PYL101: Electromagnetic waves and Quantum Mechanics

Lecture 4

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Rules and properties of the wave function

- Recall that there is Heisenberg's formalism of quantum mechanics (in terms of matrices), then Schrodinger's quantum mechanics in terms of wave functions and finally Dirac's bra-ket formalism.
- In this course we will stick to Schrodinger's quantum mechanics, i.e., wave mechanics, however it will be nice to take 'wave functions' and 'bra-ket' pictures all along while discussing some of the properties of the quantum states.

There are some notions that we need to be familiar with such as abstract Hilbert space and so on, we will talk about them also.

- Expectation values

For $A\psi(\vec{r}) = a\psi(\vec{r})$

$$\int_{-\infty}^{+\infty} \psi^*(\vec{r})\{A\psi(\vec{r})\}d^3r = a$$

The same is

$$< A > = < A >_{\psi(\vec{r})} = < \psi | A | \psi >$$

In general, matrix elements

$$< \phi | A | \psi >$$

Rules and properties of the wave function

Let's talk about things in one-dimension, all these can be generalized in higher dimensions

In Hilbert or vector space

Colum /row vectors

$$\psi(x,t) = \ < x,t \mid \psi > \ = \ \mid \psi > \quad \text{ket}$$

$$\psi^*(x,t) = \ < \psi \mid x,t > \ = \ < \psi \mid \quad \text{bra}$$

- If a wave function is normalized (represents one state of the system) at time t = 0, it will remain so for any time t later.

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

- Scalar/inner product of wave functions (normalized or not):

$$\left(\psi_1(x),\psi_2(x)\right) = \left(\psi_1^*(x)\psi_2(x)\right) = \ < \psi_1 \mid \psi_2 >$$

Rules and properties of the wave function

Problem :

Consider a system whose state is given in terms of an orthonormal set of three vectors: $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ as

$$|\psi\rangle = \frac{\sqrt{3}}{3}|\phi_1\rangle + \frac{2}{3}|\phi_2\rangle + \frac{\sqrt{2}}{3}|\phi_3\rangle.$$

(a) Verify that $|\psi\rangle$ is normalized. Then, calculate the probability of finding the system in any one of the states $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$. Verify that the total probability is equal to one.

(b) Consider now an ensemble of 810 identical systems, each one of them in the state $|\psi\rangle$. If measurements are done on all of them, how many systems will be found in each of the states $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$?

Solution :

(a) Using the orthonormality condition $\langle\phi_j|\phi_k\rangle = \delta_{jk}$ where $j, k = 1, 2, 3$, we can verify that $|\psi\rangle$ is normalized:

$$\langle\psi|\psi\rangle = \frac{1}{3}\langle\phi_1|\phi_1\rangle + \frac{4}{9}\langle\phi_2|\phi_2\rangle + \frac{2}{9}\langle\phi_3|\phi_3\rangle = \frac{1}{3} + \frac{4}{9} + \frac{2}{9} = 1.$$

Rules and properties of the wave function

Since $|\psi\rangle$ is normalized, the probability of finding the system in $|\phi_1\rangle$ is given by

$$P_1 = |\langle\phi_1|\psi\rangle|^2 = \left|\frac{\sqrt{3}}{3}\langle\phi_1|\phi_1\rangle + \frac{2}{3}\langle\phi_1|\phi_2\rangle + \frac{\sqrt{2}}{3}\langle\phi_1|\phi_3\rangle\right|^2 = \frac{1}{3},$$

since $\langle\phi_1|\phi_1\rangle = 1$ and $\langle\phi_1|\phi_2\rangle = \langle\phi_1|\phi_3\rangle = 0$.

Similarly, from the relations $\langle\phi_2|\phi_2\rangle = 1$ and $\langle\phi_2|\phi_1\rangle = \langle\phi_2|\phi_3\rangle = 0$, we obtain the probability of finding the system in $|\phi_2\rangle$:

$$P_2 = |\langle\phi_2|\psi\rangle|^2 = \left|\frac{2}{3}\langle\phi_2|\phi_2\rangle\right|^2 = \frac{4}{9}.$$

As for $\langle\phi_3|\phi_3\rangle = 1$ and $\langle\phi_3|\phi_1\rangle = \langle\phi_3|\phi_2\rangle = 0$, they lead to the probability of finding the system in $|\phi_3\rangle$:

$$P_3 = |\langle\phi_3|\psi\rangle|^2 = \left|\frac{\sqrt{2}}{3}\langle\phi_3|\phi_3\rangle\right|^2 = \frac{2}{9}.$$

