PH 107 :Quantum Physics and Applications

Particle in a infinite box potential cont..

Lecture 13: 27-01-2022

Sunita Srivastava
Department of Physics
Sunita.srivastava@iitb.ac.in

Recap

- **Particle in a box**

$$V(x) = 0 \quad \text{for } 0 < x < L$$
$$= \infty \text{ for x} < 0 \text{ or } x > L$$

- **Solutions**

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \text{ with } n = 1,2,3 \ldots \text{ for } 0 \leq x \leq L$$

$$\phi_n(x) = \ 0 \ elsewhere$$

$$E_n = \frac{\boldsymbol{\pi^2 \hbar^2 n^2}}{\boldsymbol{2mL^2}}$$

- **Properties of solutions**

1. $H\ \phi_n(x) = E_n\ \phi_n(x)\ \ , E_n\ are\ the\ eigen\ values\ corresponding\ to\ \phi_n(x)$
2. Stationary states, $\phi_n(x)$ are states of definite energy.
3. The stationary states $\phi_n(x)$are not eigenstates of the momentum operator $\hat{P}$. In other words, $\phi_n(x)$ are not states of definite momentum.
4. The expectation value of the momentum , $\langle \hat{P} \rangle = 0$.

General solutions

TISE

So, if we are given any $\Psi(x,0)$ we can write it in terms of the $\phi_n(x)$

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) = \sum_{n=1}^{\infty} c_n \, \phi_n(x)$$

TDSE

$$\Psi_n(x,t) = \sum_{n=1}^{\infty} \underbrace{c_n}_{\text{Complex coefficients}} \, \phi_n(x) \, e^{-i\frac{E_n}{\hbar}t}$$

How to we calculate the coefficients c_n?

Calculation of c_n

How to we calculate the coefficients c_n?

Let us perform $\int_0^L \phi_m^*(x)\ \Psi(x,0)\ dx$

$$\int_0^L \phi_m^*(x)\ \Psi(x,0)\ dx = \sum_{n=1}^{\infty} \int_0^L \phi_m^*(x)\ c_n \phi_n(x)\ dx$$

$$\int_0^L \phi_m{}^*(x)\ \Psi(x,0) dx = \sum_{n=1}^{\infty} \int_0^L \phi_m(x)^* c_n \phi_n(x) dx$$

Since $\int \phi_m(x)^* \phi_n(x) dx = \delta_{m,n}$

$$\sum_{n=1}^{\infty} \int_0^L \phi_m(x)^* c_n \phi_n(x) dx = \sum_{n=1}^{\infty} c_n \int_0^L \phi_m(x)^* \phi_n(x) dx = c_m$$

Thus,

$$c_m = \int_0^L \phi_m^*(x)\ \Psi(x,0)\ dx$$

Calculation of c_n

Thus, given a $\Psi(x,0)$, we can find the coefficients c_n as

$$c_n = \int_0^L \phi_n(x)^* \Psi(x,0)\,dx$$

The general solution of the TDSE as

$$\Psi_n(x,t) = \sum_{n=1}^{\infty} c_n \;\phi_n(x)\; e^{-i\frac{E_n}{\hbar}t}$$

For the infinite potential box we thus have

$$\Psi_n(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) e^{-i\left(\frac{n^2\pi^2\hbar^2}{2mL^2}\right)\frac{t}{\hbar}}$$

Normalization and Meaning of $|c_n|^2$

Is $\boldsymbol{\Psi}(\boldsymbol{x}, \mathbf{0})$ normalized?

