Quantum Mechanics

Professor Alexey Petrov

29 September 2005

Chapter 1

Physical Principles of Quantum Mechanics

1.1 Classical Description

[there would be a table]

1.2 Particle-wave Duality

Rutherford's atom: electron orbits proton.

$$d = 10^{-8}\text{ cm} \qquad E_{tot} = \frac{p^2}{2m} - \frac{e^2}{r}; \quad \frac{v}{c} = 10^{-2}, \tag{1.1}$$

i.e. electron is nonrelativistic. Since e^- moves around p: e^- is always accelerating, $a = v^2/r$, *i.e.* radiates energy! Recall Lamure formula,

$$-\frac{dE_{tot}}{dt} = P(a) = \frac{2e^2a^2}{3c^3} \tag{1.2}$$

Now, second Newton's law gives

$$F_C = m\frac{v^2}{r}, \text{ or } mv^2 = \frac{e}{r}$$

$$E_{tot} = \frac{p^2}{2m} - \frac{e^2}{r} = \frac{e^2}{2r} \tag{1.3}$$

Plugging it into Eq. (1.2) obtain that since total energy is radiated off, e^- falls onto the nucleus in about $\tau =$10^{-8} seconds

Obviously, this does not happen!!!

N. Bohr (1913) assumed the following:

1. allowed orbits are only those with:

$$mvr = n\frac{h}{2\pi} = nt$$

No radiation from allowed orbits.

2. Transitions between allowed orbits:
   $\Delta E = hv \longleftarrow$ photons, quanta particles of light

How is it possible?

De Broglie: Light can behave as particles
1927 Thus, Particles have wave properties

$$\begin{aligned} E = \;& \text{hv} \;= \tfrac{hc}{\lambda} \quad \boxed{\lambda = \tfrac{h}{p}}\; or \;\boxed{\lambda = \tfrac{\hbar}{p}} \\ E = \;& \text{pc} \end{aligned}$$

Must devise experiments that probe wave nature of matter, diffraction in interference

Clinton J. Davidson and Lester H.Germer(1927) and G.P. Thomson

1.3 Davisson - Germer Experiment: Electron Diffraction

Theory: Accelerate electrons to P:

$$\lambda = \frac{h}{P} = \frac{h}{mv} = \frac{h}{\sqrt{2mcv}} \tag{1.4}$$

for $v = 54v$:

$$\lambda_{th.} = 1.64\mathring{A}$$

Experiment: Waves: use Bragg's Law:

$$n\lambda = d\sin\theta$$

$$d_{nickel} = \underline{\underline{2.15\mathring{A}}} \sim \underline{\underline{0.092nm}} \sim \underline{\underline{10^{-8}cm}}$$

$$\text{Thus, } \lambda_{exp} = \frac{d\sin\theta}{n} \sim \frac{2.15\mathring{A}\cdot\sin 50^\circ}{l} \sim \underline{\underline{1.65\mathring{A}}}$$

Nobel Prize for de Broglie (1929) and Davisson and Thomson (1937)

Thus: depending on the "conditions" the microobject (electron) will demonstrate either particle or wave properties!

$\boxed{\text{What kind of conditions?}}$

How do we know the position of e$^-$?

What is our "basic length scale"?

Basic Length Scales:

hydrogen atom: $\Delta x \sim a_0 \sim 10^{-8}cm$

$\lambda = \frac{h}{P} \sim 10^{-8}cm$

D.-G. expt: $\Delta x \sim d \sim 10^{-8}$

$\lambda = \frac{h}{\sqrt{2meV}} \sim 10^{-8}cm$

$\boxed{\Delta x \sim \lambda} \longleftarrow$ This is when e^- demonstrates wave-like properties

This is indeed so, as in Wilson chambe:

water droplets, $r \sim r_{crit.} \sim 10^{-4}cm$

$\underline{r_{crit}}$: (internal pressure - grad p) $\sim$ (surface forces)

$$\lambda = \frac{h}{P} = \frac{h}{\sqrt{2mE}} \sim \underline{10^{-8}cm}$$

E, kinetic Energy $\geq 10eV$

Thus, $\boxed{\Delta x \gg \lambda} \longleftarrow$e$^-$ behaves as a "particle"

cannot use "trajectory" if object demonstrates wave properties.