As expected, the total probability is equal to one:

$$P = P_1 + P_2 + P_3 = \frac{1}{3} + \frac{4}{9} + \frac{2}{9} = 1.$$

Rules and properties of the wave function

(b) The number of systems that will be found in the state $|\phi_1\rangle$ is

$$N_1 = 810 \times P_1 = \frac{810}{3} = 270.$$

Likewise, the number of systems that will be found in states $|\phi_2\rangle$ and $|\phi_3\rangle$ are given, respectively, by

$$N_2 = 810 \times P_2 = \frac{810 \times 4}{9} = 360, \qquad N_3 = 810 \times P_3 = \frac{810 \times 2}{9} = 180.$$

Rules and properties of the wave function

Solved problem :

Consider a state $|\psi\rangle = \frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle$ which is given in terms of three orthonormal eigenstates $|\phi_1\rangle$, $|\phi_2\rangle$ and $|\phi_3\rangle$ of an operator $\hat{B}$ such that $\hat{B}|\phi_n\rangle = n^2|\phi_n\rangle$. Find the expectation value of $\hat{B}$ for the state $|\psi\rangle$.

Solution :

$$\langle\psi \mid \psi\rangle = \left(\frac{1}{\sqrt{2}}\langle\phi_1| + \frac{1}{\sqrt{5}}\langle\phi_2| + \frac{1}{\sqrt{10}}\langle\phi_3|\right)\left(\frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle\right) = \frac{8}{10}$$

$$\begin{aligned}\langle\psi \mid \hat{B} \mid \psi\rangle &= \left(\frac{1}{\sqrt{2}}\langle\phi_1| + \frac{1}{\sqrt{5}}\langle\phi_2| + \frac{1}{\sqrt{10}}\langle\phi_3|\right)\hat{B}\left(\frac{1}{\sqrt{2}}|\phi_1\rangle + \frac{1}{\sqrt{5}}|\phi_2\rangle + \frac{1}{\sqrt{10}}|\phi_3\rangle\right)\\ &= \frac{1}{2} + \frac{2^2}{5} + \frac{3^2}{10} = \frac{22}{10}\end{aligned}$$

Hence, the expectation value of $\hat{B}$ is given by

$$\langle\hat{B}\rangle = \frac{\langle\psi \mid \hat{B} \mid \psi\rangle}{\langle\psi \mid \psi\rangle} = \frac{22/10}{8/10} = \frac{11}{4}.$$

Note: When state function is not normalized $<A> = \frac{<\psi|A|\psi>}{<\psi|\psi>}$

Rules and properties of the wave function

- Scalar/inner product of wave functions (normalized or not):

$$\left(\psi_2(x),\psi_1(x)\right)^* = \left(\psi_1(x),\psi_2(x)\right) \neq \left(\psi_2(x),\psi_1(x)\right)$$

Outcome is a number

Write them in bra-ket notation

- Orthogonality

$$\left(\psi_1(x),\psi_2(x)\right) = 0$$

- Normalized

$$\left(\psi_2(x),\psi_2(x)\right) = 1$$

Write them in bra-ket notation

- Orthonormal set of wavefunctions

$$\left(\psi_1,\psi_2,\psi_3,\ldots.\right)$$

provided $\overset{i}{\forall}\left(\psi_i,\psi_i\right) = 1$ and $\overset{i\neq j}{\forall}\left(\psi_i,\psi_j\right) = 0$ δ_{ij}

Rules and properties of the wave function

- Forbidden operations $|\psi_1>|\psi_2>$ or $<\psi_1|<\psi_2|$

- Linear operators Any operator that obeys distributive law

$$A\{a_1\psi_1(x)+a_2\psi_2(x)+\ldots a_n\psi_n(x)\}=a_1\{A\psi_1(x)\}+a_2\{A\psi_2(x)\}+\ldots$$

Almost all operators used in quantum mechanics are linear

- Hermitian operators Any operator which for given two wave functions follows the following

$$\left.\begin{array}{l} <\psi_1|A|\psi_2> \;=\; <\psi_2|A|\psi_1>^* \\ \\ \psi_1^*(A\psi_2)=(A\psi_1)^*\psi_2 \end{array}\right\} \quad A=A^\dagger$$