We need to find whether, $\int_0^L |\Psi(x,0)|^2 dx = 1$

For that, first we need to write $\Psi^*(x,0) = \sum_{n=1}^{\infty} c_n^* \, \phi_n^*(x)$

where c_n^* and $\phi_n^*(x)$ are the complex conjugates of c_n and $\phi_n(x)$

$$|\Psi(x,0)|^2 = \Psi^*(x,0)\Psi(x,0) = \sum_{n,m=1}^{\infty} c_m^* \phi_m^*(x) c_n \phi_n(x)$$

Since, $\int_0^L |\Psi(x,0)|^2 dx = 1 \Longrightarrow \sum_{n,m=1}^{\infty} \int_0^L c_m^* \phi_m^*(x) c_n \phi_n(x) dx = 1$

$$\sum_{n,m=1}^{\infty} c_m^* c_n \int_0^L \phi_m^*(x) \phi_n(x) dx = 1$$

$$\Longrightarrow \sum_{n,m=1}^{\infty} c_m^* c_n \delta_{m,n} = 1 \;\boldsymbol{or}\; \sum_{n=1}^{\infty} c_n^* c_n = \sum_{n=1}^{\infty} |c_n|^2 = 1$$

So the normalization of $\boldsymbol{\Psi}(\boldsymbol{x}, \mathbf{0})$ requires the sum of the modulus-squared of the coefficients to add to unity.

Energy of the particle in general state $\Psi(x)$

$$\hat{H}\,\Psi(x,0) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\Psi(x,0)$$

Will it yield some $E\,\Psi(x,0)$?

$$\hat{H}\,\Psi(x) = \sum_{n=1}^{\infty} c_n\,\hat{H}\phi_n(x)$$

$$= \sum_{n=1}^{\infty} c_n\,E_n\phi_n(x)$$

$$\neq E\sum_{n=1}^{\infty} c_n\,\phi_n(x)$$

Hence $\Psi(x,0)$ is not a eigen solution.

Expectation value of energy in the general state

$$\langle \hat{H} \rangle = \bar{E} = \int_0^L \Psi^*(x,0)\hat{H}\Psi(x,0)dx$$

(assuming $\Psi(x,0)$ is normalized)

$$\bar{E} = \int_0^L \left(\sum_{m=1}^{\infty} c_m^* \, \phi_m^*(x) \sum_{n=1}^{\infty} c_n \, \hat{H}\phi_n(x) \right) dx$$

$$= \sum_{n,m=1}^{\infty} c_m^* c_n E_n \int_0^L \phi_m^*(x)\phi_n(x)dx$$

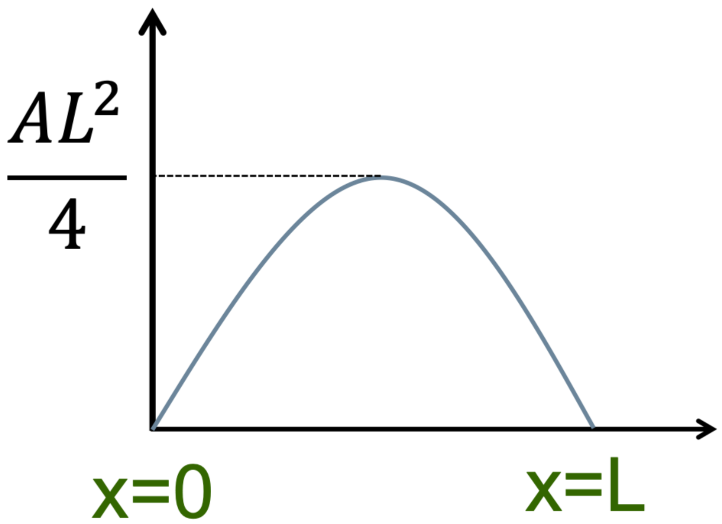
$$= \sum_{n,m=1}^{\infty} c_m^* c_n E_n \delta_{m,n}$$

$$= \sum_{n=1}^{\infty} |c_n|^2 E_n$$

$|c_n|^2$ is the probability of measuring the energy E_n in the general state $\Psi(x,0)$.

Example 1

Consider $\Psi(x) = A\ x(L-x)$ for $0 \leq x \leq L$ as an arbitrary state of a particle in a 1D rigid box.



