PHYS 320/420 Lecture 3

\[
\text{MSD } \langle \Delta_i^2 \rangle_t = \sum_i p_i(t) \Delta_i^2
\]

\[
\Delta_i = a(i-i_0)
\]

\[a = 1\text{nm}\]

\[t = 3\text{ s}\]

\[
\begin{array}{c|c|c}
\text{trial} & i-i_0 & a^2(i-i_0)^2 \\
1 & 3 & 9\text{ nm}^2 \\
2 & -2 & 4\text{ nm}^2 \\
\vdots & \vdots & \vdots \\
\end{array}
\]

average \( \Rightarrow \langle \Delta_i^2 \rangle_t = \text{nm} \)
Simplify dynamics temporarily to explicitly calculate MSD

\[ i \rightarrow i+1 \text{ w/ prob. 1} \]
\[ i \rightarrow i \quad \text{"""" 0} \]
\[ i \rightarrow i-1 \quad \text{"""" 0} \]

\(\Rightarrow\) non-random motion in one dir.

every trial will lead to same result (non-random)

avg. \(\Rightarrow\) same as one trial result

\[ t = m \delta t \quad (m \text{ time steps}) \]

\[ i = i_0 + m \]

\[ \Delta_i^2 = a^2 (i - i_0)^2 = a^2 m^2 = a^2 \left( \frac{t}{\delta t} \right)^2 \]

\[ \langle \Delta_i^2 \rangle_t = \frac{a^2}{\delta t^2} t^2 \propto t^2 \]

\[ \text{MSD} \propto t^2 \Rightarrow \text{ballistic motion} \]

\(\text{(directed, not random)}\)

\[ \text{MSD} \propto t \quad (\text{we will prove this}) \]

\(\Rightarrow\) diffusive motion
Where is ballistic regime relevant?

i) very short timescales $<< 10^{-16}$ s for objects in water

ii) if there is fuel source + "molecular motors"
   $\Rightarrow$ dragging cargo in one dir.

How do we prove MSD $\propto t$ in diffusive regime?

$\Rightarrow$ we will have to derive an equation for $P_i(t)$

$\Rightarrow$ master equation
\[ p_i(t + st) = p_i(t) - \left[ \text{loss in prob. due part. leaving } \right] \\
+ \left[ \text{gain in prob. due to part. entering } \right] \\
= p_i(t) - \frac{2w \cdot st \cdot p_i(t)}{\text{prob. you of left currently being in } i \text{ in } (t, t + st)} \\
+ \frac{w \cdot st \cdot p_{i-1}(t)}{i \rightarrow i \text{ jump prob.}} + \frac{w \cdot st \cdot p_{i+1}(t)}{i+1 \rightarrow i \text{ jump prob.}} \]

\[ \Rightarrow \frac{p_i(t + st) - p_i(t)}{st} = -2w p_i(t) \\
+ w \left( p_{i-1}(t) + p_{i+1}(t) \right) \]

On timescales \( t \gg st \), we can approximate time as continuous and treat the left-hand side as a derivative.
\[
\frac{dp_i(t)}{dt} = \underbrace{\text{loss}}_{\text{loss}} - 2w p_i(t) + w(p_{i-1}(t) + p_{i+1}(t))
\]

First example of "master equation"

Gain-loss eqn. for probability

Conservation eqn. for prob.

Note: System of equations for diff. \(i\), all coupled together

\[
\begin{align*}
1 \leftrightarrow 2 \quad \frac{dp_1(t)}{dt} &= -wp_1(t) + wp_2(t) \\
N-1 \leftrightarrow N \quad \frac{dp_N(t)}{dt} &= -wp_N(t) + wp_{N-1}(t)
\end{align*}
\]

N equations for funcs \(p_1(t), \ldots, p_N(t)\)

\[
\Rightarrow \text{figure out eqn's For } \langle i \rangle_t, \langle i^2 \rangle_t \text{ without solving master eqn. } \Rightarrow \text{solve those to get } \langle \Delta_i^2 \rangle_t \text{ MSD}
\]