Phys 330 Spring 2020

Lec #7: Schrödinger Equation

I. We want:

1. Oscillatory solutions
2. conserved probability
3. interference

$\Psi(x,t)$ complex probability amplitude

$|\Psi(x,t)|^2 \Delta x$ prob to find particle between x, $x+\Delta x$

Plane wave $\Psi_k(x,t) = e^{i(kx-\omega t)}$

$k = \frac{2\pi}{\lambda}$ $\omega = 2\pi f$

To get 1, 2 must be first order in time

$$\frac{\partial}{\partial t}\Psi_k(x,t) = -i\omega\Psi_k = (-i\omega)\left(-\frac{1}{k^2}\right)\frac{\partial^2}{\partial x^2}\Psi_k$$

$$i\frac{\partial}{\partial t}\Psi_k = -\frac{\omega}{k^2}\frac{\partial^2}{\partial x^2}\Psi_k$$

non-relativistic energy $\hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

$\omega/k^2 = \hbar/2m$

give each term dimensions of energy $\times$ Ψ_k

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi$$ free particle wave equation

observables are real numbers corresponding to eigenvalues of Hermitian operators

has real eigenvalue

Operators wear hats, $\hat{O}$ w/ eigenvalue O.

$$\hat{O}\psi = O\psi \quad \text{eigenvalue equation}$$

then Schrödinger eq. has form $E = \frac{p^2}{2m}$

$$i\hbar \frac{\partial}{\partial t} \rightarrow E = \hbar\omega$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \rightarrow \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

II Potential Energy Force $F_x = -\frac{d}{dx}V(x)$

Schrödinger is then

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi$$

Wave equation depends on V not F!   This has surprising physical consequence.

III. Probability current

$$\psi^*\left[i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi\right]$$

$$\psi\left[-i\hbar\frac{\partial}{\partial t}\psi^* = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi^* + V\psi^*\right]$$

V is real

Subtract. use notation $\dot{\psi} = \frac{\partial\psi}{\partial t}$, $\psi' = \frac{\partial\psi}{\partial x}$

$$i\hbar(\psi^*\dot{\psi} + \psi\dot{\psi}^*) = -\frac{\hbar^2}{2m}(\psi^*\psi'' - \psi\psi^{*''})$$

$$i\hbar\frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar^2}{2m}\frac{\partial}{\partial x}(\psi^*\psi' - \psi\psi^{*'})$$

imaginary part

$(\psi^*\psi')^* = (\psi\psi^{*'})$ and $z - z^* = 2i\,\mathrm{Im}\,z$

$$i\hbar \frac{\partial}{\partial t}(\psi^*\psi) = -i\frac{\hbar^2}{m}\frac{\partial}{\partial x}\left[\mathrm{Im}\left(\psi^*\frac{\partial\psi}{\partial x}\right)\right]$$

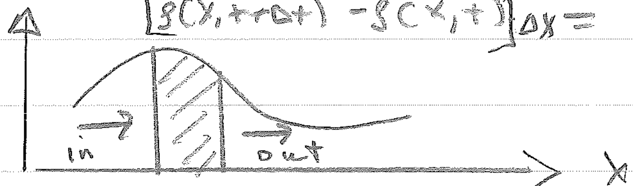
Probability density $\rho(x) \equiv \psi^*\psi = |\psi|^2$

probability current $j_x(x,t) \equiv \frac{\hbar}{m}\mathrm{Im}\left(\psi^*\frac{\partial\psi}{\partial x}\right)$

Conservation : $\boxed{\frac{\partial\rho}{\partial t} + \frac{d}{dx}j_x = 0}$

Probability flow into Δx in time Δt

$\rho(x,t)$ $\quad [\rho(x,t+\Delta t) - \rho(x,t)]\Delta x = \frac{\partial\rho}{\partial t}\Delta t\,\Delta x$



in : $j_x(x,t)\Delta t$ $\quad$ out: $j_x(x+\Delta x,t)\Delta t$

$$\frac{\partial\rho}{\partial t}\Delta t\Delta x = \Big[j_x(x,t) - \underbrace{j_x(x+\Delta x,t)}_{-\frac{d}{dx}j_x\,\Delta x\,\Delta t}\Big]\Delta t$$

probability density is conserved "fluid"

for free particle $\psi_k = Ae^{i(kx-\omega t)}$

$$j_x = |A|^2\frac{\hbar k}{m} = |A|^2(\text{Velocity})$$

IV Observables and Expectation values

Classical rules of probability —

normalization $1 = \int_{-\infty}^{\infty}\rho(x)dx = \int_{-\infty}^{\infty}|\psi|^2 dx$

expectation value of x –

$$\langle x \rangle = \int_{-\infty}^{\infty} x\, \rho(x)\, dx = \int_{-\infty}^{\infty} x\, \psi^* \psi\, dx$$

What is $\langle p \rangle$? Free particle,

$$\frac{\hbar}{i} \frac{\partial}{\partial x} e^{i(kx - \omega t)} = \underbrace{\hbar k}_{p}\, e^{i(kx-\omega t)}$$

So we can write:

$$\langle p \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i} \frac{\partial}{\partial x}(\psi)\, dx}{\int_{-\infty}^{\infty} \psi^* \psi\, dx} = \hbar k$$