1. Find *A* by normalization.

$$\int_0^L |\Psi(x)|^2\ dx = 1$$

$$\Longrightarrow |A|^2 \int_0^L x^2(L-x)^2\ dx = 1$$

$$\Longrightarrow A = \sqrt{\frac{30}{L^5}}$$

Example 1

2. How to write $\Psi(x,t)$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) e^{-i\left(\frac{n^2\pi^2\hbar^2}{2mL^2}\right)\frac{t}{\hbar}}$$

And we know how to find c_n.

$$\begin{aligned} c_n &= \int_0^L \phi_n^*(x)\Psi(x,0)\ dx \\ &= \int_0^L \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \sqrt{\frac{30}{L^5}} x(L-x)\ dx \\ &= 0\ \forall \text{ even } n \\ &= \frac{8\sqrt{15}}{(n\pi)^3}\ \forall \text{ odd } n \end{aligned}$$

Example 1:

2. How to write $\Psi(x,t)$

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) e^{-i\left(\frac{n^2\pi^2\hbar^2}{2mL^2}\right)\frac{t}{\hbar}}$$

$$\Psi(x,t) = \sqrt{\frac{30}{L}} \left(\frac{2}{\pi}\right)^3 \sum_{n=1,3,5,\ldots}^{\infty} \frac{1}{n^3} \sin\left(\frac{n\pi}{L}x\right) e^{-i\left(\frac{n^2\pi^2\hbar^2}{2mL^2}\right)\frac{t}{\hbar}}$$

Note that: $c_n \propto n^{-3}$

$\Psi(x,t)$ is $\phi_1(x)$ added to (1/27) $\phi_3(x)$,added to (1/125) $\phi_5(x)$,

and so on… $\Psi(x,t)$ should mostly have the characteristics of $\phi_1(x)$

Example 1:

3. What is the energy of the particle in the state $\Psi(x,t)$

$$\bar{E} = \sum_{n=1}^{\infty} |c_n|^2 E_n = \sum_{n=1,3,5,..}^{\infty} \left[\frac{8\sqrt{15}}{(n\pi)^3}\right]^2 \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{5\hbar^2}{mL^2}$$

Note that $\bar{E}$ is almost same as E_1

4. What is the probability of measuring the energy E_1

$$|c_1|^2 = \left[\frac{8\sqrt{15}}{(\pi)^3}\right]^2$$

Superposition of states

- A particle can be in a superposition of states that have different energies.

$$\psi(\boldsymbol{x},\boldsymbol{t}) = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}\left[\phi_1(\mathrm{x})e^{\frac{-iE_1t}{\hbar}} + \phi_2(\mathrm{x})e^{\frac{-iE_2t}{\hbar}}\right]$$

- A wavefunction that is sums of eigenfunctions with different energies are not eigenstate of the Hamiltonian.

- Eigenstates of the time-independent Schrodinger equation have a probability distribution that does not change with time:

$$|\Phi(x,t)|^2 = |\phi(x,0)|^2$$

Q1 . What happens to the probability distribution of superposed states ?

Time dependence Superposition of states

Q1 . What happens to the probability distribution of superposed states ?

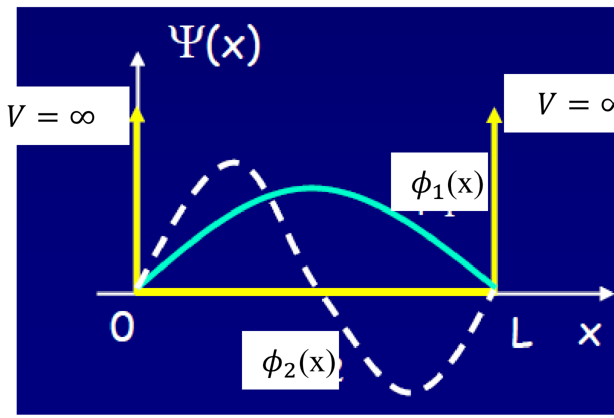
Example: At time t = 0, the particle in a box is in the superposition of the first two energy levels:

$$\psi(\boldsymbol{x},\mathbf{0}) = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}\left[\phi_1(\mathrm{x}) + \phi_2(\mathrm{x})\right]$$