Example: diagonal or those which can be diagonalized

Rules and properties of the wave function

- Hermitian operators
  - Operators corresponding to physical observables are Hermitian
  - Eigen values of Hermitian operators are real
  - Eigen vectors corresponding to two different eigen values of a Hermitian operator are orthogonal to each other

Check that the following are examples of Hermitian operators

Observable	Corresponding operator
$\vec{r}$	$\hat{\vec{R}}$
$\vec{p}$	$\hat{\vec{P}} = -i\hbar\vec{\nabla}$
$T = \frac{p^2}{2m}$	$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2$
$E = \frac{p^2}{2m} + V(\vec{r}, t)$	$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\hat{\vec{R}}, t)$
$\vec{L} = \vec{r} \times \vec{p}$	$\hat{\vec{L}} = -i\hbar\hat{\vec{R}} \times \vec{\nabla}$

Rules and properties of the wave function

- **Harmonic oscillator, or a particle of mass *m* in harmonic potential well**

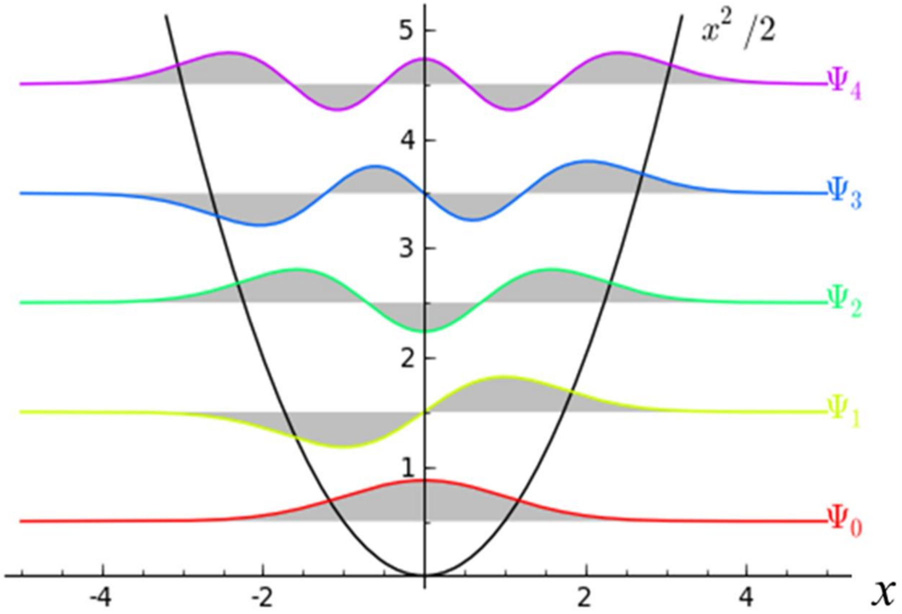
$$E_4 = \frac{9}{2}\hbar\omega$$

$$E_3 = \frac{7}{2}\hbar\omega$$

$$E_2 = \frac{5}{2}\hbar\omega$$

$$E_1 = \frac{3}{2}\hbar\omega$$

$$E_0 = \frac{1}{2}\hbar\omega$$



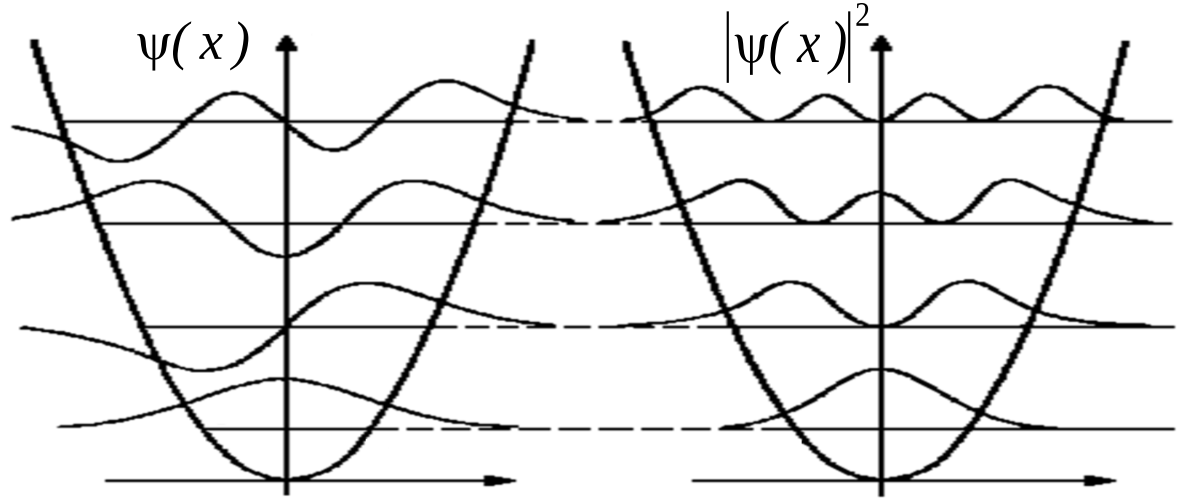
$$\Psi_0 = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-y^2/2}$$

