Ch. 13 The Schrodinger Wave Equation

Historically the governing differential equation for classical physics is

$$\vec{F}_{net} = \frac{d\vec{p}}{dt}$$

This and conservation statements are sufficient to do many problems. We have considered a paradigm shift due to the constant speed of light---relativity.

Now we must incorporate into physics the fact that all "things" have wave properties.

We will use Potential theory to describe interactions between one lump of matter and another. Recall that potential is a way to relate force, work, energy ---for path independent processes (conservation).

We will relate ----POTENTIAL $V(x, y, z, t)$ or $V(\vec{r}, t)$

to the "thing"/ "stuff"

being the wavefunction $\Psi(x, y, z, t)$ or $\Psi(\vec{r}, t)$

V---is not the electric potential, but is potential energy.

Ψ is the wavefunction--and is literally "everything".

effect

cause

We need a new dynamical equation that is not Newton's 2nd law.

The wavefunction is the thing that will "evolve in time" when exposed to a given environment (interaction, potentials, boundaries)

Review of Bohr again

- Angular momentum is not correct
- Current loops and E&M interactions --not correct
- The energies work
- The wave nature of particles has not been incorporated
- Quantization has been implanted /guessed---best we can do anyway
- Wave nature requires UNCERTAINTY PRINCIPLE
- The upper states have been considered as stationary
    - In fact--they radiate (lose energy) over a long long long time (maybe 16 ns or so for sodium……)---think about how many cycles of light this is
    - Even Schrodinger Wave equ does not handle "Relative Transition Probabilities" -----until Quantum ElectroDynamics (QED--Feynman) is incorporated
- We ought to be able to understand how atoms behave if we know the interactions---we still don't have a full grasp. S.E.---gets us MUCH MUCH MUCH CLOSER.

In the Bohr model---with circular orbits, r_n=52.9pm
And radial component of momentum was $p_r = 0$

NO UNCERTAINTY IN BOHR

DeBroglie---we must include wave nature of "stuff"

The "wavefunction" must contain all the properties

$\Psi(\vec{r},t)$

wave properties

obeys some dynamic eq — a wave eq

There are different types of descriptions of waves that result from different differential equations. Just like Newton's 2nd law---we must observe nature and infer, term by term---that the wave seems to behave like "this" and obey "this" equation.
THERE IS NO DERIVATION--STRICTLY SPEAKING.
WE CAN SHOW---IF I HAVE A WAVE ANSWER --AND PLUG IT INTO THE WAVE EQUATION---IT IS A SOLUTION (SURE --IF WE KNOW THE ANSWER FIRST, THEN IT WORKS)

Jargon and math and notation--OH MY

$$\Psi(\vec{r}, t) \quad \text{is complex} \quad (i = \sqrt{-1})$$

All physical meaning shall come from things like

$$\text{prob density} - \Psi^* \Psi$$

In one dimension the probability of a particle being between x and x+dx would be

$$= \Psi^* \Psi \, dx$$

Other than likelihood of the particle being someplace we may want to know some physical property like Energy, or Momentum, etc. These are found by allowing some Energy Operation (math stuff) to act on the wavefunction.

Like $$\Psi^* (E_{op}) \Psi$$

or if I integrate that probability over all space I'll get the

$$\int_{\text{all space}} \Psi^{*} (E_{op}) \Psi \, d\tau \quad \leftarrow \text{volume}$$

$$E_{ave}, \ \bar{E} \xrightarrow{=} \langle E \rangle$$

the "expectation" value

Instead of using integrals ---a more general notation was used to indicate adding over the entire function space----

$$\langle \Psi | \ E_{op} | \Psi \rangle$$

We could have any operator in the middle here, and our Ψ could have ---for example---many different "Fourier" components (orthogonal of course). (the frequency cross terms forming a matrix).

The Schrodinger time dep wave equation---

$$\frac{-\hbar^2}{2m} \nabla^2 \Psi(\vec{r},t) + V(\vec{r},t)\Psi(\vec{r},t) = i\hbar \frac{\partial}{\partial t}\Psi(\vec{r},t)$$

In one dimension this reduces to

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

$$\boxed{\hbar = \frac{h}{2\pi}}$$

The wave equation has spatial derivatives (which always related to potential) and time derivatives---Further--other than the constants, it is a well known form of differential equation that exhibits "wave solutions".