Thus, formulate Uncertainty Principle:

It is impossible to specify simultaneously and precisely the values of certain pairs of physical variables used to describe a system.Those variables are canonically conjugated to each other in the hamilton sense.

$$\begin{aligned} \Delta p \Delta x \geq & \quad \hbar \\ \Delta E \Delta t \geq & \quad \hbar \\ \Delta \phi \Delta L_t \geq & \quad \hbar \end{aligned}$$

1.4 Measurement and Probability in Quantum Mechanics

We talked about "measurement", what exactly do we mean?

Consider a "gedanken" experiment:
two-slit interference

Our detector, D, "measures" the signals when each electron hits it.
Therefore, measuring "intesity" or "probability" for each electron to hit a given spot on a screen.
From the Davis-Germ. experiment we know that we'll get an interderence pattern.

Lets try to explain it

If electrons are particles: each e^- goes either through slit (1) or slit (2)

Then: Probability to hit point x is

$$P = P_{slit(1)} + P_{slit(2)}$$

Interference pattern disappeared!!!! What happened? $\boxed{P \neq P_{slit(1)} + P_{slit(2)}}$

Same situation would occur if we tried to "follow" each electron, for example, by counting electrons exiting each slit wit laser impulses!

Thus,

(1) Measurement affects quantum state!
(2) Must find a new way of computing probabilities.

Thus, $\boxed{\text{wave function}}$: $\boxed{\frac{dw(q_1 t)}{dq} = |\Psi(q,t)|^2}$

Reasons for introducing $\underline{\text{wave analogy}}$,

i.e. amplitued of probability of finding a microobject in $d\vec{q}$ at t,

i.e. measrue and $\underline{\text{interpret}}$ it as probability

Let's come back to wave functions in a second and continue our gedanken experiment.

$\underline{\text{Reason:}}$ Uncertainty principle limits accuracy of the measurementas caronically-conjugated pairs of variables, such as p and x. See how it manifests itself in this experiment.

Suppose we can measure transfered momentum, ΔP from each interaction of e^- with a system of slits, i.e. employ a moving screen, B.

- We would also have to know its location, x.
- Maximum accuracy: $\frac{d}{2}$, d is the distance between maximums of the interference curve.

Recall interference formula (the condition for bright fringes):

$$\boxed{d \sin\theta = m\lambda}\ , m = 0, \pm 1, ...$$

$$\sin\theta \sim \frac{a}{e}$$

$$\text{Thus, } \boxed{\frac{a}{e} = \frac{\lambda}{d}}$$

If p is momentum of e^-, then :
after each slit each electron acquires a vertical component of momentum

$$\tan\theta_1 \; sim\theta_1 \sim \frac{p_{1y}}{p}$$

$$\tan\theta_2 \; sim\theta_2 \sim \frac{p_{2y}}{p}$$

Thus, total momentum of screen B:

$$|\vec{p}_{1y} + \vec{p}_{2y}| \sim \Delta p \sim p|\theta_1 + \theta_2|$$

can show that $|\theta_1 + \theta_2| \sim \frac{a}{e}$, $\boxed{\frac{\Delta p}{p} = \frac{a}{e}}$ Thus, $\frac{\Delta p}{p} = \frac{\lambda}{d}$, <u>but:</u> $p = \frac{h}{\lambda}$ (de Broglie)

Thus, $\boxed{d = \frac{h}{\Delta p}}$, but if you do measure and intercept disappeared

then, $\Delta x\frac{d}{2}$, $\boxed{\Delta p\Delta x\frac{h}{2}}$

<u>Thus:</u> have a particular case of uncertainty principle for Δp and Δx.
What does it mean for quantum motion and Newton's Laws?

2nd <u>Newtonian Law:</u> $\vec{F}(x) = \frac{d\vec{p}}{dt}$?
gives <u>trajectory</u> , x and p

Must be scrapped?

Yes and No:
1^{st} law (relativity principle) stands
2^{nd} law (action = reaction) stands

Thus, will see that the 2^{nd} law will remain valid in an average sense (Ehrenfest's Theorem).

