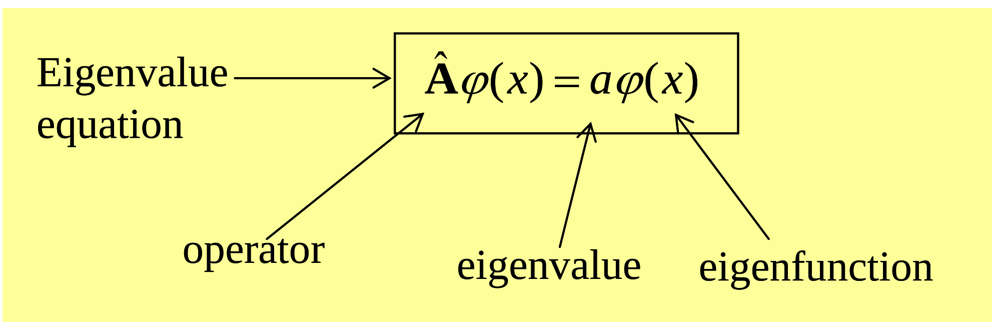
The Postulates of Quantum Mechanics
Operators, Eigenfunctions, Eigenvalues

Newtonian Physics – quantities of position, $\vec{x}$, momentum, $\vec{p}$, energy, E, number of particles, angular momentum, $\vec{J}$

From Liboff Section 3.1 Observables and Operators: 'This postulate states the following: To any self-consistently and well-defined observable in physics (call it A), such as linear momentum, energy, mass, angular momentum, or number of particles, there corresponds an operator (call it $\hat{\mathbf{A}}$) such that measurement of A yields values (call these measured values a) which are eigenvalues of $\hat{\mathbf{A}}$.

Operator (general) $\hat{\mathbf{A}}$ has an eigenvalue equation:



Examples of operators:

$$\hat{\mathbf{D}} = \frac{\partial}{\partial x} \qquad \Rightarrow \hat{\mathbf{D}}\varphi(x) = \frac{\partial \varphi(x)}{\partial x}$$

$$\hat{\Delta} = -\frac{\partial^2}{\partial x^2} = -\hat{\mathbf{D}}^2 \qquad \Rightarrow \hat{\Delta}\varphi(x) = -\frac{\partial^2 \varphi(x)}{\partial x^2}$$

Definition of Linear Operator

$$\hat{\mathbf{O}}(a\varphi_1 + b\varphi_2) = a\hat{\mathbf{O}}\varphi_1 + b\hat{\mathbf{O}}\varphi_2$$

After learning the definition of a linear operator, Dr. Shen gave us a few minutes to work through the Problem 3.3 which is to determine which operators in Table 3.1 (page 69) are linear operators. This gave us better insight into how the operator math works.

<u>These are the linear operators:</u>

$$\hat{\mathbf{D}}(a\varphi_1 + b\varphi_2) = \frac{\partial}{\partial x}(a\varphi_1 + b\varphi_2) = (a\frac{\partial}{\partial x}\varphi_1 + b\frac{\partial}{\partial x}\varphi_2) = a\hat{\mathbf{D}}\varphi_1 + b\hat{\mathbf{D}}\varphi_2$$

$$\hat{\Delta}(a\varphi_1 + b\varphi_2) = \frac{\partial^2}{\partial x^2}(a\varphi_1 + b\varphi_2) = (a\frac{\partial^2}{\partial x^2}\varphi_1 + b\frac{\partial^2}{\partial x^2}\varphi_2) = a\hat{\Delta}\varphi_1 + b\hat{\Delta}\varphi_2$$

$$\hat{\mathbf{M}}(a\varphi_1 + b\varphi_2) = \frac{\partial^2}{\partial x\partial y}(a\varphi_1 + b\varphi_2) = (a\frac{\partial^2}{\partial x\partial y}\varphi_1 + b\frac{\partial^2}{\partial x\partial y}\varphi_2) = a\hat{\mathbf{M}}\varphi_1 + b\hat{\mathbf{M}}\varphi_2$$

$$\hat{\mathbf{I}}(a\varphi_1 + b\varphi_2) = \hat{\mathbf{I}}a\varphi_1 + \hat{\mathbf{I}}b\varphi_2 = (a\varphi_1 + b\varphi_2) = a\hat{\mathbf{I}}\varphi_1 + b\hat{\mathbf{I}}\varphi_2$$

$$\hat{\mathbf{Q}}(a\varphi_1 + b\varphi_2) = \int_0^1 dx'(a\varphi_1 + b\varphi_2) = (a\int_0^1 dx'\varphi_1 + b\int_0^1 dx'\varphi_2) = a\hat{\mathbf{Q}}\varphi_1 + b\hat{\mathbf{Q}}\varphi_2$$

