Physics 115B Notes

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I. LECTURE 1

We first attempt to address the mysterious stuff such as the uncertainty principle in quantum mechanics:

$$\Delta x \Delta p \geq \frac{\hbar}{2} \tag{1}$$

$$\Delta t \Delta E \geq \frac{\hbar}{2} \tag{2}$$

In Classical mechanics, we have Noether's theorem which states that for every symmetry of the Lagrangian, there is a conserved quantity. We have some favorites: time translation gives energy conservation; space translation gives momentum conservation:

$$x \to p \tag{3}$$

$$t \to E \tag{4}$$

So we know these values are connected, by why? We start with momentum, which is a key quantity in physics. We find that it is actually really hard to define momentum. In first year, we define momentum of the Newtonian definition which calls momentum the "quantity of motion":

$$F = ma = \frac{dp}{dt}, \quad p = \int F dt = \int m\frac{dv}{dt}dt = mv \tag{5}$$

In physics 1c, we see that momentum is defined:

$$p = \gamma mv = \frac{mv}{\sqrt{1 - \left(\frac{v}{c}\right)^2}} \tag{6}$$

In our second year physics classes. we see that momentum can be defined using the de brolie definition:

$$o = \frac{h}{\lambda} \quad \text{or} \quad p = \hbar k \quad \text{with} k \equiv \frac{2\pi}{\lambda} \tag{7}$$

Then, in physics 105, we see that the generalized momentum is defined:

$$p_j = \frac{\partial \mathcal{L}}{\partial \dot{q}} \tag{8}$$

where $\mathcal{L} \equiv T - U$ (sometimes) and $\mathcal{L} = \sum_j p_j \dot{q}_j - \mathcal{H}$ from the Legendre transform and $\mathcal{H}(q, p)$ is the Hamiltonian and $\mathcal{L}(q, \dot{q})$ is the Lagrangian.

Going into our 3rd year, we learned that:

$$p = \frac{\hbar}{i}\nabla; \quad p_x = \frac{\hbar}{i}\frac{d}{dx} \tag{9}$$

In this class we are going to find that p in the generator of translations. We will also learn that:

$$\Pi = p - qA \tag{10}$$

where Π is the mechanical or kinetic observable, and p is the canonical or the conjugate momentum. They are both linear momentum (nothing to do with angular momentum). From this list, we hgave at least 9 possible definitions for p! We can rule out a few of them(mv or $\frac{\hbar}{i}\nabla$), because we want definitions to be always true. We also note a bootstrapping problem. For exmaple, in the formula $F = ma$, the definitions of F and m is quite circular which is another we're trying to avoid.

Spo here's the upshot: we shouldn't be discussing momentum at all, if we have to:

$$\vec{p} \equiv h\vec{K}, \quad \text{with} \quad |K| = \frac{1}{\lambda} \tag{11}$$

where $\vec{K}$ is the wave-vector or the spatial frequency, is a fundamental quantity, not $\vec{p}$.

What special relativity teaches us is that space and time are not separate, they are combined to create spacetime. In a change of coordinates in space (rotation), we have:

$$\begin{pmatrix} x' \\ y \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \tag{12}$$

Rotation in space corresponds to a boost in spacetime, we have an analagous rotation matrix:

$$\begin{pmatrix} ct' \\ x' \end{pmatrix} \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix} \begin{pmatrix} ct \\ x \end{pmatrix} \tag{13}$$

where

$$\cosh\theta = \gamma, \quad \gamma = \frac{1}{\sqrt{1-\beta^2}} \tag{14}$$

$$\sinh\theta = \beta\gamma, \quad \beta = \frac{v}{c} \tag{15}$$

We know that rotations preserves distances (regardless of angle θ), that is:

$$x'^2 + y'^2 = x^2 + y^2 \tag{16}$$

Meanwhile boost preserve the interval:

$$(ct')^2 - (x'^2 + y'^2 + z'^2) = (ct)^2 - (x^2 + y^2 + z^2) \tag{17}$$

this is reflected from the fact that the determinant of both matrices are 1. There is also a nice geometry intuition which is the spacetime is in fact hyperbolic.

One ugly thing is that we need to put ct so that the unit works out. In some sense, C is a historical legacy that hides the geometry. It also means that we are using two sets of units in the same setting. For more details, see Parables of the surveys in Taylor and Wheeler.

That was special relativity, now let's go back to quantum mechanics: the wave equation says:

$$\frac{1}{V^2}\frac{\partial^2 u}{\partial t^2} = \nabla^2 u = \frac{\partial^2 u}{\partial x^2} \tag{18}$$

solution looks like $u(ft - kx) = u(\phi)$. We can check it quite easily:

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial \phi}\frac{\partial \phi}{\partial t} = \dot{u}f \tag{19}$$

$$\frac{\partial^2 u}{\partial t^2} = \ddot{u}f^2 \tag{20}$$

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \phi}\frac{\partial \phi}{\partial x} = \dot{u}(-k) \tag{21}$$

$$\frac{\partial^2 u}{\partial x^2} = \ddot{x}k^2 \tag{22}$$

This gives:

$$\frac{1}{V^2} \cdot f^2\ddot{u} = k^2\ddot{u} \tag{23}$$

This, this is a solution if $\left(\frac{f}{k}\right)^2 = v^2$. We recognize that V is the phase velocity. We can show that by picking some constant $\phi_{\text{const}} = ft - kx$:

$$kx = ft - \phi_c \tag{24}$$

$$x = \frac{f}{k}t - \frac{\phi_c}{k} \tag{25}$$

$$\frac{dx}{dt} = \frac{f}{k} = v_{\text{phase}} \tag{26}$$

Here, ϕ is a scalar number. Now, we want to connect the wave equation to relativity. Things we can count don't transform under a Lorentz boost. This discussion of scalar leads us to vectors, namely four-vectors.

Everyone agree that:

$$(ct)^2 - x^2 = S^2 = \begin{pmatrix} ct & x \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} ct \\ x \end{pmatrix} = \Gamma^\mu \Gamma_\mu \tag{27}$$

We can write that:

$$ft - Kx = \phi = \begin{pmatrix} \frac{f}{c} & x \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} ct \\ x \end{pmatrix} = K^\mu \Gamma^\mu \tag{28}$$

where K^μ is the four-wave vector and Γ_μ is the four-position vector. The final product (dot/scalar product) ($K^\mu\Gamma^\mu$) is invariant under rotations (even hyperbolic rotations = boost). We can form another dot product:

$$K^\mu K_\mu = \begin{pmatrix} \frac{f}{c} & K \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \frac{f}{c} \\ K \end{pmatrix} = \left(\frac{f}{c}\right)^2 - K^2 = K_c^2 \tag{29}$$

and this value (Compton wave vector) also must be invariant. We calculate $x(hc)^2$:

$$(hf)^2 - (h\vec{k}c)^2 = (hK_c c)^2 \tag{30}$$

We define:

$$E \equiv hf \tag{31}$$

$$\vec{p} \equiv h\vec{k} \tag{32}$$

$$m \equiv \frac{hK_c}{c} \tag{33}$$

We derived the Einstein Energy-Momentum principle:

$$E^2 - \vec{p}^2 c^2 = m^2 c^4 \tag{34}$$

II. LECTURE 2

We first review the material from last class. We made 2 assumptions: 1, the geometric of spacetime is hyperbolic; 2, we have waves. We found 2 4-vectors:

$$r = (ct, \vec{r}), \quad \text{position in real space(time)} \tag{35}$$

$$k = (\frac{f}{c}.\vec{k}), \quad \text{position in reciprocal space(time)} \tag{36}$$

We can think of the second as the frequency space (or momentum space), with the first being the temporal frequency and the second as spacial frequency. From these four-vectors, we get 3 variants:

$$rr = \text{"interval" } S^2 \tag{37}$$

$$Kr = \text{phase } \phi \tag{38}$$

$$KK = \text{Compton wave-vector } K_c^2 \tag{39}$$

We define all our classical quantities based on these wave parameters. For instance:

$$\text{Energy}: \quad E \equiv hf \tag{40}$$

$$\text{Momentum}: \quad \vec{p} \equiv h\vec{K} \quad (k = 1/\lambda) \tag{41}$$

$$\text{Mass}: \quad m \equiv \frac{hK_c}{c} \tag{42}$$

$$\text{action}: \quad S \equiv h\phi \tag{43}$$

In fact, we don't need any of these "new" old-fashioned concept to do physics. (we do need them to communicate with more old-fashioned physicists.)

