

Last time: \hat{x} & \hat{p} are Fourier conjugate

using $\Psi(x,t) \times -i\hbar \frac{\partial}{\partial x} \Rightarrow \hat{E} = \hat{H} = \frac{\hat{p}^2}{2m} + V(x)$
 $= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$ (for $\Psi(x)$)

Now: Postulate 5, part 2
 Equations of motion

CM: (1) $-\frac{\partial p}{\partial t} = \frac{\partial H}{\partial x}$
 (2) $\frac{\partial x}{\partial t} = \frac{\partial H}{\partial p}$

\Rightarrow F=ma
 Verlet
 (How to do this on a computer)

QM: (1) $-\frac{\partial \psi^{(r)}}{\partial t} = \frac{\hat{H}}{\hbar} \psi^{(r)}$ (real)
 (2) $\frac{\partial \psi^{(i)}}{\partial t} = \frac{\hat{H}}{\hbar} \psi^{(i)}$ (imaginary)

Derive the Schrödinger eqn.

(1) $\hat{H} \psi^{(r)} = -\hbar \frac{\partial}{\partial t} \psi^{(r)}$

(2) $i \hat{H} \psi^{(i)} = i \hbar \frac{\partial}{\partial t} \psi^{(i)}$

add

$\hat{H} (\psi^{(r)} + i \psi^{(i)}) = i \hbar \frac{\partial}{\partial t} (\psi^{(r)} + i \psi^{(i)})$

combine
 ψ has a real part and an imaginary part

$\hat{H} \psi = i \hbar \frac{\partial}{\partial t} \psi$ → time-dependent Schrödinger eqn.

complex function w/ real & imaginary part

Easier to solve on a computer than by hand
 SUR algorithm (quantum analog of the Verlet algo)

$\frac{\partial}{\partial t} \psi^{(r)} = \frac{\psi^{(r)}(t+\Delta t) - \psi^{(r)}(t)}{\Delta t}$ [approximate derivative]

\Rightarrow $\begin{cases} \psi^{(r)}(x, t+\Delta t) = \psi^{(r)}(x, t) + \frac{\Delta t}{\hbar} \hat{H} \psi^{(i)}(x, t) \\ \psi^{(i)}(x, t+\Delta t) = \psi^{(i)}(x, t) - \frac{\Delta t}{\hbar} \hat{H} \psi^{(r)}(x, t) \end{cases}$ [Line 1 of code use postulates] [Line 2 of code]

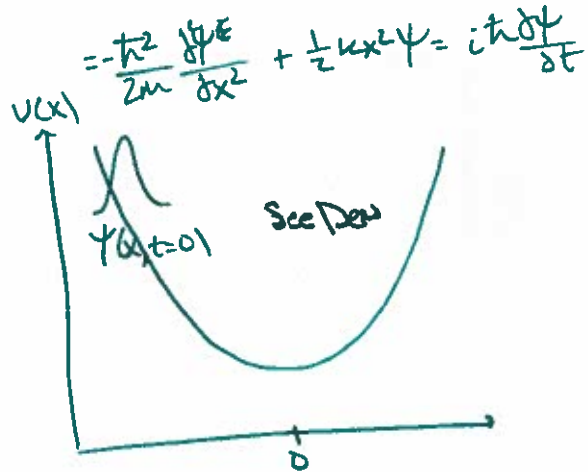
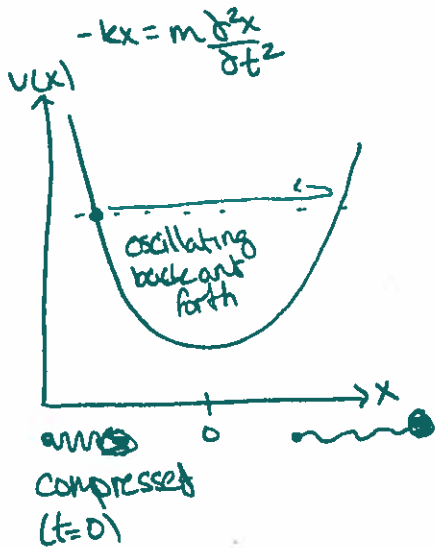
Example: Vibrating diatomic molecule = "spring"

$$F = -kx \Rightarrow V(x) = -\int F dx = \frac{1}{2} kx^2$$



In CM: plug into $F = ma$

In QM: Use Schrödinger's eqn.



$\hat{E} = i\hbar \frac{\partial}{\partial t}$ in time "representation"

similar to Fourier transform we saw previously

$\Rightarrow E \leftrightarrow \omega$ as Fourier conjugates

$$\Delta E \Delta t = \frac{\hbar}{2}; \text{ also } \Delta \omega \Delta t = \frac{1}{2} \text{ or } \Delta(\hbar\omega) \Delta t = \frac{\hbar}{2}$$

$$\Rightarrow E = \hbar\omega = \frac{\hbar}{2\pi} \frac{2\pi\omega}{\omega} \Rightarrow E = \hbar\omega \text{ (Planck's Law)}$$

Energy of any particle = to \hbar x the frequency of that particle

$$\int \int_E (\hat{H} \psi(x,t)) = i\hbar \frac{\partial}{\partial t} \psi(x,t) = \hat{H} \psi(x,E) = E \psi(x,E)$$

Time-independent Schrödinger eqn

Time-dependent & independent are Fourier Transforms of one another.