Recall waves look like-----

$$A e^{\pm i(kx - \omega t)}$$

Cartesian

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

V is potential energy of the particle — depends on configuration.

Ψ = the wavefunction — $\Psi^*\Psi$ is real

The S.W.E--is our new dynamic equation---put potential in (like forces used to be), solve the differential equation for given boundary conditions---grind math---Out comes Ψ. Then we can find any property of the system.

We will--solve some simple cases

We will--examine some properties of "answers"---meaning, if given Ψ, then find......such and such physical property.

The probability of a particle being between x_1 & x_2 is

$$= \int_{x_1}^{x_2} \underbrace{\Psi^* \Psi}_{\text{Prob density}} \, dx$$

Of course--if we make our limits all space---then we better come up with the answer "1". The probability that the particle is somewhere is "1".

To solve S.W.E---we will separate variables, and we will then assume that the potential is not time dependent.

Note big Ψ is different than ψ $\quad \Psi(x,t)$ or $\psi(x)$

Solve S.E. starting with separation of Var.

$$\Psi(x,t) = \psi(x)\, T(t) \qquad \text{big } \Psi \text{ or little } \psi$$

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

Standard for sep of variables. Try product solution, divide by product (next step).

$$T\left(\frac{-\hbar^2}{2m}\right)\psi'' + V\psi T = i\hbar\,\psi\frac{\partial T}{\partial t}$$

divide by ψT

$$\underbrace{\frac{-\hbar^2}{2m}\frac{\psi''}{\psi} + V(x)}_{\text{depends only on } x} = \underbrace{\frac{i\hbar}{T}\frac{\partial T}{\partial t}}_{\text{only on } t}$$

Assumed V is Time indep

We shall call the separation constant "E" and figure out what that might mean later.....uh (I think I know).

$$E = \frac{i\hbar}{T}\frac{\partial T}{\partial t} \qquad \partial \xrightarrow[\text{now}]{} d$$

⋮ integrate

Int const – offset in time

$$T(t) = \left(\overset{\text{Phase}}{?}\right) e^{-i(E/\hbar)t}$$

$$E = \hbar\omega \qquad (\text{or } h\nu \rightarrow \omega = 2\pi\nu)$$

Remember the entire argument of exp(stuff) must be dimensionless (since it can be expressed as a series).

So, whatever E is ---must have something in it with "h bar" and inverse time. Whatever is vibrating/oscillating/waving---it has an angular frequency ω and seems to have meaning of Energy when multiplied by "h bar" ---just like light did.

In order to solve the spatial part of Schrodinger's time INDEPENDENT equation (what is left after separating), we need to be given a specific potential like---coulomb, or hard sphere, or...something.

The separated equation looks like--spatially

$$\underbrace{-\frac{\hbar^2}{2m}\psi'' + V(x)\psi}_{\displaystyle -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)} = E\psi$$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)}_{\displaystyle E_{op}}$$

$$p_{op} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

E_{op} ∂t

so $KE_{op} = \frac{p_{op}^2}{2m}$

https://www.youtube.com/watch?v=PiZTz_CTllg

In all cases, we MUST require the wavefunction to be normalized.

$$\int_{\text{All Space}} \Psi^* \, \Psi \; d\tau \text{ or } dVol \quad \text{or} \quad dx\,dy\,dz$$

$$\text{or} \quad r^2 \sin\theta \, dr\, d\theta\, d\phi$$

$$r\, d\theta\, dz\, dr$$

The time part of the solution clearly simply complex conjugates itself away ---ONLY IF I HAVE A SINGLE FREQUENCY. ---OTHERWISE I HAVE SLOSHING TIME DEP CROSS TERMS.

Lets say we are given some ψ (it solves some potential)

$$\psi = A e^{-|x/2|} \quad \text{— find } A \text{ — Norm Const}$$

$$1 = \int_{-\infty}^{\infty} A^2 e^{-|x|} \, dx$$

$$= 2 \int_0^{\infty} A^2 e^{-|x|} \, dx$$

$$= 2 A^2 (-1) \left[\cancel{e^{-\infty}} - \overset{e^{-0}}{1} \right]$$

$$= 2A^2 \qquad A = \frac{1}{\sqrt{2}}$$

This is not dis-similar from "unitizing a vector".

$$\vec{r} = A\hat{i} + B\hat{j} + C\hat{k} \qquad \vec{r} \cdot \vec{r} = A^2 + B^2 + C^2$$

so $\hat{r} = \frac{\vec{r}}{|r|}$

find ρ — prob $x = -0.1$ to 0.1

$$\rho_{range} = \left(\frac{1}{\sqrt{2}}\right)^2 \int_{-0.1}^{0.1} e^{-|x|}\,dx$$

$$= \cancel{(\quad)}^{\cancel{2}} \int_{0}^{0.1} e^{-x}\,dx$$

$$= 1 - e^{-0.1} = \text{do}$$

Einstein did not like probability theory---? hidden variables? Field theory (is still probabilistic). The important question is "where is the energy density" or where is the ______density.