In general, expect $m \frac{d}{dt} \langle x \rangle = \langle p \rangle$

$$\frac{d}{dt} \langle x \rangle = \frac{d}{dt} \int x\, \psi^* \psi\, dx \qquad \text{limits are } \pm \infty$$

$$= \int x \left[\frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \right] dx$$

in integral,
x is an operator, not a function of time!

use $\frac{\partial}{\partial t} \psi = \frac{1}{i\hbar} \left[-\frac{\hbar^2}{2m} \psi'' + V \psi \right]$

$$\frac{\partial}{\partial t} \psi^* = \frac{-1}{i\hbar} \left[-\frac{\hbar^2}{2m} \psi^{*''} + V \psi^* \right] \qquad \underline{V \text{ real}}$$

V terms will cancel, giving

$$\frac{d}{dt}\langle x\rangle = \frac{1}{i\hbar}\left(+\frac{\hbar^2}{2m}\right)\int x\left[\psi^{*''}\psi - \psi^*\psi''\right]dx$$

$$= \frac{1}{i\hbar}\left(\frac{\hbar^2}{2m}\right)\int x\,\frac{d}{dx}\left[\psi^{*'}\psi - \psi^*\psi'\right]dx$$

integrate by parts 0 by normalizability condition

$$\frac{d}{dt}\langle x\rangle = \frac{1}{i}\left(\frac{\hbar}{2m}\right)\left\{ x[\,]\Big|_{-\infty}^{\infty} - \int [\,]\,dx\right.$$

where $[\,] \equiv \psi^{*'}\psi - \psi^*\psi'$

end-point term is zero since $\psi \xrightarrow[\pm\infty]{} 0$

$$m\frac{d}{dt}\langle x\rangle = \frac{\hbar}{i}\left(\frac{1}{2}\right)\int\left[\psi^{*'}\psi - \psi^*\psi'\right]dx$$

integrate by parts again on $\psi^{*'}\psi$ to get

$$\boxed{\langle p\rangle = m\frac{d}{dt}\langle x\rangle = \int \psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\psi\;dx}$$

momentum operator $\hat{p} = \dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$

$$\frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad \text{Kinetic energy operator}$$

Guess general form as

$$\underset{\substack{\uparrow\\ \text{observables}}}{\langle O\rangle} = \underbrace{\int \psi^*\hat{O}\psi\,dx}_{\text{rule to compute from wave function}}$$

Schrödinger becomes

$$i\hbar \frac{\partial}{\partial t}\psi = \frac{\hat{p}^2}{2m}\psi + V\psi \equiv \hat{H}\psi$$

$\hat{H} \equiv$ Hamiltonian (energy) operator

For V with no explicit time dependence, general solution is

$$\psi(x,t) = e^{-i\hat{H}t/\hbar}\,\psi(x,0)$$

↑ defined by power series

formally solves $i\hbar \frac{\partial}{\partial t}\psi(x,t) = \hat{H}\,\psi(x,t)$

V. Energy Eigenstates

$$\hat{H}\,\psi_E(x,t) = E\,\psi_E(x,t)$$

then

$$\psi_E(x,t) = e^{-iEt/\hbar}\,\psi_E(x,0) \equiv e^{-iEt/\hbar}\,\phi_E(x)$$

Get time independent Schrödinger equation

$$\boxed{-\frac{\hbar^2}{2m}\phi_E'' + V\phi_E = E\,\phi_E}$$

or $\boxed{\hat{H}\,\phi_E = E\,\phi_E}$

Energy eigenstates have *definite* energy:

$$\langle E \rangle = \int \Psi_E^* \hat{H} \Psi_E \, dx$$

$$= \int e^{iEt/\hbar} \phi_E^* \, e^{-iEt/\hbar} (\hat{H} \phi_E) \, dx$$

$$= E \underbrace{\int_{-\infty}^{\infty} \phi_E^* \phi_E \, dx}_{\text{normalized to one.}} = E$$

E has discrete (continuous) values for bound state (unbound state) solutions $\{E_i\}$

States ϕ_E are complete in the sense that any state can be written as a linear superposition (Schrödinger eq. is linear)

$$\Psi(x,t) = \sum_{i=0}^{\infty} a_i e^{-iE_i t/\hbar} \phi_{E_i}(x)$$

← integral for unbound

a_i are complex numbers. General state is not an energy eigenstate.

$$\hat{H} \Psi(x,t) = \sum_{i=0} a_i E_i e^{-iE_i t/\hbar} \phi_{E_i}(x)$$

$$\neq \text{constant } \Psi(x,t)$$

Comment on relativistic Q.M.

$$E^2 = p^2 + m^2$$

$E \to \hat{H} \to i\hbar \frac{\partial}{\partial t}$

$p \to \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ leads to Klein-Gordon equation

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \psi = -\hbar^2 \frac{\partial^2}{\partial x^2} \psi + m^2 \psi$$

Second order in time ⇒ no conserved particle. Equation describes relativistic integer Spin particles like the Spin-0 pion.

Relativistic Q.M. predicts particle number is not conserved.

The photon is always relativistic. Quantum description requires quantization of classical EM field, a relativistic quantum field theory.

So we can see why quantum description of non-relativistic electron came first.