$$\hat{\mathbf{F}}(a\varphi_1 + b\varphi_2) = F(x)(a\varphi_1 + b\varphi_2) = (aF(x)\varphi_1 + bF(x)\varphi_2) = a\hat{\mathbf{F}}\varphi_1 + b\hat{\mathbf{F}}\varphi_2$$

$$\hat{\mathbf{B}}(a\varphi_1 + b\varphi_2) = \frac{1}{3}(a\varphi_1 + b\varphi_2) = (a\frac{1}{3}\varphi_1 + b\frac{1}{3}\varphi_2) = a\hat{\mathbf{B}}\varphi_1 + b\hat{\mathbf{B}}\varphi_2$$

$$\hat{\Theta}(a\varphi_1 + b\varphi_2) = \hat{\Theta}a\varphi_1 + \hat{\Theta}b\varphi_2 = 0 = a\hat{\Theta}\varphi_1 + b\hat{\Theta}\varphi_2$$

<u>These are the non-linear operators:</u>

$$\hat{\mathbf{P}}\varphi = \varphi^3 - 3\varphi^2 - 4$$

$$\hat{\mathbf{P}}(a\varphi_1 + b\varphi_2) = \hat{\mathbf{P}}a\varphi_1 + \hat{\mathbf{P}}b\varphi_2 = a^3\varphi_1^3 - 3a^2\varphi_1^2 - 4 + b^3\varphi_2^3 - 3b^2\varphi_2^2 - 4$$

$$a\hat{\mathbf{P}}\varphi_1 + b\hat{\mathbf{P}}\varphi_2 = a\varphi_1^3 - 3a\varphi_1^2 - 4a + b\varphi_2^3 - 3b\varphi_2^2 - 4b$$

$$\hat{\mathbf{P}}(a\varphi_1 + b\varphi_2) \neq a\hat{\mathbf{P}}\varphi_1 + b\hat{\mathbf{P}}\varphi_2$$

$$\hat{\mathbf{G}}\varphi = 8$$

$$\hat{\mathbf{G}}(a\varphi_1 + b\varphi_2) = \hat{\mathbf{G}}a\varphi_1 + \hat{\mathbf{G}}b\varphi_2 = 8 + 8$$

$$a\hat{\mathbf{G}}\varphi_1 + b\hat{\mathbf{G}}\varphi_2 = 8a + 8b$$

$$\hat{\mathbf{G}}(a\varphi_1 + b\varphi_2) \neq a\hat{\mathbf{G}}\varphi_1 + b\hat{\mathbf{G}}\varphi_2$$

Operator for Linear Momentum

$$\hat{p} = -i\hbar\nabla$$

$$\hat{p}\varphi = -i\hbar\nabla\varphi = p\varphi \qquad \vec{\nabla} = \hat{\mathbf{i}}\frac{\partial}{\partial x} + \hat{\mathbf{j}}\frac{\partial}{\partial y} + \hat{\mathbf{k}}\frac{\partial}{\partial z}$$

"particle constrained to move in one dimension..."

$$\hat{p}\varphi = -i\hbar\frac{\partial}{\partial x}\varphi = p_x\varphi$$

"when you learn math, you know how to solve..."

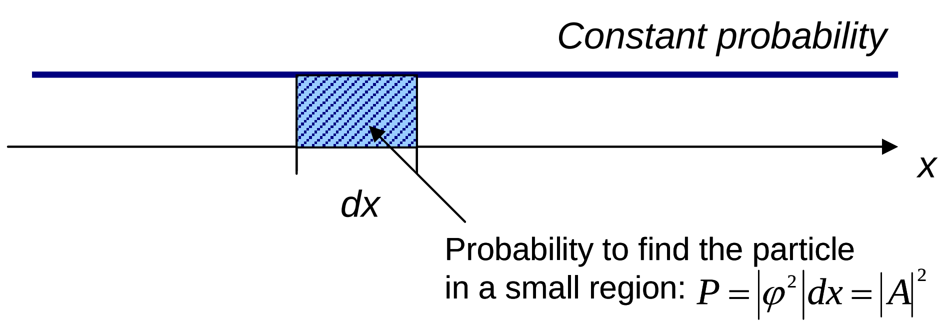
$$\varphi = A\exp\left(\frac{ip_x x}{\hbar}\right) = Ae^{ikx}$$

the eigenvalue $p_x = \hbar k$

“Let’s talk about the meaning of the wavefunction…”