If $\phi_1(\mathrm{x})$ and $\phi_2(\mathrm{x})$ are solution with different energy E_1 and E_2;

$$\psi(\boldsymbol{x},\boldsymbol{t}) = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}\left[\phi_1(\mathrm{x})e^{\frac{-iE_1t}{\hbar}} + \phi_2(\mathrm{x})e^{\frac{-iE_2t}{\hbar}}\right]$$

$$\psi(\boldsymbol{x},\boldsymbol{t}) = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}\left[\phi_1(\mathrm{x})e^{-i\omega_1t} + \phi_2(\mathrm{x})e^{-i\omega_2t}\right]$$



We define $\omega_n = \frac{E_n}{\hbar} = \frac{n^2\pi^2\hbar}{2mL^2}$ $\quad and\ \omega_n = n^2\,\omega_1$

Time dependence of Superposition of states: Particle motion in a well

Q1 . What happens to the probability distribution of superposed states ?

The probability density is given by $|\psi(x,t)|^2$

$$|\psi(x,t)|^2 = \psi * (x,t)\psi(x,t)$$

$$= \frac{1}{2}\left[\phi_1(\mathrm{x})e^{-i\omega_1 t} + \phi_2(\mathrm{x})e^{-i\omega_2 t}\right]^{*} \left[\phi_1(\mathrm{x})e^{-i\omega_1 t} + \phi_2(\mathrm{x})e^{-i\omega_2 t}\right]$$

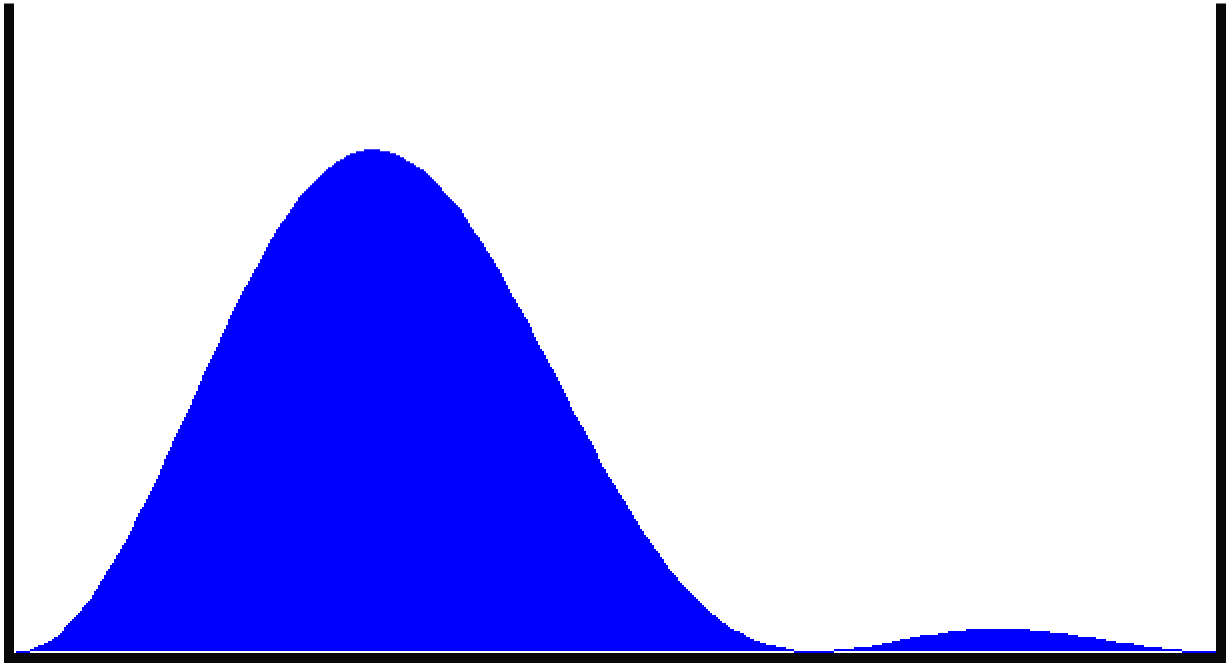
$$= \frac{1}{2}\left[\phi_1{}^{*}(\mathrm{x})e^{i\omega_1 t} + \phi_2{}^{*}(\mathrm{x})e^{i\omega_2 t}\right]\left[\phi_1(\mathrm{x})e^{-i\omega_1 t} + \phi_2(\mathrm{x})e^{-i\omega_2 t}\right]$$

$$= \frac{1}{2}\left[|\phi_1(x,t)|^2 + |\phi_2(x,t)|^2 + 2\phi_1(\mathrm{x})\phi_2(\mathrm{x})\, \boldsymbol{Cos}\,(\omega_2 - \omega_1)t\right]$$

- The most likely place to find the particle oscillates back and forth across the box.
  This oscillation occurs at frequency $\omega_2 - \omega_1 = 3\omega_1$.

