Lecture 5

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Practice Problem

When a particle of mass 9.1×10^{-28} g in a certain one-dimensional box goes from the $n=5$ level to the $n=2$ level, it emits a photon of frequency $6.0\times10^{14}\ s^{-1}$. Find the length of the box.

$$\cancel{h}\nu = (n_{upper}^2 - n_{lower}^2)\frac{h^{\cancel{2}}}{8ml^2}$$

$$l^2 = \frac{21h}{8m\nu}$$

$$l = \left(\frac{21}{8}\,\frac{6.626\times10^{-34}\ \cancel{kg}\cdot m^2\cdot \cancel{s^{-1}}}{9.1\times10^{-31}\ \cancel{kg}\cdot 6.0\times10^{14}\ \cancel{s^{-1}}}\right)^{\frac{1}{2}}$$

$$l = 1.78\times10^{-9}\ m$$ ← round to two significant figures

$$\boxed{l = 1.8\ nm}$$

Operators Continued

Distributive identities

$$(\hat{A}+\hat{B})\hat{C} = \hat{A}\hat{C} + \hat{B}\hat{C}$$ ← prove this identity

$$\hat{A}(\hat{B}+\hat{C}) = \hat{A}\hat{B} + \hat{A}\hat{C}$$

$$[(\hat{A}+\hat{B})\hat{C}]f = (\hat{A}\hat{C} + \hat{B}\hat{C})f$$

$$[(\hat{A}+\hat{B})\hat{C}]f = (\hat{A}+\hat{B})\underbrace{(\hat{C}f)}_{\text{result is a function}}$$

Definition from the last lecture:

$$(\hat{A}+\hat{B})f(x) \equiv \hat{A}f(x) + \hat{B}f(x)$$

$$[(\hat{A}+\hat{B})\hat{C}]f = \hat{A}(\hat{C}f) + \hat{B}(\hat{C}f)$$

Another definition from the last lecture:

$$\hat{A}\hat{B}f(x) \equiv \hat{A}[\hat{B}f(x)]$$

$$[(\hat{A}+\hat{B})\hat{C}]f = \hat{A}\hat{C}f + \hat{B}\hat{C}f$$

$$[(\hat{A}+\hat{B})\hat{C}]f = (\hat{A}\hat{C} + \hat{B}\hat{C})f$$

$$\boxed{\therefore (\hat{A}+\hat{B})\hat{C} = \hat{A}\hat{C} + \hat{B}\hat{C}}$$

Find the square of the operator

$\frac{d}{dx} + \hat{x}$.

Define $\hat{D} \equiv \frac{d}{dx}$; apply $(\hat{D}+\hat{x})^2$ to an arbitrary function $f(x)$.

$$(\hat{D}+\hat{x})^2 f(x) = (\hat{D}+\hat{x})[(\hat{D}+\hat{x})f]$$

$$= (\hat{D}+\hat{x})(f' + xf)$$

$$\boxed{\hat{x} \equiv x.}$$

$$= f'' + f + xf' + xf' + x^2 f$$

$$= (\hat{D}^2 + 2\hat{x}\hat{D} + \hat{x}^2 + 1)f(x)$$

$$\boxed{(\hat{D}+\hat{x})^2 = \hat{D}^2 + 2\hat{x}\hat{D} + \hat{x}^2 + 1}$$

$$(a+b)^2 = a^2 + 2ab + b^2$$

3.2 Eigenfunctions and Eigenvalues

$$\boxed{\hat{A} f(x) = \overbrace{k}^{\text{eigenvalue}} \underbrace{f(x)}_{\text{eigenfunction}}}$$

"Eigen" : German for "characteristic"

For example:

$$\frac{d}{dx} e^{2x} = \boxed{2}\boxed{e^{2x}}$$

If $f(x)$ is an eigenfunction of the linear operator $\hat{A}$ and c is any constant, prove that $cf(x)$ is an eigenfunction of $\hat{A}$ with the same eigenvalue as $f(x)$.

Definition for linear operators from the last lecture:

$A(bf) = bAf$

counterexample : $\sin(2x) \neq 2\sin(x)$

Need to prove $\hat{A}(cf) = k(cf)$

$$\hat{A}(cf) = c\hat{A}f = ckf = k(cf)$$

$$\boxed{\therefore \hat{A}(cf) = k(cf)}$$

Practice Problem

a) Find the eigenfunctions and eigenvalues of the operator $\frac{d}{dx}$.

$$\hat{A}f(x) = kf(x)$$

$$\frac{d\,f(x)}{\boxed{dx}} = k\boxed{f(x)}$$

$$\frac{1}{f(x)}\,d\,f(x) = k\,dx$$

$$\int \frac{1}{f(x)} df(x) = k \int dx$$

$$\ln f(x) = kx + \text{constant}$$

$$f(x) = e^{kx + \text{constant}}$$

$$\boxed{f(x) = ce^{kx}}$$

b) If we impose the boundary condition that the eigenfunctions remain finite as $x \to \pm\infty$, find the eigenvalues.