1.5 The Wave Function: Wave Packets

Quantum mechanics contends that the wave function contains the maximum amount of information that nature allows (Copenhagen interpretation of Quantum Mechanics)

From our gedanken experiments we derive:
$p = |\Psi|^2$, $\Psi = \Psi_1 + \Psi_2$
Thus, $p_{slit(1)} = |\Psi_1|^2$, $p_{slit(2)} = |\Psi_2|^2$
Thus, $p \neq p_{slit(1)} + p_{slit(2)}$, intensity of waves that reached the detector and were interpreted as probability.

But what about trajectory? Will have to consider $\underline{\underline{\text{wave packets}}}$.

Wave Packets

Consider the propagation of (de Broglie) matter waves in homogenious, isotropic medium:

$\sim e^{i(\vec{k}\cdot\vec{r}-wt)}$, where $\hbar w = E$ is the energy of a particle.
The phase velocity $\underline{S_{ph} = \frac{w}{k}}$.

The extent of this wave is infinite. In order to associate with a particle, one must build a superposition of plane waves of neighboring wave vectors which has a finite extent:

$$\Psi(\vec{r}, t) = \int A(\vec{k'}) exp[i(\vec{k'}\vec{r} - w't)] d^3\vec{u'} \tag{1.5}$$

Where $A\vec{k'}$ has appreciable values for $\vec{k'} \sim \vec{k}$ and “o” elsewhere

This is a $\underline{\underline{\text{wave packet.}}}$ Notice that group velocity is the velocity of the region of maximum reinforcement in the interference of several waves of approximately the same λ. Therefore, it is the velocity of a packet and of the corresponding particles. By definition: $v_{gr} = \frac{dw}{dk}$ and $v_{part} = \frac{dE}{dp}$;

$$\Longrightarrow \frac{de}{dk} = \frac{dE}{dp} = \hbar\frac{dw}{dp} \Longrightarrow dp = \hbar dk \text{ or } \underline{\underline{p = \hbar k}}.$$

Aside: consider motion of a wave packet towards the observer:

$$E = \frac{(p_x)^2}{2m} \Rightarrow \Delta E = \frac{p_x \Delta p_x}{m} = v_x \Delta p_x$$
$$\Delta t = \frac{\Delta x}{v_x} \geq \frac{\hbar}{v_x \Delta p_x} = \frac{\hbar}{\Delta E} \Longrightarrow \boxed{\Delta E \Delta t \geq \hbar}$$

<u>General Properties of a wave function:</u>

1. $\Psi(\vec{q}, t)$ is a continuous, single-valued and bounded function of q and t.

2. $\Psi(\vec{q}, t)$ is "normalizable" since our microobject is located somewhere:
   $\int_{\infty}^{\infty} d\vec{q_n} |\Psi(q_n, t)|^2 = \begin{cases} 1, & \text{for finite motion} \\ \infty, & \text{for infinite motion} \end{cases}$

3. Phase is arbitrary,
   $\Psi \longrightarrow \Psi' = e^{i\alpha}\Psi$, as $|\Psi|^2 = |\Psi'|^2$

This is an example of <u>gauge invariance</u>.
Most importantly, wave functions satisfy <u>superposition principle:</u>

If quantum system (object) can be in a state described by $\Psi_1(q_1, t)$ in which some physical quantity, f, can be measured to be f_1 <u>and</u> in a state $\Psi_2(q, t)$ in which $f \longrightarrow f_2$. Therefore, and linear combination $\Psi = C_1\Psi_1 + C_2\Psi_2, C_1, C_2$ It is possible and describes a state whose measurement will yeild either f_1 or f_2

This principle automactically implies that any differential equation that describes quantum motion must be <u>linear</u>
What is this equation?

1.6 Optical analogy: Quazi-classical wave function.

<u>Recall Optics:</u> for $\lambda \rightarrow 0$: geometrical optics light rays.

Note: $\lambda \rightarrow 0$ in the sense $\frac{\lambda}{\Delta x} \ll 1$!
This is similar to what we discussed in quantum mechanics, limits of classical trajectories, etc.

