**Schroedinger Eqn**

\[-\frac{k^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t) = \frac{-i}{\hbar} \frac{\partial}{\partial t} \psi(x,t)\]

**Diffusion Eqn**

\[\rho(x,t) = \text{concentration at } x,t\]

\[T(x,t) = \text{temperature at } x,t\]

\[D \frac{\partial^2}{\partial x^2} \rho(x,t) = \frac{\partial}{\partial t} \rho(x,t)\]

**NB**

\[\int dx \mid \psi(x,t) \mid^2 = 1\]

but

\[\int dx \rho(x,t) = 1 \quad \text{or conservation of}\]

\[\int dx \varphi(x,t) = 1 \quad \text{or conservation of}\]

**Why this form for diffusion Eqn**

\[\begin{align*}
T_{ip} & \\
\hline
\text{do not expect particles or heat flow} & \\
\frac{\partial \rho}{\partial t} & = 0
\end{align*}\]

\[\begin{align*}
\text{similary} & \\
\frac{\partial \rho}{\partial t} & = 0 \\
\text{so} & \\
\frac{\partial \rho}{\partial x} & \neq 0 \text{ does not induce} \frac{\partial \rho}{\partial t} \neq 0
\end{align*}\]

\[\text{Need} \frac{\partial^2 \rho}{\partial x^2} \neq 0\]

\[\text{sign is also correct}\]
How problem: Given \( p(x) = \delta(x) \) compute \( p(x,t) \)

**Solution:**
\[ p(x,t) = f(x)g(t) \]
\[ D f''(x) g = f g'(t) \]
\[ D f'' = \frac{g'}{g} = -Dk^2 \]
\[ f(x) = e^{ikx}, \quad g(t) = e^{-Dk^2t} \]

**General:**
\[ \int a(k) e^{ikx-Dk^2t} \frac{dk}{\sqrt{2\pi}} = p(x,t) \]
\[ a(k) = \int dx e^{-ikx} p(x,0) \sim \frac{1}{\sqrt{2\pi}} \text{ for } \delta(x) \]

\[ p(x,t) = \int \frac{dk}{2\pi} e^{ikx-Dk^2t} \]
\[ = \int \frac{dk}{2\pi} e^{-Dt(k^2 - \frac{i{kx}}{2} \frac{2}{Dt})} \]
\[ = \int \frac{dk}{2\pi} e^{-Dt(k - \frac{i}{2Dt})^2 + \frac{t}{2Dt}(\frac{i}{2Dt})^2} e^{x^2/4Dt} \]
\[ = \frac{1}{\sqrt{4\piDt}} e^{-x^2/4Dt} \]
\[ p(x,t) = \frac{1}{\sqrt{4\piDt}} e^{-x^2/4Dt} \]

Note still normalized
Numerical Solution to Diff. Eqn

- We will do this in a few weeks after learning/reviewing C.
- Prelude to Riemann problem if numerical soln of 5th Eqn?

Discretize $x \rightarrow dx$
$t \rightarrow dt$

$f(x+dx) = f(x) + f'(x)dx + \frac{1}{2} f''(x)dx^2 + \ldots$

$f(x-dx) = f(x) - f'(x)dx + \frac{1}{2} f''(x)dx^2 + \ldots$

$\Rightarrow f(x+dx) + f(x-dx) = 2f(x) + f''(x)dx^2$

$f''(x) = \frac{f(x+dx) - 2f(x) + f(x-dx)}{dx^2}$

$\Rightarrow \frac{p(x,t+dt) - p(x,t)}{dt} = d \frac{p(x+dx,t) - 2p(x,t) + p(x-dx,t)}{dx^2}$

$p(x,t+dt) = \frac{ddt}{(dx)^2} [p(x+dx,t) - 2p(x,t) + p(x-dx,t)] + p(x,t)$
Change notation to emphasize discrete $x, t$

\[ x_n = n \, dx \]

\[ t_m = m \, dt \]

\[ p(n, m+1) = \frac{D}{(dx)^2} \left[ p(n+1, m) - 2 \, p(n, m) + p(n-1, m) \right] + p(n, m) \]

Normalization \[ \sum_n p(n, m+1) = \sum_n p(n, m) \]

Why?

Save memory \[ p_{\text{new}}(n) \] just show $p$ at two times.
\[ \frac{D}{dt} \frac{\partial f}{\partial x^2} \text{ must be small} \]

Consider \[ \frac{D}{dt} \frac{\partial f}{\partial x^2} = \frac{1}{2} \]

\[ p(n, m+1) = \frac{1}{2} \left[ p(n+1, m) + p(n-1, m) \right] \]

\[ \text{new value at } n = \text{average of adjacent values earlier} \]

\( t=0 \)
\( m=0 \)
\[ \begin{array}{ccccccc}
  & n=-3 & -2 & -1 & 0 & 1 & 2 & 3 \\
(0) & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
  & 0 & 0 & 1/2 & 0 & 1/2 & 0 & 0 \\
  & 0 & 1/4 & 0 & 1/2 & 0 & 1/4 & 0 \\
  & 1/8 & 0 & 3/8 & 0 & 3/8 & 0 & 1/8 \\
\end{array} \]

* Recognize this as binomial coefficients/Pascal's triangle?*

* Relation between diffusion and random walk because if random walk with \( p(\text{left}) = p(\text{right}) = 1/2 \) would get exact same table for probabilities if these final locations*

* \( D \frac{dt}{dx^2} \approx 1/2 \) is too big. Diffusion does not have these zero values separating non-zero values*
\[ p(n, m+1) = 0.8 \ p(n, m) + 0.1 \ [ p(n+1, m) + p(n-1, m) ] \]

\[ \frac{d t}{d x}^2 = 0.1 \]

\[ \begin{array}{ccccccc}
M & -3 & -2 & -1 & 0 & 1 & 2 & 3 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 0.1 & 0.8 & 0.1 & 0 & 0 \\
2 & 0 & 0.01 & 0.16 & 0.66 & 0.16 & 0.01 & 0 \\
3 & 0.001 & 0.024 & 0.195 & 0.560 & 0.195 & 0.024 & 0.001 \\
\end{array} \]

Much more reasonable for diffusion.