$$k = a + ib$$

$$f(x) = c\boxed{e^{ax}}\,e^{ibx}$$

If $a < 0$, then $f(x) \to \infty$ as $x \to -\infty$

If $a > 0$, then $f(x) \to \infty$ as $x \to \infty$

$\therefore$ $a = 0$, $\boxed{k = ib}$

Commutators Revisited

On a Rubik's cube, a commutator is in the form

R L R' L' Jorja

R U R' U' Kate

r R r' R' Thomas

Operations that overlap completely or do not overlap at all commute; operations that partially overlap do not commute.

3.3 Operators and Quantum Mechanics

Linear momentum in classical mechanics

$$P_x \equiv m v_x, \quad P_y \equiv m v_y, \quad P_z \equiv m v_z$$

$$v_x = \frac{P_x}{\ldots}, \quad T = \frac{1}{2} m v_x^2$$

$$H = \frac{p_x^2}{2m} + V(x)$$

In quantum mechanics,

$$\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}, \quad \hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}, \quad \hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

$$\frac{\hbar}{i}\cdot\frac{i}{i} = \frac{i\hbar}{i^2} = -i\hbar$$

$$\hat{p}_x = -i\hbar\frac{\partial}{\partial x}, \quad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}, \quad \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$

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

$$\hat{p}_y^2 = -\hbar^2\frac{\partial^2}{\partial y^2}, \quad \hat{p}_z^2 = -\hbar^2\frac{\partial^2}{\partial z^2}$$

$$\boxed{\hat{V}(x) = V(x)\cdot} \quad \boxed{\hat{T} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}$$

$$\boxed{\hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)}$$

Is $\Psi(x)$ for the one-dimensional PIAB an eigenfunction of $\hat{p}_x$?

$$\Psi(x) = \left(\frac{2}{\ell}\right)^{\frac{1}{2}} \sin\left(\frac{n\pi x}{\ell}\right)$$

$$\hat{p}_x \Psi(x) = -i\hbar \frac{d}{dx}\left[\left(\frac{2}{\ell}\right)^{\frac{1}{2}} \sin\left(\frac{n\pi x}{\ell}\right)\right]$$

$$\hat{p}_x \Psi(x) = -\frac{n\pi i\hbar}{\ell}\left(\frac{2}{\ell}\right)^{\frac{1}{2}} \cos\left(\frac{n\pi x}{\ell}\right)$$

$$\hat{p}_x \Psi(x) \neq k\Psi(x)$$

$\therefore$ $\Psi(x)$ for PIAB is <u>not</u> an eigenfunction of $\hat{p}_x$.

Despite this, whenever we make a measurement for p_x, we must still get one of the eigenvalues for $\hat{p}_x$.

$$\hat{p}_x^2 \Psi(x) = -\hbar^2 \frac{d^2}{dx^2}\left[\left(\frac{2}{\ell}\right)^{\frac{1}{2}} \sin\left(\frac{n\pi x}{\ell}\right)\right]$$

$$= \frac{n^2\pi^2\hbar^2}{\ell^2}\left(\frac{2}{\ell}\right)^{\frac{1}{2}}\sin\left(\frac{n\pi x}{\ell}\right)$$

$$\therefore \hat{p}_x^2\,\psi(x) = \frac{n^2h^2}{4\ell^2}\psi(x)$$

$$E = \frac{n^2h^2}{8m\ell^2}$$

$\psi(x)$ is an eigenfunction of $\hat{p}_x^2$.

Notation for a three-dimensional, many-particle system:

Laplacian operator, ∇^2

$$\boxed{\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}}$$

One particle in three dimensions:

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(x,y,z)\psi = E\psi$$

n-particles in three dimensions :

$$\hat{T} = \underbrace{-\frac{\hbar^2}{2m_1}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2}\right)}_{\text{particle 1}}$$

$$\underbrace{-\frac{\hbar^2}{2m_2}\left(\frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2}\right)}_{\text{particle 2}} - \ldots$$

$$\underbrace{-\frac{\hbar^2}{2m_n}\left(\frac{\partial^2}{\partial x_n^2} + \frac{\partial^2}{\partial y_n^2} + \frac{\partial^2}{\partial z_n^2}\right)}_{\text{particle n}}$$

$$\hat{T} = -\sum_{i=1}^{n} \frac{\hbar^2}{2m_i} \nabla_i^2$$

$$\boxed{\hat{H} = -\sum_{i=1}^{n} \frac{\hbar^2}{2m_i} \nabla_i^2 + V(x_1, y_1, \ldots z_n)}$$