Quantum Mechanics Tutorial III

Engineering Physics

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Operators in Quantum Mechanics:

- Operators are the tools that extract the information from the wavefunction.
- An operator $\hat{A}$ may be thought of as "something" that operates on a function to produce another function:

$$\hat{A}\, f(x) = g(x)$$

Where, f & g are the functions of x.

- In most cases, the operators in quantum mechanics are linear. The linear operators have the following properties:

$$\hat{A}\,[f(x) + g(x)] = \hat{A}f(x) + \hat{A}g(x)$$

$$\hat{A}\,[cf(x)] = c\,\hat{A}f(x)$$

where c is a constant (c can be a complex number: c = a + ib, i = √ (-1)

Linear operators:

- x (multiplication by x):

$$x[f(x) + g(x)] = xf(x) + xg(x)$$

- d/dx (differentiation with respect to x):

$$\frac{d}{dx}[f(x) + g(x)] = \frac{d}{dx}f(x) + \frac{d}{dx}g(x)$$

A nonlinear operators:

- √ (square root operator):

$$\sqrt{f(x) + g(x)} \neq \sqrt{f(x)} + \sqrt{g(x)}$$

Operators associated with various observable quantities:

$f(x)$	Any function of position, such as x, or potential V(x)	$f(x)$
p_x	x component of momentum (y and z same form)	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
E	Hamiltonian (time independent)	$\frac{p_{op}^2}{2m} + V(x)$
E	Hamiltonian (time dependent)	$i\hbar\frac{\partial}{\partial t}$
KE	Kinetic energy	$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
L_z	z component of angular momentum	$-i\hbar\frac{\partial}{\partial \phi}$

Eigenvalues and Eigenfunctions:

An *Eigenfunction* of an operator $\hat{A}$ is a function Ψ such that the application of $\hat{A}$ on Ψ gives Ψ times a constant.

$$\hat{A}\,\Psi = k\,\Psi$$

where k is a constant called the *eigenvalue*.

Examples:

- The operator d/dx has an eigenfunction e^{kx} with eigenvalue k :

$$d/dx\,(e^{kx}) = ke^{kx}$$

- The operator d^2/dx^2 has a set of eigenfunctions of the form {cos kx; k = real number} and $-k^2$ is the eigenvalue:

$$d^2/dx^2\,[\cos kx] = d/dx\,[-k \sin kx] = -k^2[\cos kx]$$

➢ **Now check $[coskx + isinkx]$ is eigenfunction for operator d^2/dx^2 or not?**

Expectation value:

Suppose $\hat{A}$ is a quantum mechanical operator and Ψ is the wavefunction. Then, the expectation value of A is given by the following expression:

$$< A > = \frac{\int_{-\infty}^{+\infty} \Psi^*(x)\, \hat{A}\, \Psi(x)\, dx}{\int_{-\infty}^{+\infty} \Psi^*(x)\, \Psi(x)\, dx}$$

Since the wavefunction must be normalized,

$$\int_{-\infty}^{+\infty} \Psi^*(x)\, \Psi(x)\, dx = 1$$

$$\therefore < A > = \int_{-\infty}^{+\infty} \Psi^*(x)\, \hat{A}\, \Psi(x)\, dx$$

Useful Integral:

Gamma functions: $\Gamma(n) = \int_0^{\infty} x^{n-1} e^{-x} dx$ for $n > 0, \Gamma(n+1) = n\Gamma(n)$;

$\Gamma(n) = (n-1)!$ for n is poistive integer. $\Gamma(1) = 1$ and $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$

- A particle considered to move along x-axis in the domain $0 \le x \le L$ has a wave function $\psi(x) = N \sin\left(\frac{n\pi x}{L}\right)$, where n is an integer. Normalize the wave function and find the expression for N and evaluate the expectation value of its momentum. [Note: N is known as normalization constant]

The normalization condition gives

$$\int_{-\infty}^{\infty} \Psi^* \Psi\, dx = 1$$

For this wave function

$$N^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \quad \text{or} \quad N^2 \int_0^L \frac{1}{2}\left(1 - \cos\frac{2n\pi x}{L}\right) dx = 1$$