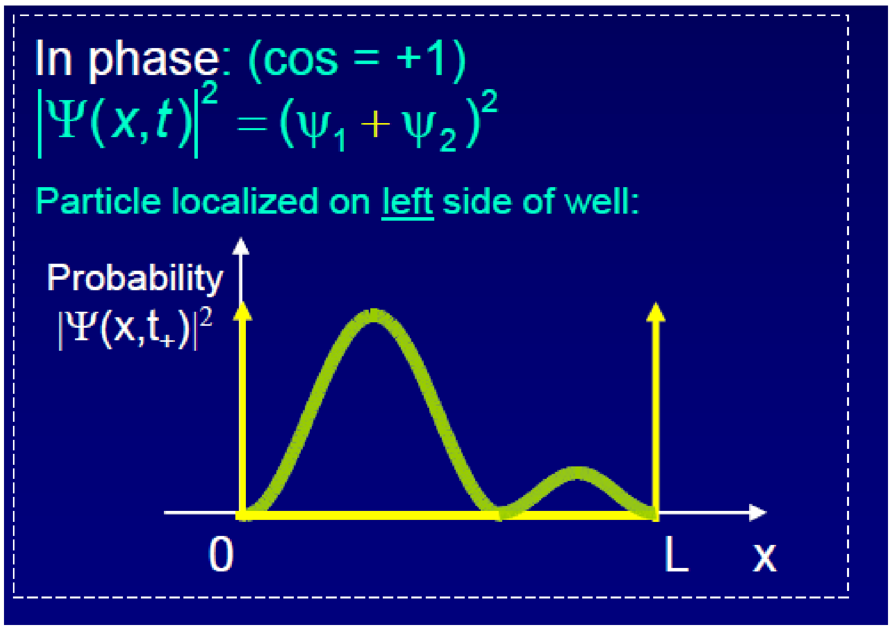
- The two terms have different energies so they oscillate in and out of phase.

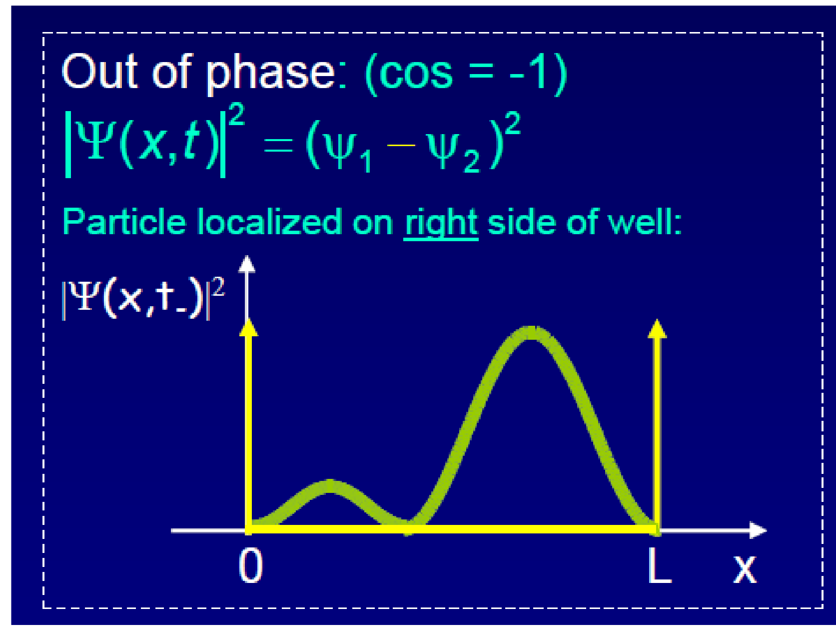
Probability distribution of superposed states.