Let's demonstrate that we can consider classical mechanics as a limiting case of wave mechanics (QM).

Let's consider a a probability function $|\Psi(x)|^2$ and in the reciprocal space $|\bar{\Psi}(k)|^2$. We know that its spread are inverse of each other: $\sigma_x \sim \frac{1}{\sigma_k}$, or the uncertainty principle: $\sigma_x \sigma_k \geq \frac{1}{4\pi}$.

Classically, the "probability function" in position and momentum space would just be a delta-function (since they are well-localized). Well, it seems like this violate the uncertainty principle.

The resolution of this seemingly paradox is that we do in fact has $\sigma_x \sim \frac{1}{\sigma_k}$. Classically, we have $\bar{x} >> \sigma_x$ and $\bar{k} >> \sigma_k$. Or:

$$\frac{\sigma_x}{\bar{x}} \to 0 \quad \text{as} N(\text{number of particles}) \to \text{large} \tag{44}$$

$$\frac{\sigma_k}{\bar{k}} \to 0 \quad \text{as} N(\text{number of particles}) \to \text{large} \tag{45}$$

There's no contradiction here. In one dim: $\bar{x} \sim N$ and $\sigma_x \sim \sqrt{N}$; $\bar{k} \sim N$ and $\sigma_k \sim \sqrt{N}$. Thus, both distributions look like delta-function in the classical limit: "object" can be well-localized in real and reciprocal space.

Classical "objects"(waves) follow the path where the phase(action) is stationary. With this wave interpretation, we can justify the classical postulate.

Consider we have two paths from (x_1, y_1) to (x_2, y_2) separate by δ_y. We enforce the phase in stationary:

$$-\phi = \vec{k} \cdot \vec{r} - f \tag{46}$$

$$= \int \vec{k} \cdot d\vec{r} - f dt \tag{47}$$

This way we allow for a potential, i.e. $\vec{k}$ and f might change over the path. We require ϕ ton be a min or max (extremum) along the path: $\delta\phi = 0$.(Marion and Thorton "modified Hamilton's principle"). We get:

$$-\phi = \int (k\dot{r} - f)dt \quad \text{where} \dot{r} \equiv \frac{dr}{dt} \tag{48}$$

Here the integrand in the Lagrangian: $\mathcal{L} = h\dot{\phi}$. We have:

$$\delta\phi = 0 = \int (\delta k\dot{r} + k\delta\dot{r} - \delta f)dt \tag{49}$$

then

$$\int k\delta\dot{r}dt = \int k\delta dr = \int kd(\delta r) = k\delta r\Big|_1^2 - \int \delta r dk \tag{50}$$

The surface term disappear:

$$0 = \int (\delta k\dot{r} - \delta r\dot{k} - \frac{\partial f}{\partial r}\delta r - \frac{\partial f}{\partial k}\delta k)dt \tag{51}$$

$$= \int \left[\delta k \left(\dot{r} - \frac{\partial f}{\partial k}\right) - \delta r \left(\dot{k} + \frac{\partial f}{\partial r}\right)\right] dt \tag{52}$$

For this to be true, both terms nee to be 0, this means that:

$$\dot{r} = \frac{\partial f}{\partial k} \tag{53}$$

$$\dot{k} = -\frac{\partial f}{\partial r} \tag{54}$$

This is our equation of motion. The first is also our group velocity $v_{\text{group}} = \frac{\partial \mathcal{H}}{\partial p}$ (compared to $v_{\text{phase}} = \frac{f}{k}$). We time the second equation by h:

$$\dot{p} = \frac{d\vec{p}}{dt} = -\frac{\partial \mathcal{H}}{\partial \vec{r}} = -\frac{\partial}{\partial \vec{r}}(T+U) = -\frac{\partial}{\partial \vec{r}}U = -\nabla U \equiv \vec{F} \tag{55}$$

This gives us $\vec{F} = \frac{d\vec{p}}{dt}$ which is Newton's 2nd law. Using this analysis, we can write:

$$\frac{df}{dt} = \frac{\partial f}{\partial r}\frac{dr}{dt} + \frac{\partial f}{\partial k}\frac{dk}{dt} + \frac{\partial f}{\partial t} \tag{56}$$

$$= \frac{\partial f}{\partial r}\frac{\partial f}{\partial k} - \frac{\partial f}{\partial k}\frac{\partial f}{\partial r} + \frac{\partial f}{\partial t} = \frac{\partial f}{\partial t} \tag{57}$$

This tells us that if Hamiltonian is time independent, then energy is conserved. The equation $\dot{k} = -\frac{\partial f}{\partial r}$ is Noether's theorem. If f(i.e. $\mathcal{H}$) is independent of some coordinate q. then the "momentum conjugate to q is conserved:

$$\frac{\partial f}{\partial x} = 0 \rightarrow k_x, p_x \text{ is conserved} \tag{58}$$

$$\frac{\partial f}{\partial \theta} = 0 \rightarrow L \text{ is conserved} \tag{59}$$

We have recovered all of classical physics from our discussion of wave. We don't really need $\vec{p}, E, S$.... We can rewrite the energy momentum relation as follows:

$$f^2 - \vec{k}^2 = m^2 \tag{60}$$

For QM, we are much better off without them. The classical quantum mechanical uncertainty principle says:

$$\Delta x \Delta p \geq \frac{\hbar}{2} \tag{61}$$

$$\Delta t \Delta E \geq \frac{\hbar}{2} \tag{62}$$

where now we can write:

$$\Delta x \Delta k \geq \frac{1}{4\pi} \quad (k = \lambda) \tag{63}$$

$$\Delta t \Delta f \geq \frac{1}{4\pi} \tag{64}$$

III. LECTURE 3

Now we see that we don't need E, p, S.... Now for a few examples. The first example was the uncertainty principle which we did in the first lecture. The second example is the Schrodinger equation and momentum in quantum mechanics. The schrodinger equation:

$$-\hbar\frac{\partial\Psi}{\partial t} = \mathcal{H}\Psi \tag{65}$$

$$-i\hbar\frac{\partial\Psi}{\partial x} = p\Psi \tag{66}$$

where $\omega = 2\pi f = 2\pi/T$ amd $k = 2\pi/\lambda = 1\Theta$ depending on our conversion. Unit of ω is radians/s $(1/s)$; the unit of f is cycles/s $(1/s)$. In our standard notation, this could be a bit confusing. We can also write:

$$i\frac{\partial\Psi}{\partial t} = \hat{\omega}\Psi \tag{67}$$

$$-i\frac{\partial\Psi}{\partial x} = \hat{k}\Psi \quad \text{where} \quad k = \frac{2\pi}{\lambda} \tag{68}$$

We want to answer the question: How does the wavefunction change in time? In traditional units, the answer would be according to the Hamiltonian (momentum), or according to its frequency (spatial frequency) in the modern units.

