For $1 \leq i \leq N$:

\[
\frac{p_i(t + \delta t) - p_i(t)}{\delta t} = -2W p_i(t) + W(p_{i-1}(t) + p_{i+1}(t))
\]

In "continuum limit" (interested in dynamics on timescales $t \gg \delta t$), we can approximate this as:

\[
\frac{dp_i(t)}{dt} = \frac{\text{loss}}{\text{gain}} = -2W p_i(t) + W(p_{i-1}(t) + p_{i+1}(t))
\]

our first "master equation": gain-loss equation for time evolution of $p_i(t)$

Similar reasoning can apply to much more general context, where system has some set of states $i$ and undergoes random transitions between them at certain rates.

Useful for modeling many biological processes, from simple molecular diffusion to genetic regulation to spreading of epidemics.
Note that master equation in above form is valid for $1 \leq i \leq N$. What about $i=1$ or $i=N$?

\[
\begin{align*}
\frac{dP_1(t)}{dt} &= -WP_1(t) + WP_2(t) \\
\frac{dP_N(t)}{dt} &= -WP_N(t) + WP_{N-1}(t)
\end{align*}
\]

Putting everything together, the master equation looks like matrix multiplication:

\[
\frac{d\vec{P}}{dt} = \sum_{j=1}^{N} \Omega_{ij} P_j \quad \text{where} \quad \Omega_{ii} = \begin{cases} -W & i=1 \\ -2W & 1 < i < N \\ -W & i=N \end{cases} \\
\Omega_{ij} = \begin{cases} W & i=j-1 \\ W & i=j+1 \\ 0 & \text{otherwise} \end{cases}
\]

or \[
\frac{d\vec{P}}{dt} = \Omega \cdot \vec{P}
\]

where \[
\vec{P} = \begin{pmatrix} P_1 \\ P_2 \\ \vdots \\ P_N \end{pmatrix}
\]

\[
\Omega = \begin{pmatrix}
W & -W & \cdots & -W \\
-W & W & \cdots & -W \\
\vdots & \vdots & \ddots & \vdots \\
-W & -W & \cdots & W \\
\end{pmatrix}
\]

This structure of a matrix-vector equation is very general. If you have a random process with transitions between states $i=1, \ldots, N$, then
\[ \frac{dp_i}{dt} = \sum_j \Omega_{ij} p_j \]

where \( \Omega_{ij} \) = probability rate for transition from \( j \rightarrow i \) (if \( i \neq j \))

\( \Omega \) represents a network of states:

The elements of \( \Omega \) will be different for each problem we encounter. \( \Omega = \text{transition matrix} \)

What about diagonal elements \( \Omega_{ii} \)?

These have a fixed form due to the necessity of preserving the normalization of probability.

\[ \sum_i p_i(t) = 1 \text{ for all } t \]

\[ \frac{d}{dt} \sum_i p_i(t) = 0 \]

\[ \Rightarrow \sum_i \sum_j \Omega_{ij} p_j(t) = 0 \]

\[ \Rightarrow \sum_j \left[ \sum_i \Omega_{ij} \right] p_j(t) = 0 \]

This must be true for all \( p_j(t) > 0 \)

so: \[ \sum_i \Omega_{ij} = 0 \] [columns of \( \Omega \) must sum to zero]

\[ \Omega_{jj} = -\sum_{i \neq j} \Omega_{ij} = -\text{total rate of escape from state } j \]

Usually when setting up the problem, we specify \( \Omega_{ij} \) [the transition rates], and then choose \( \Omega_{jj} \) to satisfy the above requirement.
To get the MSD, we need the moments of $p_i$.

From the master equation, we can derive equations for any of the moments:

$$\langle i^n \rangle_t = \sum_{i=1}^{n} i^n p_i(t)$$

$$\frac{d \langle i^n \rangle_t}{dt} = \sum_{i} i^n \frac{dp_i}{dt}$$

$$= \sum_{i,j} i^n \Omega_{ij} P_j$$

$$= \sum_{j, i \neq j} i^n \Omega_{ij} P_j + \sum_{j} j^n \Omega_{jj} P_j$$

$$= \sum_{j, i \neq j} (i^n - j^n) \Omega_{ij} P_j$$

$$= \sum_{j} a_j^{(n)} P_j$$

where $a_j^{(n)} = \sum_{i} (i^n - j^n) \Omega_{ij}$ “jump moments”

For our diffusion transition matrix

$$a_j^{(1)} = \begin{cases} w & j=1 \\ 0 & 1 \leq j \leq N \\ -w & j=N \end{cases}$$

$$a_j^{(2)} = \begin{cases} 3w & j=1 \\ 2w & 1 \leq j \leq N \\ (1-2N)w & j=N \end{cases}$$

$$\frac{d \langle i \rangle_t}{dt} = w P_i(t) - w P_N(t)$$

$$\frac{d \langle i^2 \rangle_t}{dt} = 2w \sum_{j=2}^{N-1} P_j(t) + 3w P_i(t) + (1-2N)w P_N(t)$$