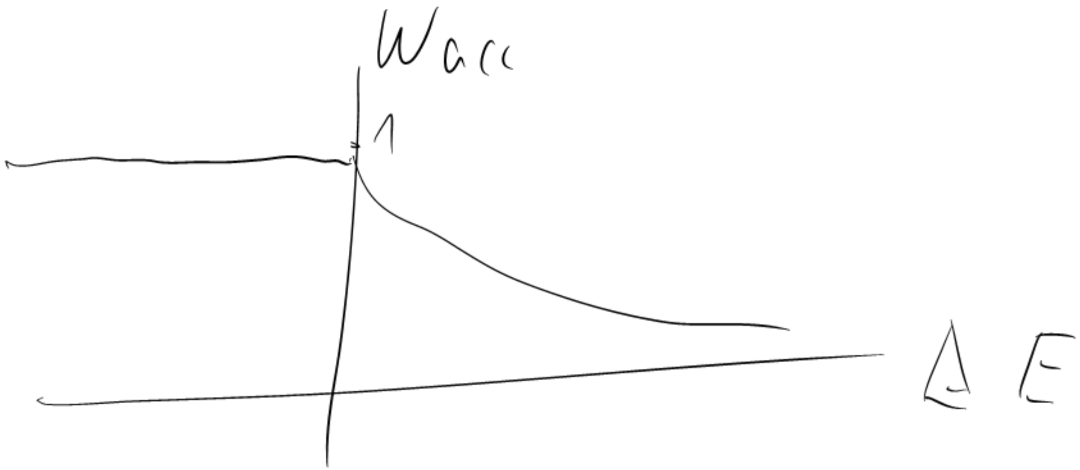


8 possibilities

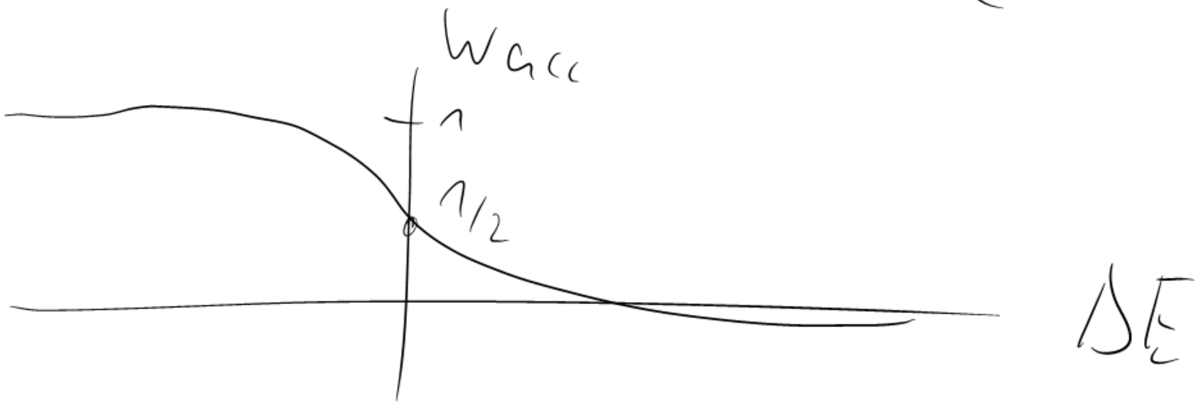
Remark: It IS possible to base MC on such event lists, but this is more complicated, involving WAITING TIME distributions → then detailed balance can be satisfied. "event-driven" simulations, "n-fold way"

[Bortz / Lebowitz / Kalos 70s]

Metropolis: $w_{acc} = \min\left(1, \exp(-\beta \Delta E)\right)$



"Heat bath" $w_{acc} = \frac{1}{2}\left[1 - \tanh\left(\frac{\beta \Delta E}{2}\right)\right]$



$$\frac{W_{acc}(\vec{x} \to \vec{y})}{W_{acc}(\vec{y} \to \vec{x})} = \frac{1 - \tanh\left(\frac{\beta \Delta E}{2}\right)}{1 + \tanh\left(\frac{\beta \Delta E}{2}\right)} =$$

$$= \frac{\cosh\left(\frac{\beta \Delta E}{2}\right) - \sinh\left(\frac{\beta \Delta E}{2}\right)}{\cosh\left(\frac{\beta \Delta E}{2}\right) + \sinh\left(\frac{\beta \Delta E}{2}\right)} =$$

$$= \frac{\exp\left(-\frac{\beta \Delta E}{2}\right)}{\exp\left(\frac{\beta \Delta E}{2}\right)} = \exp(-\beta \Delta E) \quad \text{OK}$$