Now the 3rd example. The plane wave in traditional units:

$$\Psi = \Psi_0 e^{\phi(\vec{p}\cdot r - \vec{E}t)/\hbar} \tag{69}$$

where in our new units (more concise and more physical):

$$\Psi = \Psi_0 e^{i(\vec{k}\vec{r} - \omega t)} \tag{70}$$

In Griffiths, the Fourier transform is defined:

$$\Psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} e^{ipx/\hbar}\bar{\Psi}(p)dp \tag{71}$$

and

$$\Psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-ikx}\bar{\Psi}(k)dk \tag{72}$$

where $k = \frac{2\pi}{\lambda}$ or we can write

$$\Psi(x) = \int_{-\infty}^{\infty} e^{2\pi ik\cdot x}\bar{\Psi}(k)dk \tag{73}$$

where $k = \frac{1}{\lambda}$.

In some sense, the Fourier transform in Dirac notation:

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar} \tag{74}$$

and in new units:

$$\langle k|x\rangle = e^{-2\pi i k\cdot x} \tag{75}$$

there are many more examples (9n chapter 6, time evolution, translations, boost, rotation operators...) Before we can use E, p we must convert it out of traditional units. Using 2 line summary, we have two defined constants: c relates to x and t; while h relates to x, t to m. While the numerical meaning of c, it does indicates that we have a limiting velocity. Also, we don't have a physical distinction between E, f or $\vec{p}, \vec{k}$.

We now move to QM and talk about the postulates of QM (ch3).

1. pure states are described by vectors(rays) $|\Psi\rangle$ in Hilbert space.

2. every observable is described by an operator A acting in this space

3. Measurements of the observable only return eigenvalues of A.

4. Principle of spectral decomposition: $A|u_n\rangle = a_n|u_n\rangle$ (abbrv to $A_0|n\rangle = n|n\rangle$)
   and $p(n) = |\langle n|\Psi\rangle|^2$. In the discretw, non-degenerate case: $|\Psi\rangle = \sum c_n|n\rangle$ and $P(n) = |c_n|^2$.
   In the Dirac notation,

   $$|\Psi\rangle = \mathbb{1}|\Psi\rangle = (\sum_n |n\rangle\langle n|)|\Psi\rangle = \sum_n |n\rangle\langle n|\Psi\rangle = \sum_n |n\rangle c_n \tag{76}$$

   . This is called closure or "completeness". There are some "obvious" extensions, if we have some degeneracy:

   $$P(n) = \sum_{i=1}^{g_n} |\langle n_i|\Psi\rangle|^2 \tag{77}$$

   where g_n is the degree of degeneracy and the $|n_i\rangle$ are the g_n orthonormal vectors spanning the subspace with eigenvalue n.

   If our basis are continuous:

   $$dP(\alpha) = |\langle\alpha|\Psi\rangle|^2 d\alpha \tag{78}$$

   is the probability of finding a result in $[\alpha, \alpha + d\alpha]$, where $|\alpha\rangle$ is the eigenvector corresponding to the eigenvalue α

5. If measuring A on $|\Psi\rangle$ gives n, the state of the system immediately after the measurement is the normalized projection: $\frac{P_n|\Psi\rangle}{\sqrt{\langle\Psi|P-n|\psi\rangle}}$. For the discrete, non-deg case, our projection operator is $p_n = |n\rangle\langle n|$ and $\frac{|n\rangle\langle n|\Psi\rangle}{\sqrt{\langle\Psi|n\rangle\langle n|\Psi\rangle}} = |n\rangle$

6. The time evolution of $|\Psi\rangle$ is governed by the Schrodinger equation:

$$i\hbar\frac{d}{dt}|\Psi(t)\rangle = \mathcal{H}(t)|\Psi(t)\rangle \tag{79}$$

or:

$$i\frac{d}{dt}|\Psi(t)\rangle = \hat{\omega}(t)|\Psi(t)\rangle \tag{80}$$

To summarize:

1. States $|\Psi\rangle$ are in Hilber space
2. Observables are Hermitian operators
3. Measurements give eigenvalues
4. spectral decomposition
5. measurements project (wavefunction collapse)
6. time evolution (Schrodinger equation)

Previously, we wrote $|\Psi\rangle = \sum_n c_n|n\rangle$. We can consider the result of a measurement:

$$\langle n|\Psi\rangle = \langle n|\sum_m c_m|m\rangle \tag{81}$$

$$= \sum_m c_m\langle n|m\rangle \tag{82}$$

$$= \sum_m c_m\delta_{nm} = c_n \tag{83}$$

or:

$$\langle n|\Psi\rangle = \langle n|\mathbb{1}|\Psi\rangle \tag{84}$$

$$= \langle n|\sum_m |m\rangle\langle m|\Psi\rangle \tag{85}$$

A better way to understand the Dirac notation is to see the analogy to regular vectors in linear algebra. All

Dirac Notation	regular vectors
Ket $\|\Psi\rangle$	Column $\vec{a}$
bra $\langle\Psi\|$	Row $\vec{b}$
Inner product $\langle\psi\|\phi\rangle$	$\vec{b}\cdot\vec{a}$
Operator (time evolution $e^{-i\mathcal{H}t/\hbar}$)	rotation R
Matrix element $\langle\phi\|e^{-i\mathcal{H}t/\hbar}\|\psi\rangle$ (time evolve $\|\Psi\rangle$ and then project on $\|\Psi\rangle$)	$\vec{b}R\vec{a}$ (rotate $\vec{a}$ and then project on $\vec{b}$)

these statements are independent of basis. We can pick a specific coordinate system:

$$\begin{pmatrix} bx & b_y & b_z \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_x \\ a_y \\ a_z \end{pmatrix} \tag{86}$$

Then we have:

$$\vec{a} = (\vec{a}\cdot\hat{x})\hat{x} + (\vec{a}\cdot\hat{y})\hat{y} + (\vec{z}\cdot\hat{z})\hat{z} \tag{87}$$

In Dirac Notation:

$$\mathbb{1}|\Psi\rangle = \sum |n\rangle\langle n|\Psi\rangle \tag{88}$$

IV. LECTURE 4

Completeness means that our basis vectors span the space:

$$\mathbb{1} = \sum |n\rangle\langle n| \tag{89}$$

We define:

$$\hat{x} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad \hat{y} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \hat{z} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \rightarrow \quad \text{with regular vectors} \tag{90}$$

We have:

$$
\begin{aligned}
\mathbb{1} &= \hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z} & (91)\\
&= \begin{pmatrix}1\\0\\0\end{pmatrix}\begin{pmatrix}1 & 0 & 0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix}\begin{pmatrix}0 & 1 & 0\end{pmatrix} + \begin{pmatrix}0\\0\\1\end{pmatrix}\begin{pmatrix}0 & 0 & 1\end{pmatrix} & (92)\\
&= \begin{pmatrix}1 & 0 & 0\\0 & 0 & 0\\0 & 0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0 & 0\\0 & 1 & 0\\0 & 0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0 & 0\\0 & 0 & 0\\0 & 0 & 1\end{pmatrix} = \begin{pmatrix}0 & 0 & 0\\0 & 0 & 0\\0 & 0 & 1\end{pmatrix} & (93)\\
&= \mathbb{1} & (94)
\end{aligned}
$$

$$
\begin{aligned}
\vec{a} &= \mathbb{1}\vec{a} = \mathbb{1}\mathbb{1}\vec{a} & (95)\\
&= \sum_{j=x,y,z} \hat{j}(\hat{j}\cdot\vec{a}) = \sum_{i,j} \hat{i}(\hat{i}\hat{j})(\hat{j}\vec{a}) & (96)
\end{aligned}
$$

and

$$
\sum_{i,j} \hat{i}\cdot\hat{j} = \begin{pmatrix}\hat{x}\hat{x}' & \hat{x}\hat{y}' & \hat{x}\hat{z}'\\ \hat{y}\hat{x}' & \hat{y}\hat{y}' & \hat{y}\hat{z}'\\ \hat{z}\hat{x}' & \hat{z}\hat{y}' & \hat{z}\hat{z}'\end{pmatrix} \tag{97}
$$

we have:

$$
\begin{pmatrix}a_x\\a_y\\a_z\end{pmatrix} = \begin{pmatrix}\hat{x}\hat{x}' & \hat{x}\hat{y}' & \hat{x}\hat{z}'\\ \hat{y}\hat{x}' & \hat{y}\hat{y}' & \hat{y}\hat{z}'\\ \hat{z}\hat{x}' & \hat{z}\hat{y}' & \hat{z}\hat{z}'\end{pmatrix}\begin{pmatrix}a'_x\\a'_y\\a'_z\end{pmatrix} = \begin{pmatrix}\cos\theta & \sin\theta & 0\\ -\sin\theta & \cos\theta & 0\\ 0 & 0 & 1\end{pmatrix} \tag{98}
$$