$$\Psi_1 = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2}y\, e^{-y^2/2}$$

$$\Psi_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}}(2y^2 - 1)\, e^{-y^2/2}$$

$$\Psi_3 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}}(2y^3 - 3y)e^{-y^2/2}$$

$$\alpha = \frac{m\omega}{\hbar} \qquad y = \sqrt{\alpha}\, x$$



Rules and properties of the wave function

$$< x >_{n=0} = \int_{-\infty}^{+\infty} \psi_0^*(x) x \psi_0(x) dx$$

Use normalized wave functions

$$< x >_{n=3} = \int_{-\infty}^{+\infty} \psi_3^*(x) x \psi_3(x) dx$$

$$< p >_{n=0} = \int_{-\infty}^{+\infty} \psi_0^*(x) p_x \psi_0(x) dx = -i\hbar \int_{-\infty}^{+\infty} \psi_0^*(x) \frac{\partial \psi_0(x)}{\partial x} dx$$

$$< p >_{n=3} = \int_{-\infty}^{+\infty} \psi_3^*(x) p_x \psi_3(x) dx = -i\hbar \int_{-\infty}^{+\infty} \psi_3^*(x) \frac{\partial \psi_3(x)}{\partial x} dx$$

Check $<x^2>$, $<p^2>$ in $\Psi_n(x)$ state

Rules and properties of the wave function

- **Superposition principle** A quantum state can be represented as a superposition of two or more quantum states each of which satisfy SE

$$\psi(x,t) = c_1\psi_1(x,t) + c_2\psi_2(x,t) + \ldots c_n\psi_n(x,t)$$

$$= \sum_{i=1}^{n} c_i\psi_i(x,t)$$

$$\boxed{|\psi> = \sum_{i=1}^{n} c_i|\psi_i>}$$

- **Probability** of finding the system (microscopic particle) in a given state

$$\int_{-\infty}^{\infty}\psi^*(x,t)\psi(x,t)dx = \int_{-\infty}^{\infty}\left(\sum_{i=1}^{n} c_i\psi_i(x,t)\right)^*\left(\sum_{i=1}^{n} c_i\psi_i(x,t)\right)dx$$

$$= \sum_{i=1}^{n}|c_i|^2\int_{-\infty}^{\infty}\psi_i^*(x,t)\psi_i(x,t)dx = \sum_{i=1}^{n}|c_i|^2$$

Rules and properties of the wave function

- Probability of finding the system (microscopic particle) in one of the states out of many n possible eigen states

$$P_j = \left| \int_{-\infty}^{\infty} \psi_j^*(x,t)\psi(x,t)dx \right|^2 = \left| \int_{-\infty}^{\infty} \psi_j^*(x,t)\left(\sum_{i=1}^{n} c_i\psi_i(x,t) \right)dx \right|^2$$

$$= \left| \int_{-\infty}^{\infty} \psi_j^*(x,t)\left(\sum_{i=1}^{n} c_i\psi_i(x,t) \right)dx \right|^2 = \left| c_j \right|^2$$

Total probability $$P = \sum_{i=1}^{n} P_i = 1$$

Check, all eigen states and the general state (linear superposition of all) should be normalized

Rules and properties of the wave function

- **Test problem**

$$|\psi\rangle = \begin{pmatrix} i \\ 7 \\ i-10 \end{pmatrix}; \quad |\phi\rangle = \begin{pmatrix} i-10 \\ 7i \\ 1 \end{pmatrix};$$

(a) Find the corresponding bra <| of each

(b) Find the scalar/inner products $\langle\phi|\psi\rangle; \ \langle\psi|\psi\rangle; \ \langle\phi|\phi\rangle; \ \langle\psi|\phi\rangle$

(c) Check $\langle\psi|\langle\phi|; \ \langle\phi|\langle\phi|; \ \langle\phi|\langle\psi|;$