Then,

$$N^2 \frac{L}{2} = 1 \quad \text{or} \quad N = \sqrt{\frac{2}{L}}$$

So now the normalized wave function is,

$$\sqrt{\frac{2}{L}} \sin(n\pi x/L)$$

The momentum operator is defined as-

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

$$\therefore < \hat{p}_x > = \int_0^L \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi\, dx = -i\hbar \frac{2}{L} \frac{n\pi}{L} \int_0^L \sin\frac{n\pi x}{L} \cos\frac{n\pi x}{L} dx = -i\hbar \frac{n\pi}{L^2} \int_0^L \sin\frac{2n\pi x}{L} dx = 0$$

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➢ Obtain an expression for the energy levels (in MeV) of a neutron confined to a one dimensional box $1.00 \times 10^{14}\ m$ wide. What is the neutron's minimum energy?

We know that the allowed energies for a particle in a box: $E_n = \frac{n^2h^2}{8mL^2}$ n=1,2,3,...

Each permitted energy is called an energy level and integer n that specifies an energy level E_n is called its quantum number.

Mass of neutron $m = 1.67 \times 10^{27}\ kg$, Width of box $L = 1.00 \times 10^{12}\ m$

$$\therefore E_n = \frac{n^2h^2}{8mL^2}$$

$$= \frac{(n^2)(6.63 \times 10^{-34}\ \mathrm{J.s})^2}{8(1.67 \times 10^{-27}\mathrm{kg})(1.0 \times 10^{-12}\ \mathrm{m})^2}$$

$$= 20.5\ n^2\ \mathrm{MeV}$$

The minimum energy, corresponding to n = 1 , is 20.5 MeV.

➢ A proton in a one dimensional box has an energy of 400 keV in its first excited state. How wide is the box?

From the expression of energy, we have

$$L = n\sqrt{\frac{h^2}{8\ m\ E_n}}$$

The first excited state corresponds to n =2 .

$$\therefore L = 2\sqrt{\frac{(6.63 \times 10^{-34}\ \mathrm{J.s})^2}{8\ (1.67 \times 10^{-27}\mathrm{kg})\ (400 \times 10^3\ eV)\ (1.6 \times 10^{-19}\ J/eV)}}$$

$= 4.53 \times 10^{-14}\ m$

$= 45.3\ fm$

(1) A particle of mass m, which moves freely inside an infinite potential well of length a, has the following initial wave function at t = 0

$$\psi(x,0) = \frac{A}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right)$$

where A is real constant.

(a) find A so that $\psi(x,0)$ is normalized.

(b) If measurement of energy are carried out, what are the values that will be found and what are the corresponding probabilities? Calculate the average energy

(c) find the wave function $\psi(x,t)$ at any letter time t.

(d) Determine the probability of finding the system at a time t in the state $\phi(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{5\pi x}{a}\right) e^{-\frac{iE_5 t}{\hbar}}$; then determine the probability of finding it in the state $\chi(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) e^{-\frac{iE_2 t}{\hbar}}$.

Solution: Since the function

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad \text{--- (1)}$$

$$\psi(x,0) = \frac{A}{\sqrt{2}} \phi_1(x) + \sqrt{\frac{3}{10}} \phi_3(x) + \frac{1}{\sqrt{10}} \phi_5(x) \quad \text{--- (2)}$$

(a) Normalization of above equation

$$\int_0^a \psi^*(x,0)\, \psi(x,0)\, dx = 1$$

$$\int_0^a \left\{ \frac{A}{\sqrt{2}} \phi_1(x) + \sqrt{\frac{3}{10}} \phi_3(x) + \frac{1}{\sqrt{10}} \phi_5(x) \right\}^* \left\{ \frac{A}{\sqrt{2}} \phi_1(x) + \sqrt{\frac{3}{10}} \phi_3(x) + \frac{1}{\sqrt{10}} \phi_5(x) \right\} dx = 1$$

$$\frac{A^2}{2}\int_0^a \phi_1^*(x)\,\phi_1(x)\,dx + \frac{3}{10}\int_0^a \phi_3^*(x)\,\phi_3(x)\,dx + \frac{1}{10}\int_0^a \phi_5^*(x)\,\phi_5(x)\,dx = 1$$

$$\frac{A^2}{2} + \frac{3}{10} + \frac{1}{10} = 1$$

$$A = \sqrt{\frac{6}{5}} \quad \text{hence}$$

$$\psi(x,0) = \sqrt{\frac{3}{5}}\,\phi_1(x) + \sqrt{\frac{3}{10}}\,\phi_3(x) + \frac{1}{\sqrt{10}}\,\phi_5(x) \qquad (3)$$