13.2---the separated S.W.E

13.2 separated diffeq

Time indep S.E. – one dim ?

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \bar{V}(x)\,\psi = E\,\psi$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \bar{V}\right)\psi = E\,\psi$$

$$\underbrace{\qquad\qquad\qquad\qquad}_{}$$

Energy operator
1st term is kinetic energy op } Hamiltonian operator

$$\boxed{E_{op}\,\psi(x)} = E\,\psi(x)$$

The solutions to the Separated Schrodinger equation
are $\psi_n(\vec{r})$ Eigenfunction (vector)

Which are called "stationary states"---the "standing wave states"---and may be one, two, three dimensions --depending on the problem given. The time dep. has been separated out. "n" is just a label for ordering the many possible solutions to the differential equation that can satisfy the boundary conditions.

E_n = Energy of ψ_n state

Eigenvalue

Just like we may have many vector components $\hat{i}, \hat{j}, \hat{k}$
or many Fourier components

$\sin\left(n \frac{\pi x}{L}\right)$

All added together to make a specific vector or specific waveform, we may have many Eigen functions added to make up a specific resulting waveform.

Just as $\hat{i}, \hat{j}, \hat{k}$ are perpendicular and normalized---so are the ψ_n

ψ_n form an ortho-normal basis set (normalized and have a Perpendicular like rule.).

If $\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi = (\overline{KE})\,\psi$

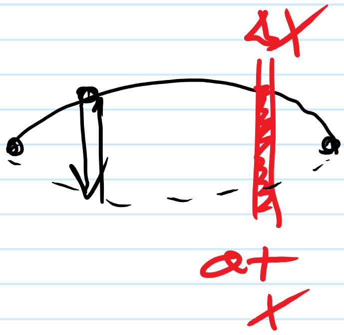
then note $\frac{p^2}{2m} = \overline{KE}$

is satisfied by $P_{op} = \frac{\hbar}{i}\frac{d}{dx}$

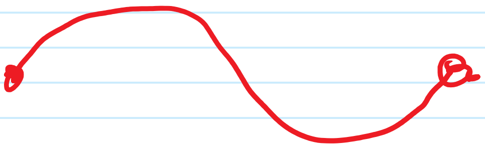
$P_{op}\,\psi = \text{mom}\;\psi$

Any measurement result can be found by "hitting" the state with an operator (allowing the differential operator for that measurement to act on the wave function). The operators are well known---The wavefunctions must be found by solving the differential equation for a given potential and given boundary conditions= a specific given problem.

A string may do



This vibrational standing wave mode on a string has a "this much energy on average" at any location range along the string.
The average speed or KE or p--stays same at a given x.
It is a stationary state.



This is a different stationary state---has it's own "probability" density. The two different states have different frequencies---and they may be added to give a time dependent sloshing state (a particle moving between the ends may be many states added).

Questions you may have---and must avoid asking

What is waving---I DON'T KNOW--BUT THERE ARE WAVE PROPERTIES

When I measure something--don't I know the answer absolutely --so there is no uncertainty.

SURE--TRY THE EXPERIMENT AGAIN--YOU WILL GET THE PROBABILITY DISTRIBUTION. APPARENTLY THINGS DO NOT HAPPEN FOR A REASON.

Doesn't the wave function evolve deterministically----YES--THE PROBABILITY DISTRIBUTION IS A SOLUTION TO A DETERMINISTIC EQUATION---AND NO ONE REALLY UNDERSTANDS THE MECHANISM OF THE
"RELIGEOUS HOKUM" ---CALLED WAVEFUNCTION COLLAPSE--- yet that is the Copenhagen model suggested by Bohr ~100 years ago--and it has stuck. Observation causes the entire entangled universe to change (instantly).