- The most likely place to find the particle oscillates back and forth across the box.

$$|\psi(x,t)|^2 = \frac{1}{2}\left[|\phi_1(x,t)|^2 + |\phi_2(x,t)|^2 + 2\phi_1(\mathrm{x})\phi_2(\mathrm{x})\,\boldsymbol{Cos}\,(\omega_2 - \omega_1)t\right]$$





This oscillation occurs at frequency $\omega_2 - \omega_1 = 3\omega_1$.

The motion of the probability density comes from the changing interference between terms in $\psi(x,t)$ that have different energy.

Measuring energy of superposed states

Q2 . What happens when we measure the energy of a particle whose wave function is a superposition of more than one energy state ?

If the wave function is in an energy eigenstate (E1, say), then we know with certainty that we will obtain E1 (unless the apparatus is broken).

If the wave function is a superposition $\psi(\boldsymbol{x},\mathbf{0}) = [a\phi_1(\mathrm{x}) + b\phi_2(\mathrm{x})]$

of energies E_1 and E_2, then we aren't certain what the result will be. However:

We know with certainty that we will only obtain E_1 or E_2 !!

To be specific, we will never obtain $(E_1+E_2)/2$, or any other value.

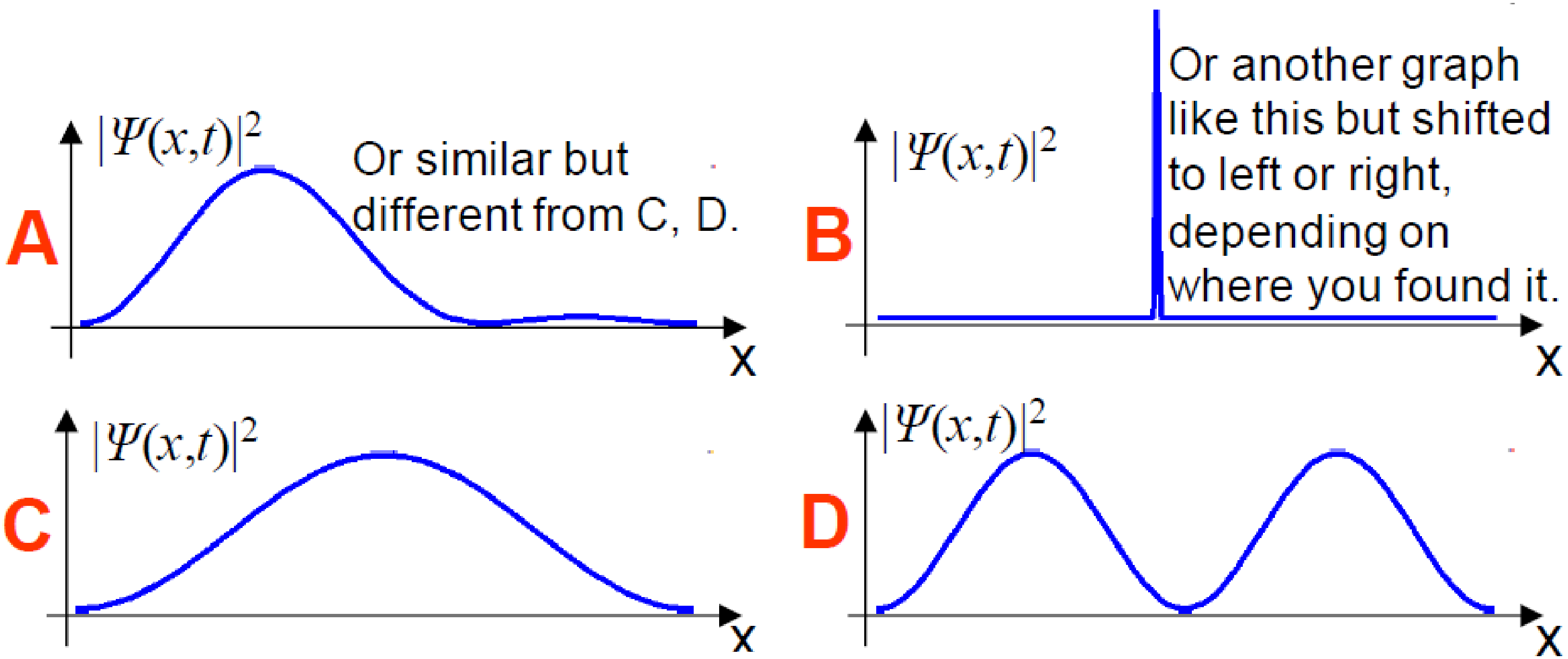
What about a and b?