(b) – Hamiltonian of free particle is $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$, the expectation value of $\hat{H}$ with respect to $\phi_n(x)$ is

$$E = \int_0^a \phi_n^*(x)\,\langle H\rangle\,\phi_n(x)\,dx$$

$$E = \int_0^a \left\{\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\right\}^* \left\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right\}\left\{\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\right\} dx$$

$$= -\frac{\hbar^2}{ma}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\times\left\{-\sin\left(\frac{n\pi x}{a}\right)\left(\frac{n\pi}{a}\right)^2\right\} dx$$

$$= \frac{n^2\pi^2\hbar^2}{ma^3}\int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$= \frac{n^2\pi^2\hbar^2}{ma^3}\left\{a/2\right\} = \frac{n^2\pi^2\hbar^2}{2ma^2} \qquad (4)$$

If measurement is carried out on the system, we would obtain $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$ with a corresponding probability of $P_n(E) = |\langle\phi_n|\psi\rangle|^2$. Since the initial wave function (3) contains only three eigen-states of $\hat{H}$, $\phi_1(x)$, $\phi_3(x)$, and $\phi_5(x)$, the result of

The energy measurements along with the corresponding probabilities are

$E_1 = \frac{\pi^2 \hbar^2}{2ma^2}$, $E_2 = \frac{9\pi^2\hbar^2}{2ma^2}$, $E_3 = \frac{25\pi^2\hbar^2}{2ma^2}$

$P_1(E_1) = |\langle\phi_1|\psi\rangle|^2 = \frac{3}{5}$

$P_3(E_3) = |\langle\phi_3|\psi\rangle|^2 = \frac{3}{10}$

$P_5(E_5) = |\langle\phi_5|\psi\rangle|^2 = \frac{1}{10}$

The average energy is

$$E = \sum_n P_n E_n = \frac{3}{5}E_1 + \frac{3}{10}E_3 + \frac{1}{10}E_5 = \frac{29\pi^2\hbar^2}{10ma^2}$$

(c) As the initial state $\psi(x,0)$ is given be eq. (3), the wave function $\psi(x,t)$ at any letter time t is

$$\psi(x,t) = \sqrt{\frac{3}{5}}\,\phi_1(x)\,e^{-\frac{iE_1t}{\hbar}} + \sqrt{\frac{3}{10}}\,\phi_3(x)\,e^{-\frac{iE_3t}{\hbar}} + \frac{1}{\sqrt{10}}\,\phi_5(x)\,e^{-\frac{iE_5t}{\hbar}} \quad \text{--- (4)}$$

Put all the corresponding values.

(d) first, let us express $\phi(x,t)$ in terms of $\phi_n(x)$

$$\phi(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{5\pi x}{a}\right)e^{-\frac{iE_5t}{\hbar}} = \phi_5(x)\,e^{-\frac{iE_5t}{\hbar}} \quad \text{--- (5)}$$

The probability of finding the system at a time t in the state $\phi(x,t)$ is

$$P = |\langle\phi|\psi\rangle|^2 = \left|\int_0^a \phi^*(x,t)\,\psi(x,t)\,dx\right|^2$$

$= \frac{1}{10} \left| \int_0^a \phi_5^*(x)\, \phi_5(x)\, dx \right|^2 = \frac{1}{10}$

since $\langle \phi | \phi_1 \rangle = \langle \phi | \phi_3 \rangle = 0$ and $\langle \phi | \phi_5 \rangle = e^{\frac{iE_5 t}{\hbar}} \frac{1}{10}$

Similarly, since $\chi(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \exp\left(-\frac{iE_2 t}{\hbar}\right)$