Free particle unconstrained with no boundary conditions in x-direction

$$\varphi = A\exp\left(\frac{ip_x x}{\hbar}\right) = Ae^{ikx}$$



Δp=0 $\quad$ $\Delta p\Delta x$ can’t be defined at the same time

Δx=∞ $\quad$ – Heisenberg’s equation

$$\Delta p\Delta x \geq \hbar$$

$$\varphi(x+\lambda) = \varphi(x)$$

‘Wave’ Function: $Ae^{ik(x+\lambda)} = Ae^{ikx}e^{ik\lambda} = Ae^{ikx}$ $\qquad k\lambda = 2\pi \qquad \lambda = \dfrac{2\pi}{k}$

$$\lambda = \frac{h}{p}$$ de Broglie hypothesis

Operator for Energy – Generally write the Hamiltonian

$$\hat{H} = -\frac{p_x^2}{2m} + V(x) \qquad \text{one - dimensional}$$

$$p^2 = \left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right) = -\hbar^2\frac{\partial^2}{\partial x^2}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \qquad \text{one - dimensional}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(x) \qquad \text{three - dimensional}$$

Hamiltonian operator and eigenvalue equation

$$\hat{H}\varphi(x) = E\varphi(x) \quad \text{Time - Independent Schrodinger Equation}$$

For simplicity: particle in free space (V(x)=0), one-dimensional

$$\hat{H}\varphi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2} = E\varphi(x)$$

$$k^2 = \frac{2mE}{\hbar^2}$$

$$\frac{\partial^2\varphi(x)}{\partial x^2} + k^2\varphi(x) = 0$$

Solve to get standing wave (please review mathematics):

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

Ae^{ikx} is motion in positive x - direction

Be^{-ikx} is motion in negative x - direction

$$\hat{p}\varphi = \hbar k\varphi$$

$$\hat{H}\varphi = \frac{p}{2m}(\hat{p}\varphi) = \frac{\hat{p}(\hbar k\varphi)}{2m} = \frac{\hbar k}{2m}(\hat{p}\varphi) = \frac{(\hbar k)^2}{2m}\varphi$$

☼ **Homework: Please solve the free particle (no potential in free space) by yourself – do the math for all the operations. Give a proof that the Hamiltonian and the linear momentum operators for a free particle have common eigenfunctions. 3.6, 3.7**

Measurement in Quantum Mechanics – Postulate

One particle can exist in many possible states:

$$\varphi(x) = \sum_n c_n \varphi_n(x)$$

Postulate as written in Section 3.2: "Measurement of the observable A that yields the value a leaves the system in the state φ_A, where φ_A is the eigenfunction of $\hat{\mathbf{A}}$ that corresponds to the eigenvalue a.

$$\hat{H}\varphi_i = E_i \varphi_i$$

Dirac Delta Function

Consider $\hat{x}$ - if you measure a system and find the particle at position *x*, it will remain at *x*. The operator equation is:

$$\hat{x}\delta(x - x') = x'\delta(x - x')$$

The original definition of the Delta function:

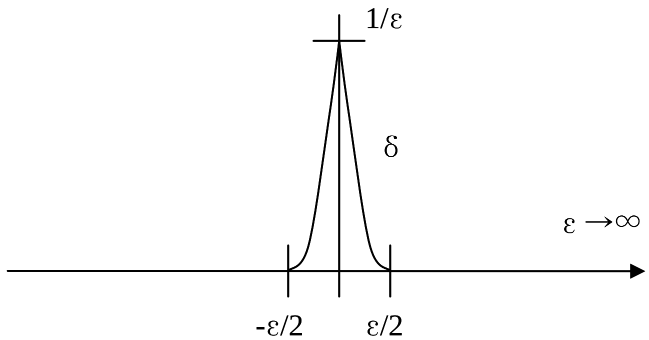
$$\int_{-\infty}^{\infty} f(x')\delta(x - x')dx' = f(x)$$

$$\int_{-\infty}^{\infty} \delta(x - x')dx' = 1$$

In terms of a single variable:

$$\int_{-\infty}^{\infty} f(y)\delta(y)dy = f(0)$$

$$\int_{-\infty}^{\infty} \delta(y)dy = 1$$



Use integration by parts [(vu)'=v'u+vu'] and the definition of the Delta function to show that $y\delta'(y) = -\delta(y)$, note $fy\delta\Big|_{-\infty}^{\infty} = 0$:

$$\int_{-\infty}^{\infty} f(y)y\delta'(y)dy = \int_{-\infty}^{\infty} \frac{d}{dy}(fy\delta)dy - \int_{-\infty}^{\infty} \delta \frac{d}{dy}(yf)dy = -\int_{-\infty}^{\infty} \delta(y)\left(\delta\frac{df}{dy} + f\right)dy = -\int_{-\infty}^{\infty} \delta(y)f(y)dy$$