Draw analogy from optics:

Recall: $u(\vec{r},t) = a' \exp\,(i\,\underbrace{(\vec{k}\cdot\vec{r} - wt)}_{\text{goes to } \infty \text{ if } \lambda \longrightarrow 0}) = a' \exp\, i(\frac{}{\lambda} - wt)$

large phase

For waves that are not plane waves, but for which geometrical approximation still work:

$$u = ae^{i\phi}$$

ϕ, "eikonal", large for $\lambda \rightarrow 0$; a, smooth function of r
estimate derivative of $a(x_i)$:

$$\frac{\partial a}{\partial x_i} \sim \frac{\Delta a}{\Delta x_i} \sim \frac{a}{\Delta x_i}$$

$$\frac{\partial^2 a}{\partial (x_i)^2} \sim \frac{a}{\Delta (x_i)^2}$$

Recall wave equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^t} = 0$$

or

$$\frac{\partial^2 u}{\partial {x_i}^2};\; x_i = (\vec{r}, ict)$$

apply to (x)!!!

$$\frac{\partial^2 u}{\partial {x_i}^2} = \frac{\partial}{\partial x_i}\left(\frac{\partial a}{\partial x_i}e^{i\phi} + ia\frac{\partial \phi}{\partial x_i}e^{i\phi}\right) =$$

$$\left(\frac{\partial^2 a}{\partial {x_i}^2} + 2i\frac{\partial a}{\partial x_i}\frac{\partial \phi}{\partial x_i} + ia\frac{\partial^2 \phi}{\partial {x_i}^2} \text{ - } a\left(\frac{\partial \phi}{\partial x_i}\right)^2\right)e^{i\phi}$$

since ϕ^2 is "large" : $\boxed{a\phi^2 \gg (a, a\phi)}$ thus $\boxed{(\frac{\partial \phi}{\partial x_i})^2 = 0}$ $\longleftarrow$ *eikonel equation*

$$\text{thus, } \underbrace{\left(\frac{\partial \phi_o}{\partial \vec{r}}\right)^2}_{} = \frac{1}{c^2}\underbrace{\left(\frac{\partial \phi_o}{\partial t}\right)^2}_{}$$

$$\frac{w^2}{c}\vec{n} = \vec{k} \qquad \frac{w^2}{c^2} = k^2$$

$$\text{Thus, } \boxed{\frac{\partial \phi_o}{\partial \vec{r}} = \vec{k}}$$

Write: $\phi_o = \int \frac{\partial \phi_o}{\partial \vec{r}} d^3\vec{r}$

$$\delta\phi_o = \delta \int \frac{\partial \phi_o}{\partial \vec{r}} d^3\vec{r} = \int d^3 r \delta(\frac{\partial \phi_o}{\partial \vec{r}}) = 0$$

$$\text{Thus, } \boxed{\delta\phi_o = \delta\phi = 0}$$

Fermat's principle of optics: A light ray takes a path which is stationary with respect to the optical path length.
Recall: Classical mechanics: Least action principle,

$$\boxed{\delta S = 0}$$

Since classical mechanics is a limite pf wave mechanics (Quantum Mechanics), we can ssure that:

$$\Phi_{q.c.} = ae^{i\phi} \text{ , } \phi \longrightarrow 0, \underline{\text{and}}\ S = const.\phi$$

This constant is called Plank's constant $\underline{\hbar}$! thus, $S = \hbar\phi$ and $\Psi_{q.c.} = ae$!

Note: since $\Psi \longrightarrow \infty$ in "geometric limit", $S \gg \hbar$ for classical objects.

Example: Moving car $m \simeq 1000kg$
$v \simeq 10m/s$
$\Delta t \simeq 10s$

Therefore, $S = \int L dt = \frac{mv^2}{2}\Delta t = 0.5 \times 10^6 J \cdot s$! $\hbar = 1.05^{-36} J \cdot s$!
Thus, $S \gg \hbar$!

1.7 Correspondence Principle

Let's formulate correspondence principle

In quantum mechanics, each physical quantity corresponds to an operator whose action on Ψ_{qc} reduces to multiplication of Ψ_{qc} by a cprresponding physical quantity.

$$L \longrightarrow \hat{L}\Psi_{qc} = L\Psi_{qc}$$