$= \phi_2(x) \exp\left(-\frac{iE_2 t}{\hbar}\right)$, we

can easily show that the probability for finding the system in the state $\chi(x,t)$ is zero:

$$P = |\langle \chi | \psi \rangle|^2 = \left| \int_0^a \chi^*(x,t)\, \psi(x,t)\, dx \right|^2 = 0$$

since $\langle \chi | \phi_1 \rangle = \langle \chi | \phi_3 \rangle = \langle \chi | \phi_5 \rangle = 0$

(2) — A particle of mass m, which moves freely inside an infinite potential well of length a, is initially in the state

$$\psi(x,0) = \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right)$$

(a) find $\psi(x,t)$ at any ~~left~~ later time t

(b) Calculate the probability density $\rho(x,t)$ and the current density, $\vec{J}(x,t)$.

(c) Verify that the probability is conserved i.e. $\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{J}(x,t) = 0$

Solution:-

(a) Since $\psi(x,0)$ can be expressed in terms of $\phi_n(x)$

$= \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$ as

$$\psi(x,0) = \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right) \quad \text{--- (1)}$$

$$= \sqrt{\frac{3}{10}}\, \phi_3(x) + \frac{1}{\sqrt{10}}\, \phi_5(x)$$

we can write

$$\psi(x,t) = \sqrt{\frac{3}{5a}} \sin\left(\frac{3\pi x}{a}\right) e^{-\frac{iE_3 t}{\hbar}} + \frac{1}{\sqrt{5a}} \sin\left(\frac{5\pi x}{a}\right) e^{-\frac{iE_5 t}{\hbar}}$$

$$= \sqrt{\frac{3}{10}}\, \phi_3(x)\, e^{-\frac{iE_3 t}{\hbar}} + \frac{1}{\sqrt{10}}\, \phi_5(x)\, e^{-\frac{iE_5 t}{\hbar}} \quad \text{--- (2)}$$

we have $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$

(b) Since $\rho(x,t) = \cancel{\psi^*(x,t)\,\psi(x,t)}\ \psi^*(x,t)\,\psi(x,t)$

using eq. (2)

$$\rho(x,t) = \left(\sqrt{\frac{3}{10}}\, \phi_3(x)\, e^{\frac{iE_3 t}{\hbar}} + \frac{1}{\sqrt{10}}\, \phi_5(x)\, e^{\frac{iE_5 t}{\hbar}}\right) \times$$
$$\left(\sqrt{\frac{3}{10}}\, \phi_3(x)\, e^{-\frac{iE_3 t}{\hbar}} + \frac{1}{\sqrt{10}}\, \phi_5(x)\, e^{-\frac{iE_5 t}{\hbar}}\right)$$

$$= \frac{3}{10}\phi_3^2(x) + \frac{\sqrt{3}}{10}\phi_3(x)\,\phi_5(x)\left[e^{i(E_3-E_5)t/\hbar} + e^{-i(E_3-E_5)t/\hbar}\right] + \frac{1}{10}\phi_5^2(x)$$

Since $E_3 - E_5 = 9E_1 - 25E_1 = -16E_1$

$$= \frac{-8\pi^2\hbar^2}{ma^2}$$

$$\rho(x,t) = \frac{3}{10}\phi_3^2(x) + \frac{\sqrt{3}}{5}\phi_3(x)\,\phi_5(x)\cos\left(\frac{16E_1 t}{\hbar}\right) + \frac{1}{10}\phi_5^2(x)$$

$$= \frac{3}{5a}\sin^2\left(\frac{3\pi x}{a}\right) + \frac{2\sqrt{3}}{5a}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\cos\left(\frac{16E_1 t}{\hbar}\right)$$

$$+ \frac{1}{5a}\sin^2\left(\frac{5\pi x}{a}\right) \quad \text{——— (3)}$$

Since the system is one-dimensional, the action of the gradient operator on $\psi(x,t)$ and $\psi^*(x,t)$ is given by $\vec{\nabla}\psi(x,t) = \left(\frac{d\psi(x,t)}{dx}\right)\vec{i}$ and $\vec{\nabla}\psi^*(x,t) = \left(\frac{d\psi^*(x,t)}{dx}\right)\vec{i}$