Quantum mechanics problems are often just a change of basis. It might be easy to write $V(x)$. but easier to solve it in $\psi\bar(k)$. One example is the infinite square well: Suppose:

$$
\psi(x) = \begin{cases} A & 0 < x < \frac{L}{2}\\ 0 & \text{else}\end{cases}
$$

We normalize in the Dirac notation:

$$
\begin{aligned}
\langle\psi|\psi\rangle = 1 = \langle\psi|\mathbb{1}|\psi\rangle &= \langle\psi|\int dx|x\rangle\langle x||\psi\rangle & (99)\\
&= \int dx\langle\psi|x\rangle\langle x|\psi\rangle = \int dx\psi^*(x)\psi(x) & (100)\\
&= \int_0^{L/2} dx A^* A = A^2\frac{L}{2} \to A = \sqrt{\frac{2}{L}} & (101)
\end{aligned}
$$

Let's say we want this state $|\psi\rangle$ in the $|k\rangle$ representation:

$$\bar{\psi}(k) = \langle k|\psi\rangle = \langle k|\mathbb{1}|\psi\rangle \tag{102}$$
$$= \int dx \langle k|x\rangle\langle x|\psi\rangle = \int_0^{L/2} e^{-2\pi i k x}\sqrt{\frac{2}{L}}\psi(x)dx \quad \text{where we pick} \quad k = \frac{1}{\lambda} \tag{103}$$
$$= \sqrt{\frac{2}{L}}\frac{1}{-2\pi i k}e^{-2\pi i k x}|_0^{L/2} \tag{104}$$
$$= \sqrt{\frac{2}{L}}\frac{1}{2\pi i k}(-e^{-2\pi i k\frac{L}{2}}+1) = \sqrt{\frac{2}{L}}\frac{e^{-2\pi i k\frac{L}{4}}}{2\pi i k}(e^{2\pi i k\frac{L}{4}} - e^{-2\pi i k\frac{L}{4}}) \tag{105}$$
$$= \sqrt{\frac{2}{L}}\frac{e^{-2\pi i k\frac{L}{4}}}{2\pi i k L/4}\frac{L}{4}\sin\left(\frac{2\pi k L}{4}\right) \tag{106}$$
$$= \sqrt{\frac{2}{L}}e^{-2\pi i k\frac{L}{4}}\,\text{sinc}\left(\frac{2\pi k L}{4}\right) \quad \text{where} \quad \text{sinc}(x) = \frac{\sin x}{4} \tag{107}$$

We can see that the normalization is the inverse of our previous normalization. This is familiar from single slit diffraction (narrow in real space $\rightarrow$ wide reciprocal space). The second term (exponential) is a phase factor. (in Chapter 6, we will see that it is a translation operator that translates by $\frac{L}{4}$)

Now we have two bases $\psi(x), \bar{\psi}(k)$. We shall move to a 3rd basis (we are using the short hand $|\psi_n\rangle = |n\rangle$):

$$c_n = \langle n|\psi\rangle = \langle n|\mathbb{1}|\psi\rangle = \langle n|\int dx|x\rangle\langle x||\psi\rangle \tag{108}$$
$$= \int dx\langle n|x\rangle\langle x|\psi\rangle \tag{109}$$
$$= \int dx\varphi_n^*(x)\psi(x) \quad \text{where} \quad \varphi_n(x) = \frac{2}{L}\sin\left(\frac{n\pi x}{L}\right),\ n = 1, 2, ... \tag{110}$$
$$= \int_0^{L/2} dx\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) = \frac{2}{L}\frac{-L}{n\pi}\cos\left(\frac{n\pi x}{L}\right)|_0^{L/2} = \frac{2}{n\pi}\left(1-\cos\frac{n\pi}{2}\right) \tag{111}$$

So we have:

$$c_1 = \frac{2}{\pi} \quad c_2 = \frac{2}{\pi}(1-\cos\pi) = \frac{2}{\pi} \quad c_3 = \frac{2}{3\pi} \quad c_4 = 0, \quad \text{and} \quad \sum_n^\infty |c_n|^2 = 1 \tag{112}$$

We see that the completeness relation holds.

We can describe our state in 3 different ways:

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \int dx|x\rangle\langle x||\psi\rangle = \int_0^{L/2} dx|x\rangle\sqrt{\frac{2}{L}} \tag{113}$$
$$= \int dk|k\rangle\langle k|\psi\rangle = \int_{-\infty}^{\infty} dk|k\rangle\sqrt{\frac{L}{2}}e^{-\frac{2\pi i k L}{4}}\,\text{sinc}\left(\frac{2\pi k L}{4}\right) \tag{114}$$
$$= \sum|\varphi_n\rangle\langle\varphi_n|\psi\rangle = \frac{2}{\pi}|1\rangle + \frac{2}{\pi}|2\rangle + \frac{2}{3\pi}|3\rangle + ... \tag{115}$$

with

$$\langle x|\varphi_n\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad \langle x|\psi\rangle = \frac{2}{\pi}\sqrt{\frac{2}{L}}\left[\frac{\sin\pi x}{L} + \frac{\sin 2\pi x}{L} + \frac{\sin 3\pi x}{L} + ...\right] \tag{116}$$

To summarize:

$$\mathbb{1} = \int dx|x\rangle\langle x| = \int dk|k\rangle\langle k| = \int dp|p\rangle\langle p| = \sum|\varphi_n\rangle\langle\varphi_n| \tag{117}$$

and these are the energy eigenstates for a bound state.

$$|\psi\rangle = \int dx|x\rangle\langle x|\psi\rangle \tag{118}$$
$$= \int dk|k\rangle\langle k|\psi\rangle \tag{119}$$
$$= \int dp|p\rangle\langle p|\psi\rangle \tag{120}$$
$$= \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle \tag{121}$$

and:

$$c_n = \langle\varphi_n|\psi\rangle \tag{122}$$
$$= \langle\varphi|\mathbb{1}|\psi\rangle \tag{123}$$
$$= \int dx\langle\varphi_n|x\rangle\langle x|\psi\rangle \tag{124}$$
$$= \int dx\varphi_n^*(x)\psi(x)... \tag{125}$$

This should be familiar from chapter 2 of Griffiths Couple identities:

$$|\psi\rangle = \mathbb{1}\mathbb{1}|\psi\rangle \tag{126}$$
$$\mathbb{1}|\psi\rangle = \int dx|x\rangle\langle x|\psi\rangle \tag{127}$$
$$\mathbb{1}\mathbb{1}|\psi\rangle = \int dx'|x'\rangle\langle x'|\int dx|x\rangle\langle x|\psi\rangle \tag{128}$$
$$= \int dx'dx|x'\rangle\langle x'|x\rangle\langle x|\psi\rangle \tag{129}$$
$$\langle x'|x\rangle = \delta(k-k') \tag{130}$$
$$\langle x'|x\rangle = \delta(k-k') \tag{131}$$
$$\langle n'|n\rangle = \langle\phi_{n'}|\psi_n\rangle = \delta_{n'n} \tag{132}$$

