Lecture 3
Free Particle Problem

Dirac Momentum Operator:

$\hat{p}_x : -i\hbar \dfrac{d}{dx}$ → a differential operator.

Dirac Position Operator:

x : multiplication by x → usual classical mechanics position functions

This is to ensure consistency with the Heisenberg principle, i.e., $\hat{x}(\hat{p}_x \Psi) - \hat{p}_x(\hat{x}\,\Psi) \neq 0$.

The action of these operators (for example) can be understood in terms of their effect on a function:

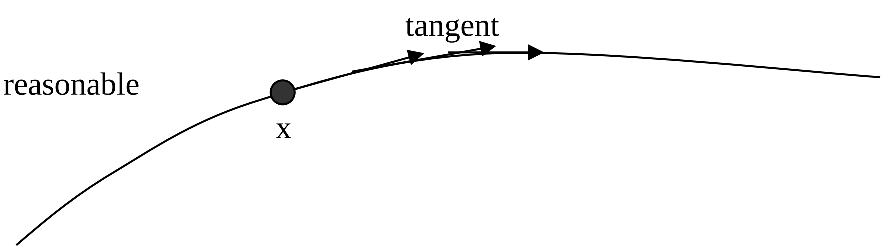
$$x\,f(x) = xf(x) \qquad \text{If } f(x) = x+1\text{, then } x\,f(x) = x^2 + x$$

$$\hat{p}_x\,f(x) = -i\hbar\frac{d}{dx}\,f(x) = -i\hbar$$

Logically possible Motivation for the choice (not a proof)

$\hat{p}_x$ (momentum) generates translations in x. In general, one can do this by drawing the tangent at position x and taking an incremental step along the tangent.

Thus $\dfrac{d}{dx}$ is reasonable



$\hbar$ needed for dimensionality and de-Broglie $\lambda = \dfrac{h}{p}$

What about $i = \sqrt{-1}$? [Needed to keep the measurable values real…]

With these details, we can now construct $\hat{H}$:

$$\underset{\substack{\text{Kinetic}\\ \text{operator}}}{\hat{H} = \hat{T}} \quad + \quad \underset{\substack{\text{Potential}\\ \text{operator}}}{\hat{V}}$$

From Classical Mechanics in one dimension,

$$H = \frac{1}{2m} p_x^2 + V(x)\,; \quad m = \text{mass}$$

To turn it into operators in Quantum Mechanics, we “put hats”

$$\hat{H}\ddot{x} = \frac{1}{2m} \hat{p}_x^2 + \hat{V}(x)$$

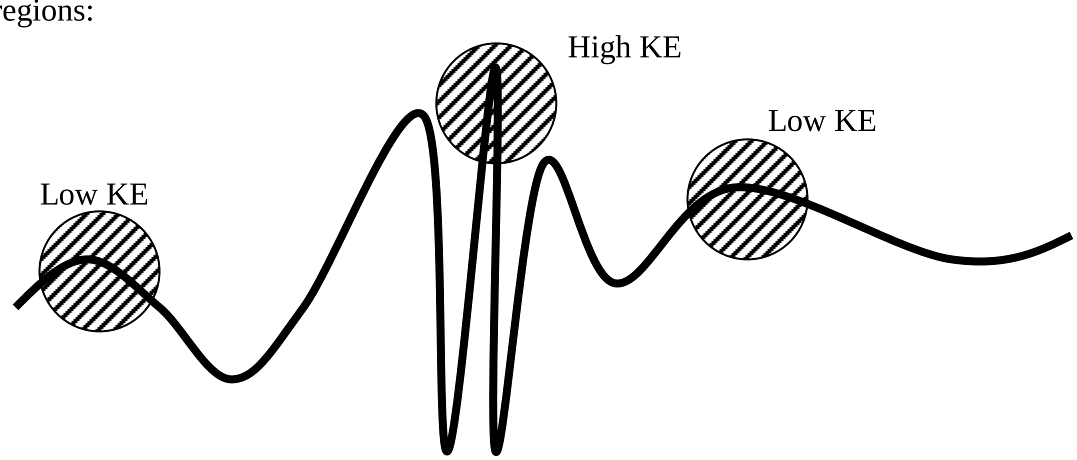
Note: $\hat{p}_x^2$ means $\hat{p}_x \hat{p}_x$, i.e., apply $\hat{p}_x$ twice.

$$\therefore \quad \hat{H} = \left(\frac{1}{2m}\right)\left(-i\hbar \frac{d}{dx}\right)\left(-i\hbar \frac{d}{dx}\right) + \hat{V}(x) = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{K} + \hat{V}(x)$$

Note: 2nd order derivative & not $\left(\frac{d}{dx}\right)^2$

$\therefore \quad \hat{T}\Psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx}$ $\Rightarrow$ In quantum mechanics, the kinetic energy is related to the <u>curvature</u> of the wavefunction $\Psi(x)$.