we can thus write the current density

$$\vec{J}(x,t) = \frac{i\hbar}{2m}\left(\psi(x,t)\frac{d\psi^*(x,t)}{dx} - \psi^*(x,t)\frac{d\psi(x,t)}{dx}\right)\vec{i} \quad \text{——— (3a)}$$

using eq. (2) we have

$$\frac{d\psi(x,t)}{dt} = \frac{3\pi}{a}\sqrt{\frac{3}{5a}}\cos\left(\frac{3\pi x}{a}\right)e^{-\frac{iE_3 t}{\hbar}} + \frac{5\pi}{a}\frac{1}{\sqrt{5a}}\cos\left(\frac{5\pi x}{a}\right)e^{-\frac{iE_5 t}{\hbar}} \quad \text{——— (4)}$$

$$\frac{d\psi^*(x,t)}{dt} = \frac{3\pi}{a}\sqrt{\frac{3}{5a}}\cos\left(\frac{3\pi x}{a}\right)e^{\frac{iE_3 t}{\hbar}} + \frac{5\pi}{a}\frac{1}{\sqrt{5a}}\cos\left(\frac{5\pi x}{a}\right)e^{\frac{iE_5 t}{\hbar}} \quad \text{——— (6)}$$

So

$$\psi\frac{d\psi^*}{dx} - \psi^*\frac{d\psi}{dx} = -2i\pi\frac{\sqrt{3}}{5a^2}\left[5\sin\left(\frac{3\pi x}{a}\right)\cos\left(\frac{5\pi x}{a}\right) - 3\sin\left(\frac{5\pi x}{a}\right)\cos\left(\frac{3\pi x}{a}\right)\right]\times\sin\left(\frac{E_3 - E_5}{\hbar}t\right) \quad \text{——— (7)}$$

Inserting (7) into (3a)

$$\vec{J}(x,t) = -\frac{\pi\hbar}{m}\frac{\sqrt{3}}{5a^2}\left[5\sin\left(\frac{3\pi x}{a}\right)\cos\left(\frac{5\pi x}{a}\right) - 3\sin\left(\frac{5\pi x}{a}\right)\cdot\cos\left(\frac{3\pi x}{a}\right)\right]\sin\left(\frac{16E_1 t}{\hbar}\right)\vec{i} \quad \text{——— (8)}$$

(c) Performing the time derivative of (3) and using expression $\frac{32\sqrt{3}E_1}{5a\hbar} = \frac{16\pi^2\hbar\sqrt{3}}{(5ma^3)}$, since $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$, we obtain

$$\frac{\partial \rho}{\partial t} = -\frac{32\sqrt{3}E_1}{5a\hbar}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\sin\left(\frac{16E_1 t}{\hbar}\right)$$

$$= \frac{-16\pi^2\hbar\sqrt{3}}{5ma^2}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\sin\left(\frac{16E_1 t}{\hbar}\right) \longleftarrow (9)$$

Now taking the divergence of (8), we end up with

$$\vec{\nabla}\cdot\vec{J}(x,t) = \frac{dJ(x,t)}{dx}$$

$$= \frac{16\pi^2\hbar\sqrt{3}}{5ma^2}\sin\left(\frac{3\pi x}{a}\right)\sin\left(\frac{5\pi x}{a}\right)\sin\left(\frac{16E_1 t}{\hbar}\right) \longleftarrow (10)$$

The addition of (9) and (10) confirms the conservation of probability

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}\cdot\vec{J}(x,t) = 0 \quad \text{——— (11)}$$

(i) $f(x)$ = Any function of position, such as x, or potential $V(x)$ $f(x)$

$$p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$E = \frac{p_{op}^2}{2m} + V(x) \quad \text{(time independent)}$$

$$E = i\hbar\frac{\partial}{\partial t} \quad \text{(time dependent)}$$

$$K.E = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

① $\frac{d}{dx}(e^{kx}) = ke^{kx}$

② $\frac{d^2}{dx^2}(\cos kx) = -k^2 \cos kx$

③ $\cos kx + i \sin kx$ is the eigen function for operator $\frac{d^2}{dx^2}$ or not

Expectation value :-

Suppose $\hat{A}$ is a quantum mechanical