For infinite square well:

$$\langle n|x\rangle = \left(\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{2}\right)\right)^* \tag{133}$$

$$\langle x|n\rangle = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{2}\right) \tag{134}$$

Other interesting cases

$$\langle\psi|\psi\rangle = \int dx\langle\psi|x\rangle\langle x|\psi\rangle \quad \text{and} \quad \langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-2\pi ipx/\hbar} \tag{135}$$

We attempt to write $|\psi\rangle = |x\rangle$:

$$|x\rangle = \mathbb{1}|x\rangle = \int dx'|x'\rangle\langle x'|x\rangle \tag{136}$$

$$= \int dx'|x'\rangle\delta(x-x') \tag{137}$$

$$\psi(x) = \langle x'|x\rangle = \delta(x-x') \tag{138}$$

V. LECTURE 5

: On Monday, we were talking about some useful identities, such as:

$$\langle x'|x\rangle = \delta(x-x') \tag{139}$$

$$\langle k'|k\rangle = \delta(k-k') \tag{140}$$

One thing we didn't get to is that:

$$|\psi\rangle = \mathbb{1}\mathbb{1}|\psi\rangle = \mathbb{1}|\psi\rangle \tag{141}$$

$$= \int dp|p\rangle\langle p|\int dx|x\rangle\langle x|\psi\rangle \tag{142}$$

$$= \int\int dpdx|p\rangle\langle p|x\rangle\psi(x) \tag{143}$$

$$= \cap dp|p\rangle\langle p|\psi\rangle = \int dp|p\rangle\bar{\psi}(p) \tag{144}$$

If we compare this with the definition of the Fourier transform, it basically tells us:

$$\langle p|x\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{ipx}{\hbar}} \tag{145}$$

$$\langle k|x\rangle = \frac{1}{\sqrt{2\pi}}e^{-ikx} \quad \text{where} \quad k = \frac{2\pi}{\lambda} \tag{146}$$

$$\langle k|x\rangle = e^{-i2\pi kx} \quad \text{where} \quad k = \frac{1}{\lambda} \tag{147}$$

This is just elegant notation, nothing deep mathematically here. Now, we look at other Dirac notations that are essential. We need to know how to form the adjoint, or the Hermitian conjugate.

1. $c \to c^*$
2. $|\varphi\rangle \to \langle\varphi|$
3. $\langle\psi| \to \ker\psi$
4. $A \to A^\dagger \quad (A^\dagger = (A^T)^* = (A^*)^T)$
5. Reverse the other of the factors

$$(\lambda\langle u|A|v\rangle|\omega\rangle|\psi\rangle)^\dagger = |\psi\rangle\langle\psi|\langle v|A^\dagger|u\rangle\lambda^* \tag{148}$$

$$= \lambda^*\langle v|A^\dagger|u\rangle|\psi\rangle\langle\omega| \tag{149}$$

Say we have:

$$A|\psi\rangle = \lambda|\psi\rangle \tag{150}$$

where we call A the operator, the $|\psi\rangle$ is the eigenket, λ is the eigenvalue (maybe complex). Now say $A = A^\dagger$ (meaning that A is Hermitian). Then, the expectation value of A is given:

$$A = \langle\psi|A|\psi\rangle = \langle\psi|\lambda|\psi\rangle = \lambda\langle\psi|\psi\rangle = \lambda \tag{151}$$

Then:

$$(\langle\psi|A|\psi\rangle)^\dagger = \langle\psi|A^\dagger|\psi\rangle = \langle\psi|A|\psi\rangle = \lambda = \lambda^* \tag{152}$$

so we have $(\lambda)^\dagger = \lambda^*$, for $A = A^\dagger$. Thus, the eigenvalues λ must be real. So, we require that measurements return real results $\to$ operators corresponding to observables must be Hermitian. We then follows that:

$$A|\psi\rangle = \lambda|\psi\rangle \tag{153}$$

$$\langle\psi|A^\dagger = |\psi\rangle A = |\psi\rangle\lambda^* = \langle\psi|\lambda \tag{154}$$

$$|\psi\rangle A = |\psi\rangle\lambda \tag{155}$$

$$\langle\psi|A|\psi\rangle = \langle\psi|\lambda|\psi\rangle = \lambda\langle\psi|\psi\rangle \tag{156}$$

This is true for any ket $|\varphi\rangle$, no necessarily an eigenket. These are groundwork for an awesome theorem: Twp eigenvectors of a Hermitian operator corresponding to different eigenvalues are orthogonal. Say we have:

$$A|\psi\rangle = \lambda|\psi\rangle \tag{157}$$

$$A|\varphi\rangle = \mu|\varphi\rangle \tag{158}$$

This gives:

$$\langle\psi|A|\varphi\rangle = \mu\langle\psi|\varphi\rangle \tag{159}$$

$$\langle\psi|A|\varphi\rangle = 1\langle\psi|\varphi\rangle \tag{160}$$

$$0 = (\mu - \lambda)\langle\psi|\mathrm{var}\phi\rangle \tag{161}$$

So if $\mu \neq \lambda$, then we have $\langle\psi|\varphi\rangle = 0$. ($|\psi\rangle$ and $|\varphi\rangle$ are orthogonal). Thus, we can see that that the momentum eigenstates with different momenta are orthogonal. The inifinite square well Hamiltonian eigenstates with different energies are orthogonal. (same with the Harmonic oscillator)

Now we start Chapter 4 of Griffiths. (QM in 3D). We start with our Schrodinger equation:

$$i\hbar = \frac{\partial|\psi\rangle}{\partial t} = \mathcal{H}|\psi\rangle \tag{162}$$

or better:

$$-\frac{\partial}{\partial t}|\psi\rangle = \hat{\omega}|\psi\rangle \tag{163}$$

Here we have

$$p_i \longrightarrow \frac{\hbar}{i}\frac{\partial}{\partial x} \quad \text{or} \quad p \longrightarrow \frac{\hbar}{i}\nabla \tag{164}$$

For now, let's say that ψ is scalar. Recall where $\mathcal{H}$ comes from. We set $c = 1$:

$$E^2 - p^2 = m^2 \tag{165}$$

and

$$E = \sqrt{m^2 + p^2} = m\sqrt{1 + \left(\frac{p}{m}^2\right)} = m\left(1 + \frac{1}{2}\left(\frac{p}{m}\right)^2 + ...\right) \tag{166}$$

We ignore the first term which is the constant and we add a potential:

$$\mathcal{H} = \frac{\vec{p}^2}{2m} + V(\vec{r}) \tag{167}$$

We know that:

$$\vec{p}^2 = \vec{p} \cdot \vec{p} = -\hbar^2 \nabla^2 \tag{168}$$

where the Laplacian is:

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{169}$$

So:

$$i\hbar \frac{\partial \psi}{\partial t} = \mathcal{H}\psi = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) |\psi\rangle \tag{170}$$