Pictorially, therefore, if $\Psi(x)$ looks as below which can be correlated to the low and high energy regions:



Thus, solving for $\hat{H}\Psi = E\Psi$ means solving the differential equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + \hat{V}(x)\Psi(x) = E\Psi(x)$$

Given a specific V(x) and E, we would like to solve for the state $\Psi(x)$ of the quantum system. $\Psi(x)$ is known as the wave function.

In quantum mechanics, once you know Ψ for a system, then all the observables for the system can be determined (Like in classical mechanics, once you know {x(t),p_x(t)} then you know everything about the system).

However, determining Ψ can be quite difficult and it turns out that, in general, Ψ can be complex!

CASE 1

Free particle in one dimension:

No force is acting $\Rightarrow$ V(x) = constant $\equiv 0$

Then: $-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi(x)$

which is a simple linear 2nd order differential equation and we can solve this exactly.

Rewriting the above expression, we get:

$$\frac{d^2\Psi}{dx^2} = -\left(\sqrt{\frac{2mE}{\hbar^2}}\right)^2 \Psi(x) \equiv -k^2\Psi(x)\text{, where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

The general solution for this 2nd order differential equation is:

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}$$

Plane wave moving to “right” | Plane wave moving to “left”

a positive term before the x means a wave travelling towards positive x (i.e. right) & vice versa

Wavefunction is a complex function…

Interpretation?

Max Born’s probability density…

An interpretation of wave function was provided by Max Born (1926). For a one-dimensional case, probability of finding a particle between x and x + dx is given by

$\left|\Psi(x)\right|^2 dx \equiv \Psi^*(x)\Psi(x)dx,$ where $\Psi^*(x)$ is the complex conjugate of $\Psi(x)$. Thus, $\left|\Psi(x)\right|^2$ is the probability density that the particle is in state *y*(x) and position x.

If the particles are moving from right to the left initially, then A = 0, B ≠ 0

Similarly, if the particles are moving from left to the right initially, then A ≠ 0, B = 0

$$\Psi(x) = Ae^{ikx}$$

Note that a positive term before the x means a wave travelling towards positive x. To measure energy, we apply $\hat{H}$ on $\Psi(x)$, i.e.,

$$\hat{H}\Psi(x) \equiv -\frac{\hbar^2}{2m}\frac{d^2Be^{-ikx}}{dx^2} = \left(\frac{\hbar^2k^2}{2m}\right)\left(Be^{-ikx}\right) \equiv \left(\frac{\hbar^2k^2}{2m}\right)\Psi(x)$$

$$\text{Thus, } E = \frac{\hbar^2k^2}{2m}$$

⇒ that if a particle has momentum $p_x = \pm\hbar k$, then the corresponding energy is given by $\frac{p_x^2}{2m}$.

There is no difference from classical mechanics (CM) since here in quantum mechanics (QM) case also p_x can take arbitrary values (integer, non-integer) & we get continuous energy values.

From a wavefunction view, the higher is the momentum indicating massive particles (or CM), higher is the energy and the wavefunction "wiggles" around a lot more. This also follows from the fact that higher energy requires more curvature in the wavefunction resulting in the "wiggles". If we look at the real part of Ψ, i.e., $A\cos\left(kx\right)$, the oscillatory part, i.e., the cosine function can be rewritten as $\cos\left(\frac{p_x.x}{\hbar}\right) \approx \cos\left(\frac{x}{\lambda_{de-Broglie}}\right)$ bringing back the de-Broglie prediction that as particles get massive the associated wavelength gets smaller and smaller to be insignificant !

However, all these will change as soon as this free particle is "confined" to certain part in space!

We deal with that in the next class.