$|a|^2$ and $|b|^2$ are the probabilities of obtaining E_1 and E_2, respectively. That's why we normalize the wave function to make $|a|^2 + |b|^2 = 1$.

The "Collapse" of the Wave Function

Q3 . What does the probability density of this particle looks like immediately after measuring the energy ?

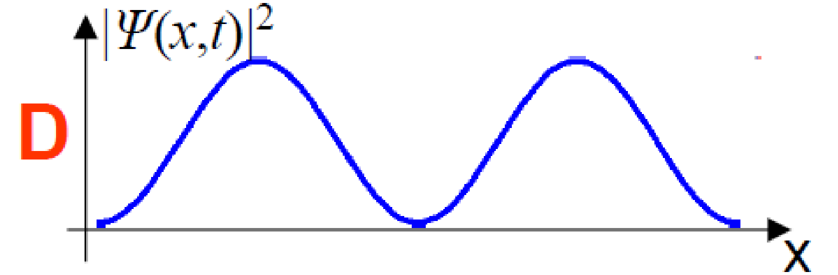
$$\psi(\boldsymbol{x},\boldsymbol{t}) = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}\left[\phi_1(\mathrm{x})e^{\frac{-iE_1t}{\hbar}} + \phi_2(\mathrm{x})e^{\frac{-iE_2t}{\hbar}}\right]$$



The "Collapse" of the Wave Function

$$\psi(\boldsymbol{x},\boldsymbol{t}) = \frac{\mathbf{1}}{\sqrt{\mathbf{2}}}\left[\phi_1(\mathrm{x})e^{\frac{-iE_1t}{\hbar}} + \phi_2(\mathrm{x})e^{\frac{-iE_2t}{\hbar}}\right]$$

Q4 . What is the state of the particle if E_2 is observed ?



- We start out with $\psi(\boldsymbol{x},\boldsymbol{t})$, before we make the measurement, we can't predict the result of an energy measurement with certainty.