Thus, closure in 3D is different:

$$1D: \quad \mathbb{1} = \int dx |x\rangle\langle x| \tag{171}$$

$$3D: \quad \mathbb{1} = \int d^3r |\vec{r}\rangle\langle \vec{r}| \tag{172}$$

Normalization is:

$$1 = \langle \psi | \psi \rangle = \langle \psi | \mathbb{1} | \psi \rangle \tag{173}$$

$$= \langle \psi | \int d^3\vec{r} |\vec{r}\rangle\langle \vec{r} | \psi \rangle \tag{174}$$

$$= \int d^3\vec{r} \langle \psi | \vec{r}\rangle\langle \vec{r} | \psi \rangle \tag{175}$$

$$= \int d^3\vec{r} \psi^*(\vec{r}) \psi(\vec{r}) = 1 \tag{176}$$

Sometimes we can use separation of variables and that is the case here:

$$\Psi(x, y, z, t) = A(x)B(y)C(z)D(t) \tag{177}$$

Then we plug this guess into the Shrodinger equation:

$$i\hbar ABC\dot{D} = -\frac{\hbar^2}{2m}(\ddot{A}BCD + A\ddot{B}CD + AB\ddot{C}D) + V(\vec{r})ABCD \tag{178}$$

Then, divided by Ψ:

$$i\hbar \frac{\dot{D}}{D} = -\frac{\hbar}{2m} \left(\frac{\ddot{A}}{A} + \frac{\ddot{B}}{B} + \frac{\ddot{C}}{C} \right) = E \text{ (constant)} \tag{179}$$

Say we have an infinite square well in 3D:

$$V(\vec{r}) \begin{cases} 0 & \text{for } x, y, z \text{ in} [0, L] \\ \infty & \text{else} \end{cases}$$

Starting from the Shrodinger equation:

$$i\hbar\frac{\dot{D}}{D} = -\frac{\hbar^2}{2m}\left(\frac{\ddot{A}}{A}+\frac{\ddot{B}}{B}+\frac{\ddot{C}}{C}\right)+V(\vec{r}) \tag{180}$$

we have:

$$D = e^{-i\omega t} \tag{181}$$

with $E \equiv \hbar\omega$. Then:

$$-\frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2) \equiv E \tag{182}$$

$$A = \sqrt{\frac{2}{L_x}}\sin\left(\frac{n_x\pi x}{2x}\right) \quad \text{with} \quad n_x = 1,2,3,\text{...and} \quad K_x = \frac{n_x\pi}{L_x} \tag{183}$$

$$B = \sqrt{\frac{2}{L_y}}\sin\left(\frac{n_y\pi y}{2y}\right) \quad \text{with} \quad n_y = 1,2,3,\text{...and} \quad K_y = \frac{n_y\pi}{L_y} \tag{184}$$

$$C = \sqrt{\frac{2}{L_z}}\sin\left(\frac{n_z\pi z}{2z}\right) \quad \text{with} \quad n_z = 1,2,3,\text{...and} \quad K_z = \frac{n_z\pi}{L_z} \tag{185}$$

For our next important case:

$$V(\vec{r}) = V(|\vec{r}|) = V(r) \tag{186}$$

For example, the Hydrogen atom. The Laplacian in the spherical coordinate:

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{187}$$

We again assume separability:

$$\Psi(x,y,z,t) = R(r)Y(\theta,\phi)D(t) \quad \text{where} \quad D = e^{-i\omega t} \tag{188}$$

The time-independent Shrodinger equation:

$$\mathcal{H}\psi = E\psi \quad \text{where} \quad \psi = RY \tag{189}$$

VI. LECTURE 6

We are looking at the special case that $V(\vec{r}) = V(r)$. We also assumed separability as usual. In this case, $\Psi = \psi(r)\phi(t)$ and $\phi(t) = e^{-i\omega t}$ as usual. This leaves us the time-independent Schrodinger equation:

$$\mathcal{H}\psi = E\psi \quad \text{where } E \text{ is the separation constant} \tag{190}$$

Our Hamiltonian:

$$\mathcal{H} = \frac{p^2}{2m} + V(r) \tag{191}$$

and the Schrodinger equation:

$$\frac{p^2}{2m}\psi = (E - V(r))\psi \tag{192}$$

We use separation of variables again:

$$\psi = R(r)Y(\theta,\phi) \quad \text{using} \quad \nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \tag{193}$$

Putting this all together, we have:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{R}\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial R}{\partial r} + \frac{1}{Y}\frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial Y}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]\right) = E - V(r) \tag{194}$$

Then, we times $\left(-\frac{2m}{\hbar^2}r^2\right)$ on both sides:

$$\frac{1}{R}\frac{\partial}{\partial r}r^2\frac{\partial R}{\partial r} + \frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\frac{\partial Y}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = \left(-\frac{2m}{\hbar^2}r^2\right)(E - V(r)) \tag{195}$$

$$\frac{1}{R}\frac{\partial}{\partial r}r^2\frac{\partial R}{\partial r} + \left(+\frac{2m}{\hbar^2}r^2\right)(E - V(r)) = -\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\frac{\partial Y}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] \tag{196}$$

On the left side, we have a function of r only, and on the right, we have a function of (θ,ϕ) only. We set this quantity to be constant and call it $l(l+1)$ in anticipation of future results.

We are going to solve the angular equation first. We use the separation of variable again:

$$Y(\theta,\phi) = \Theta(\theta)\Psi(\phi) \tag{197}$$

$$= A(\theta)B(\phi) \tag{198}$$

Then,

$$\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\frac{\partial Y}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = -l(l+1)Y \;\rightarrow\; Y = AB \tag{199}$$

$$\frac{1}{A}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\dot{A} + \frac{1}{\sin^2\theta}\frac{\ddot{B}}{B} = -l(l+1) \tag{200}$$

We take the last equation and times $\sin^2\theta$:

$$\frac{1}{A}\sin\theta\frac{\partial}{\partial\theta}\sin\theta\dot{A} + l(l+1)\sin^2\theta = -\frac{\ddot{B}}{B} = \text{constant} = m^2 \tag{201}$$

So the left hand side, we have a function of θ only, and the right hadn side a function of ϕ only. We set this constant to be constant and call it m^2 (not mass!!). So we have:

$$-\ddot{B} = Bm^2 \tag{202}$$

the solution is then:

$$B = Ae^{im\phi} + B'e^{-im\phi} \tag{203}$$

$$= A\sin m\phi + B'\cos m\phi \tag{204}$$

This reduce to $B = e^{im\phi}$ (Griffiths says m can be $+$ or $-$).

$$\frac{1}{A}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\dot{A} + l(l+1)\frac{1}{\sin^2\theta} = m^2 \tag{205}$$

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\dot{A} + (l(l+1)\frac{1}{\sin^2\theta} - m^2)A = 0 \tag{206}$$

The solutions are:

$$A(\theta) = A'P_l^m(\cos\theta) \tag{207}$$

where:

$$P_l^m(x) \equiv (-1)^m(1-x^2)^{m/2}\left(\frac{\partial}{\partial x}\right)^m P_l(x) \tag{208}$$

This is called the associated Legendre function. Here:

$$P_l(x) \equiv \frac{1}{2^l l!}\left(\frac{\partial}{\partial x}\right)^l (x^2-1)^l \tag{209}$$

is the Legendre polynomial. Now, we can write our total solution:

$$Y(\theta,\phi) = A(\theta)B(\phi) \tag{210}$$

and the so called shperical harmonics are:

$$Y_l^m(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}e^{im\phi}P_l^m(\cos\theta) \tag{211}$$

The Y_l^m are normalized and orthogonal, or orthonormal. That is, if we integrate it over a sphere, it gives 0 or 1:

$$\int_0^{2\pi}\int_0^{\pi} d\phi\sin\theta d\theta\,[Y_l^m(\cos\theta)]^*\,Y_{l'}^{m'}(\cos\theta) = \delta_{ll'}\delta_{mm'} \tag{212}$$

This comes up in QM and also in the cosmic microwave background. That solves the angular part of the problem (the radial part $V(r)$ has not come in at all).

