transfer matrix

$$\pi(x,t+\Delta t) = \pi(x,t) - \frac{1}{2}\pi(x,t)A(x,x+\Delta x) - \frac{1}{2}\pi(x,t)A(x,x-\Delta x)$$
$$+ \frac{1}{2}\pi(x+\Delta x,t)A(x+\Delta x,x) + \frac{1}{2}\pi(x-\Delta x,t)A(x-\Delta x,x)$$
$$= \frac{1}{2}\pi(x,t)\left[2 - A(x,x+\Delta x) - A(x,x-\Delta x)\right]$$
$$+ \frac{1}{2}\pi(x+\Delta x,t)A(x+\Delta x,x) + \frac{1}{2}\pi(x-\Delta x,t)A(x-\Delta x,x)$$

discretized form: $\pi(x,t) = \pi(x_i,t_i)$, $m = \frac{L}{\Delta x}$, $x \pm \Delta x = x_i \pm \frac{L}{m} = x_{i\pm1}$,
$t \pm \Delta t = t_{n\pm1}$

$$\pi(x_i,t_{n+1}) = \frac{1}{2}\pi(x_i,t_n)\left[2 - A(x_i,x_{i+1}) - A(x_i,x_{i-1})\right]$$
$$+ \frac{1}{2}\pi(x_{i+1},t_n)A(x_{i+1},x_i) + \frac{1}{2}\pi(x_{i-1},t_n)A(x_{i-1},x_i)$$

Define: $A_{i,i+1} = A(x_i,x_{i+1})$, $A_{i,i-1} = A(x_i,x_{i-1})$
$A_{i+1,i} = A(x_{i+1},x_i)$, $A_{i-1,i} = A(x_{i-1},x_i)$
$\pi_i^{n+1} = \pi(x_i,t_{n+1})$, $\pi_{i-1}^n = \pi(x_{i-1},t_n)$ … …

$$\Rightarrow \pi_i^{n+1} = \frac{1}{2}\left[A_{i-1,i}\,\pi_{i-1}^n + (2 - A_{i,i-1} - A_{i,i+1})\,\pi_i^n + A_{i+1,i}\,\pi_{i+1}^n\right]$$

Boundary conditions:

(1) reflecting boundary at lower position x_0:
(when reach equilibrium step_in = step_out)

$$\pi_0^{n+1} = \frac{1}{2}\left[(2 - A_{0,1})\pi_0^n + A_{1,0}\pi_1^n\right]$$

reflecting boundary at upper position x_m:

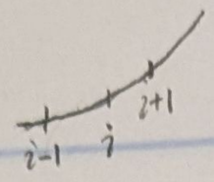
$$\pi_m^{n+1} = \frac{1}{2}\left[A_{m-1,m}\pi_{m-1}^n + (2 - A_{m,m-1})\pi_m^n\right]$$

(2) absorbing boundary at lower position x_0: $\pi_0 = 0$
absorbing boundary at upper position x_m: $\pi_m = 0$

Metro_accept: $A(a \to b) = \min\left[1, e^{-\beta(U(b)-U(a))}\right]$ ~piece_wise function

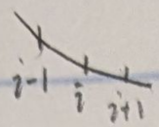
Criteria_accept: $A(a \to b) = \dfrac{e^{-\beta(U(b)-U(a))}}{1 + e^{-\beta(U(b)-U(a))}}$

$$= \frac{1}{e^{\beta(U(b)-U(a))} + 1}$$ ~ Analytical function



Metro_accept: if $U_{i+1} > U_i$: $A_{i,i+1} = e^{-\beta(U_{i+1}-U_i)}$, $A_{i+1,i} = 1$

else : $A_{i,i+1} = 1$, $A_{i+1,i} = e^{-\beta(U_i - U_{i+1})}$



if $U_{i-1} < U_i$: $A_{i,i-1} = 1$, $A_{i-1,i} = e^{-\beta(U_i - U_{i-1})}$

else : $A_{i,i-1} = e^{-\beta(U_{i-1}-U_i)}$, $A_{i-1,i} = 1$

Criteria_accept: $A_{i,i+1} = \dfrac{1}{\exp(\beta U_{i+1} - \beta U_i) + 1}$, $A_{i,i-1} = \dfrac{1}{\exp(\beta U_{i-1} - \beta U_i) + 1}$

$A_{i+1,i} = \dfrac{1}{\exp(\beta U_i - \beta U_{i+1}) + 1}$, $A_{i-1,i} = \dfrac{1}{\exp(\beta U_i - \beta U_{i-1}) + 1}$

transfer matrix:

Re

$$
\begin{pmatrix} \pi_0^{n+1} \\ \pi_1^{n+1} \\ \pi_2^{n+1} \\ \vdots \\ \pi_{m-2}^{n+1} \\ \pi_{m-1}^{n+1} \\ \pi_m^{n+1} \end{pmatrix}
= \frac{1}{2}
\begin{pmatrix}
2-A_{0,1} & A_{1,0} & & & & & \\
A_{0,1} & 2-A_{1,0}-A_{1,2} & A_{2,1} & & & & \\
 & A_{1,2} & 2-A_{2,1}-A_{2,3} & A_{3,2} & & & \\
 & & \ddots & \ddots & \ddots & & \\
 & & & A_{m-3,m-2} & 2-A_{m-2,m-3}-A_{m-2,m-1} & A_{m-1,m-2} & \\
 & & & & A_{m-2,m-1} & 2-A_{m-1,m-2}-A_{m-1,m} & A_{m,m-1} \\
 & & & & & A_{m-1,m} & 2-A_{m,m-1}
\end{pmatrix}
\begin{pmatrix} \pi_0^{n} \\ \pi_1^{n} \\ \pi_2^{n} \\ \vdots \\ \pi_{m-2}^{n} \\ \pi_{m-1}^{n} \\ \pi_m^{n} \end{pmatrix}
$$

Ab

Ab

Re