- However, after the measurement, we know with certainty that E = E_2 and

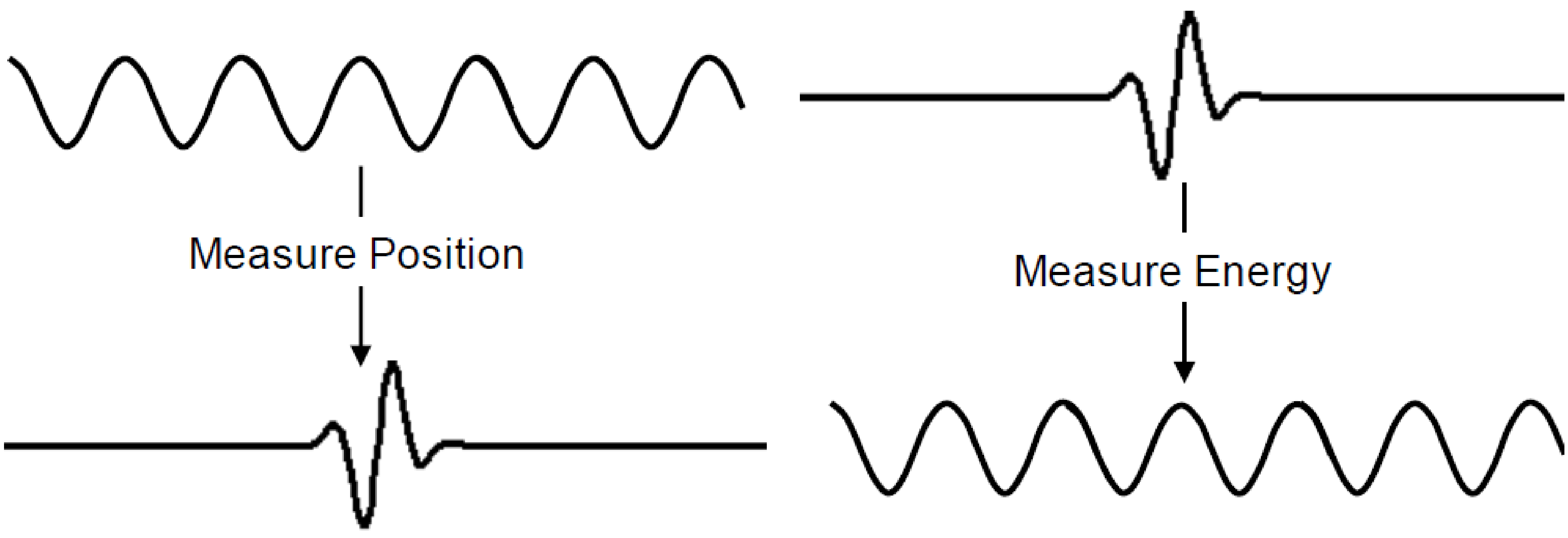
  the wave function must now be $\psi(\boldsymbol{x},\boldsymbol{t}) = \phi_2(\mathrm{x})e^{\frac{-iE_2t}{\hbar}}$

- That is, the wave function has "collapsed" to the state that corresponds with the result we obtained.

- This is one of the weirder features of QM, and is the principal reason that Einstein never accepted QM as a complete theory.

Notes on position and energy

- Energy eigenstates: spread out in space.
- Position eigenstates: localized in space.
- This is why you cannot know both at the same time (wave packet vs plane waves)
- Measuring position messes up energy and vice versa.



Example 2:

Assume: $$\Psi(x,0) = \sqrt{\frac{2}{5L}}\sin\left(\frac{\pi}{L}x\right) + \sqrt{\frac{8}{5L}}\sin\left(\frac{4\pi}{L}x\right)$$

1. Normalise the above given wave-function

We can re-write the above function as below such that Ψ (x, 0) is normalized

$$\Psi(x,0) = \sqrt{\frac{1}{5}}\phi_1(x) + \frac{2}{\sqrt{5}}\phi_4(x)$$

It is easy to see that $$\sum_{n=1}^{\infty}|c_n|^2 = \frac{1}{5} + \frac{4}{5} = 1$$

Example 2:

2. Average value of Energy, $\bar{E} = \sum_{n=1}^{\infty} |c_n|^2 \ E_n = \frac{1}{5} \ E_1 + \frac{4}{5} \ E_4$

$$= \frac{1}{5} \ \left(\frac{\pi^2 \hbar^2}{2mL^2} \right) + \frac{4}{5} \ \left(\frac{16\pi^2 \hbar^2}{2mL^2} \right) = 6.5 \ \left(\frac{\pi^2 \hbar^2}{mL^2} \right)$$

3. If no measurement is performed, what is the state of the particle at time t?

$$\Psi(x,t) = \sqrt{\frac{1}{5}} \phi_1(x) e^{-i\frac{E_1}{\hbar}t} + \frac{2}{\sqrt{5}} \phi_4(x) e^{-i\frac{E_4}{\hbar}t}$$

4. If a measurement is performed such that the value of energy is measured to be E_4, what is the state of the particle at time *t* after the measurement?

$$\Psi(x,t) = \phi_4(x) \ e^{-i\frac{E_4}{\hbar}t}$$

Measurements in Quantum mechanics

- A measurement returns a specific value for one or more aspects of a quantum state (like position or energy).
- The measurement itself changes the wave function. (Remember for instance Heisenberg's uncertainty relation.)
- The fact that it actually must change the wave function lies at the heart of the problem of the interpretation of quantum mechanics!
- Unlike classical physics, measurement in QM doesn't just find something that was already there – **it CHANGES the system**!