Now we look at the radial part:

$$\frac{\partial}{\partial r}r^2\frac{\partial R}{\partial r} + R\left(\frac{2m}{\hbar^2}r^2\right)(E - V(r)) = l(l+1)R \tag{213}$$

We apply change of variables $u = rR$, $R = \frac{u}{r}$, and $\frac{\partial R}{\partial r} = \frac{1}{r}\frac{\partial u}{\partial r} - \frac{u}{r^2} = \frac{1}{r^2}\left(r\frac{\partial u}{\partial r} - u\right)$. Then:

$$\frac{\partial}{\partial r}r^2\frac{\partial R}{\partial r} = \frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r} - u\right) \tag{214}$$

$$= \frac{\partial u}{\partial r} + r\frac{\partial^2 u}{\partial r^2} - \frac{\partial u}{\partial r} \tag{215}$$

$$= r\frac{\partial^2 u}{\partial r^2} \tag{216}$$

Then:

$$r\frac{\partial^2 u}{\partial r^2} + \frac{2m}{\hbar}ru(E - V(r)) = l(l+1)\frac{u}{r} \tag{217}$$

$$-\frac{\hbar^2}{2m}\frac{d^2 u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \tag{218}$$

This last equation is called the radial equation, it looks just like our time independent Schrodinger equation $\mathcal{H}\psi = E\psi$ for $\mathcal{H} = \frac{p^2}{2m} + V(x)$. Here:

$$V_{\text{eff}} = V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2} \tag{219}$$

The second term is our new centrifugal term. This term being positive means it's repulsive. Still, we haven't said anything about $V(r)$. Some of the possibilities include

1. Infinite square well. For $l = 0$, it's just the square well. For $l \neq 0$, we have special function.

2. Finite Square Well

3. Hydrogen Atom

VII. LECTURE 7

From the previous lecture, we arrived at the radial equation:

$$-\frac{\hbar^2}{2m}\frac{d^2 u}{dr^2} + \left[V(r) + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \tag{220}$$

The Hydrogen atom has potential:

$$v(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \tag{221}$$

We know that potential is an energy which we can think as a frequency (i.e. inverse time or distance). The $\frac{1}{r}$ part has unit 1/distance. Thus, the middle part $\frac{e^2}{4\pi\epsilon_0}$ should be dimensionless. Here, the $1/4\pi$ suggests spherical symmetry. (This appears here because the MKS system is rationalized). In the MKS system, the capacitance takes form:

$$C = \frac{A\epsilon\epsilon}{d} \tag{222}$$

There is no 2π because this is in cartesian. Here, we also have:

$$\epsilon \to 8.85 \times 10^{-12} F/s \tag{223}$$

This is completely a historical legacy. In fact, it would be nice if capacitance is to be measured in meters. Back to the original equation, the e^2 is where the physics is. We have:

$$\frac{e^2}{4\pi\epsilon_0\hbar c} \equiv \alpha = \frac{1}{137} << 1 \tag{224}$$

where α is called the fine constant which is completely independent of the units. For the Hydrogen atom, we attribute the potential to the proton and assume that it is stationary. We plug it into the radial equation and solve it:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu \tag{225}$$

We call this term in the middle:

$$\left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right] \tag{226}$$

the effective potential V_{eff}. We note that there is a gap called the centrifugal barrier(why planets don't fall into the sun). Now, we define:

$$\kappa \equiv= \frac{\sqrt{-2mE}}{\hbar} \tag{227}$$

where $\hbar\kappa = \sqrt{-2mE}$ is a momentum, in fact, it is the Bohr momentum (semi-classical momentum). We see that:

$$\frac{\hbar^2\kappa^2}{2m} = -E \tag{228}$$

Then:

$$\frac{E}{\kappa^2}\frac{d^2u}{dr^2} + \left[\frac{-e^2}{4\pi\epsilon_0 r} - \frac{E}{\kappa^2}\frac{l(l+1)}{r^2}\right]\kappa = Eu \tag{229}$$

$$\frac{1}{\kappa^2}\frac{d^2u}{dr^2} + \left[\frac{-e^2\kappa}{4\pi\epsilon_0 rE\kappa} - \frac{1}{\kappa^2}\frac{l(l+1)}{r^2}\right]\kappa = u \tag{230}$$

We define $\rho = \kappa r$:

$$\frac{d^2u}{d\rho^2} + \left[-1 - \frac{e^2\kappa}{4\pi\epsilon_0\rho} - \frac{1}{\kappa^2}\frac{l(l+1)}{r^2}\right]u = 0 \tag{231}$$

We define:

$$\rho_0 = -\frac{e^2\kappa}{4\pi\epsilon E} = \frac{e^2\kappa 2m}{4\pi\epsilon\hbar^2\kappa^2} = \frac{2\alpha mc}{\hbar\kappa} \tag{232}$$

Then,

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right] u \tag{233}$$

Now we review the Bohr Model: First, we write down the expression for Energy:

$$E = \frac{1}{2}mv^2 = \frac{e^2}{4\pi\epsilon r} \tag{234}$$

We then assume circular orbit:

$$\frac{mv^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2} \tag{235}$$

Then, we say that the angular momentum is quantized in the unit of $\hbar$:

$$mvr = n\hbar \tag{236}$$

We solve the three equations:

$$pr = n\hbar \tag{237}$$

$$\hbar kr = n\hbar \tag{238}$$

$$\frac{2\pi}{\lambda}r = n \tag{239}$$

so we have:

$$2\pi r = n\lambda \tag{240}$$

Another important theorem is the virial theorem, which states that:

$$U \propto r^n \rightarrow \langle T\rangle = \frac{n}{2}\langle u\rangle \tag{241}$$

In out case where $n = -1$, we haveL

$$\langle T\rangle = -\frac{1}{2}\langle u\rangle \tag{242}$$

Then,

$$E = \langle T\rangle + \langle u\rangle = -\frac{1}{2}\langle u\rangle + \langle u\rangle = \langle u\rangle/2 \tag{243}$$

also:

$$E = \langle T \rangle - 2\langle T \rangle = -\langle T \rangle \tag{244}$$

We write down the results in Regan's favorite units:

$$E = -\frac{1}{2}\frac{\alpha^2 mc^2}{n^2} \tag{245}$$

$$r = \frac{n^2}{\alpha}\frac{\hbar c}{mc^2} \tag{246}$$

$$\frac{v}{c} = \frac{\alpha}{n} \tag{247}$$

where,

$$\hbar c = 197\text{eV} \cdot \text{nm} \tag{248}$$

$$mc^2 = 511 \times 10^3\text{eV} \tag{249}$$

$$\frac{e^2}{4\pi\epsilon_0} = 1.44\text{eV} \cdot \text{nm} \tag{250}$$

. So, we know that:

$$E, \frac{1}{r} \propto \frac{1}{n^2} \tag{251}$$

$$v, p \propto \frac{1}{n} \tag{252}$$

$$\lambda, L = rp \propto n \tag{253}$$

Note that:

$$\frac{v}{c} = \frac{\alpha}{n} \tag{254}$$

$$vn = c\alpha \tag{255}$$

$$mvn = mc\alpha \tag{256}$$

Earlier, we have:

$$\rho_0 = \frac{2\alpha mc}{\hbar\kappa} = \frac{2mvn}{\hbar\kappa} = \frac{2pn}{p} = 2n \tag{257}$$

In some sense, ρ_0 is a dimensionless number where $\rho = \kappa r$. Previously, we had arrived at:

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right] u \tag{258}$$

Now, we look at the asymptotic behavior where $\rho \to \infty$. We have:

$$\frac{d^2u}{dp^2} = u \tag{259}$$

The solution is given $u = Ae^{-\rho} + Be^{\rho}$ and the second term dissappear since it blow up as ρ foes to ∞. Thus, we have $u = Ae^{-\rho}$ for large ρ. Then, for $\rho \to 0$, we have $\frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2}u$. The solution is given:

$$u = c\rho^{l+1} + D^{-l} \tag{260}$$

$$\dot{u} = c(l+1)\rho^{l} - Dl\rho^{-(l+1)} \tag{261}$$

$$\ddot{u} = cl(l+1)\rho^{l-1} + Dl(l+1)\rho^{-(l+2)} = \frac{l(l+1)u}{\rho^2} \tag{262}$$

So, we have $u = C\rho^{l+1}$ for small ρ. Now, we factor out the asympotic behavior:

$$u(\rho) = \rho^{l+1}e^{-\rho}V(\rho) \tag{263}$$

Then,

$$\dot{u} \equiv \frac{\partial u}{\partial \rho} = (l+1)\rho^{l}e^{-\rho}v + \rho^{l+1}(-1)e^{-\rho}v + \rho^{l+1}e^{-\rho}\dot{v} \tag{264}$$

$$= \rho^{l}e^{-\rho}[(l+1-\rho)v + \rho\dot{v}] \tag{265}$$

$$\ddot{u} = l\rho^{l-1}e^{-\rho}[\,] + \rho^{l}(-1)e^{-\rho}[\,] + \rho^{l}e^{-\rho}[-v + (l+1-\rho)\dot{v} + \dot{v} + \rho\ddot{v}] \tag{266}$$

$$= \rho^{l}e^{-\rho}\left(\left[\frac{l(l+1-\rho)v}{\rho} + l\dot{v}\right] - ((l+1-\rho)v + \rho\dot{v}) - v + (l+2-\rho)\dot{v} + \rho\ddot{v}\right) \tag{267}$$

$$= \rho^{l}e^{-\rho}\left(v\left(-2 - 2l + \rho + \frac{l(l+1)}{\rho}\right) + \dot{v}\,(2l + 2 - 2\rho) + \rho\ddot{v}\right) \tag{268}$$

$$= \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]\rho^{l+1}e^{-\rho}v(\rho) \tag{269}$$

So, we have:

$$v(-2l - 2 + \rho + \frac{l(l+1)}{\rho}) + 2\dot{v}(l+1-\rho) + \rho\ddot{v} = \left[\rho - \rho_0 + \frac{l(l+1)}{\rho}\right]v \tag{270}$$

$$p\ddot{v} + 2(l+1-\rho)\dot{v} + (\rho_0 - 2(l+1))v = 0 \tag{271}$$

Then, we assume a power series for solution:

$$V(\rho) = \sum_{j=0}^{\infty} c_j\rho^{j} \tag{272}$$

Taking the derivative:

$$\dot{v} = \sum_{j=0} jc_j\rho^{j-1} = \sum_{k=-1}^{\infty}(k+1)c_{k+1}\rho^{k} = \sum_{k=0}^{\infty}(k+1)c_{k+1}\rho^{k} \tag{273}$$

Second derivative:

$$\ddot{v} = \sum_{k=0} k(k+1)c_{k+1}\rho^{k-1} \tag{274}$$

Then:

$$\sum_{k=0}\Big[k(k+1)c_{k+1}\rho^k + 2(l+1-\rho)(k+1)c_{k+1}\rho^k + (\rho_0 - 2(l+1))c_k\rho^k\Big] = 0 \qquad (275)$$

This expression must hold for every power of ρ individually: We use:

$$-2(k+1)c_{k+1}\rho^{k+1} = -2kc_k\rho^k \qquad (276)$$

to simplify:

$$k(k+1)c_{k+1} + 2(l+1-\rho)(k+1)ck + 1 + (\rho_0 - 2(l+1))c_k = 0 \qquad (277)$$

$$k(k+1)c_{k+1} + 2(l+1)(k+1)ck + 1 + (\rho_0 - 2(l+1))c_k - 2kc_k = 0 \qquad (278)$$

Then:

$$c_{k+1}(k(k+1) + 2(l+1)(k+1)) = c_k(2k - \rho_0 + 2(l+1)) \qquad (279)$$

$$c_{k+1} = \frac{2(k+l+1) - \rho_0}{(k+1)(k+2(l+1))}c_k \qquad (280)$$

This last equation is our recursion relation which can be used to determine all the terms in this power series. We notice that for large K:

$$c_{k+1} = \frac{2k}{k(k+1)}c_k = \frac{2c_k}{k+1} \qquad (281)$$

$$c_k = \frac{2^k c_0}{k!} \qquad (282)$$

If this is true for all k,

$$v(\rho) = \sum_{k=0}^{\infty} c_k\rho^k = \sum \frac{2^k}{k!}\rho^k c_0 = \sum \frac{(2\rho)^k}{k!}c_0 = e^{2\rho}c_0 \qquad (283)$$

since we know that $e^x = \sum_{n=0}^{\infty}\frac{x^n}{n!}$. THi simplies:

$$u(\rho = e^{-\rho}\rho^{l+1}v(\rho) = e^{-\rho}\rho^{l+1}e^{2\rho}c_0 \propto e^{\rho} \qquad (284)$$

However, this blows up at $\rho \to \infty$, and this is unacceptable. We put a restraint on the power series: k can not $\to \infty$. This recursion series must terminate. So, for $k = \text{some}N$, we must find $c_n = 0$ (but $c_{n-1} \neq 0$) and $c_{n+1} = 0$. Our recursion relation gives:

$$c_{k+1} = \frac{2(k+l+1) - \rho_0}{(k+1)(k+2(l+1))}c_k \qquad (285)$$

Then:

$$c_N = 2(N+l) - \rho_0 = 0 \qquad (286)$$

This tells us:

$$2(N+l) = \rho_0 = 2n \quad \text{(from the Bohr model)} \tag{287}$$

We know that $N + l = n$. So, in other words, for this series to terminate, we need $N, l, n \in$ integers. We note that:

$$\rho_0 = 2n = \frac{-e^2\kappa}{4\pi\epsilon E} = \frac{-e^2}{4\pi\epsilon}\frac{\sqrt{-2mE}}{\hbar} = \frac{-e^2}{4\pi\epsilon_0\hbar}\sqrt{\frac{-2m}{E}} \tag{288}$$

then,

$$4n^2 = \left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 \cdot \frac{-2m}{E} \tag{289}$$

$$E = -\left(\frac{e^2}{4\pi\epsilon_0\hbar c}\right)^2 \frac{mc^2}{2n^2} = -\frac{1}{2}\alpha^2\frac{mc^2}{n^2} \quad \text{(Bohar Formula)} \tag{290}$$

So, we have redefined Bohr's semiclassical formula using the full Schrodinger equation. Bohr assumed the quantization of angular moment. Where, we derived it by following from the angular periodicity of Ψ and its asymptotic behavior.

To recap, we first apply the separation of variables:

$$\Psi = \Theta R\phi \tag{291}$$

We get three separation constants: $l, (l+1)$ and m. We have the quantized n from the radial term and lastly E from the time dependent term. We write the radial term again:

$$\left[\frac{\hbar}{2m}\left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}\right) + v(r)\right] u = Eu \quad \text{where} \quad u \equiv rR \tag{292}$$

We note that the terms in the parenthesis is $\frac{p^2}{2m}$ combining the parallel and perpendicular terms:

$$\frac{p^2}{2m} = \frac{\vec{p}_{\parallel}^2}{2m} + \frac{\vec{p}_{\perp}^2}{2m} \tag{293}$$

$$= \frac{\vec{p}_{\parallel}^2}{2m} + \frac{L^2}{2mr^2} \quad \text{where} \quad \vec{L} \equiv \vec{r} \times \vec{p} = |r||p_{\perp}| \tag{294}$$