Intro to Quantum Mechanics I

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This is an advanced undergraduate course. Offered in Fall 2013 at Columbia University. Required Course textbook: Griffiths, *Introduction to Quantum Mechanics.* Office Hours: Mon 1:00-2:00.

Contents

1 Introduction

Lecture 1 (9/3/13)

We will cover chapters 1-5, and go through some exact solvable problems: 3D problems, identical particles, etc.

1.1 Quantum Description

1900 Plank found mathematical curves to fit radiation from hot objects by assuming energy was quantized. 5 years later, 1905, Einstein, in his spare time not working on general relativity, explained photoelectric effect. Bohr 1913 used standing waves explained spectrum of H atoms, He^{+}ion, but his method didn't work for other things. 1925 Heisenberg invented matrix mechanics, same year Schrodinger invented wave mechanics, and Schrodinger showed that two mechanics were equivalent. Thus quantum mechanics was born.

Vocabularies (momentum, spins) in quantum mechanics have quite different meaning of in classical mechanics.

In classical mechanics, states of a system of particles is completely specified through Newton's law if we know all positions and velocities of all particles at a given time, and the system is labeled by

$$\{\vec{x}_\alpha, \vec{v}_\alpha\} \text{ or } \{\vec{x}_\alpha, \vec{p}_\alpha\}$$

In classical mechanics, one studies the system in terms of Lagrangian and Hamiltonian

$$L(\text{positions, velocities}) \implies \text{equation of motion}$$

in most cases

$$L = \text{KE}-\text{PE}$$

Hamiltonian

$$H(\text{positions, momentums}) \implies \text{equation of motion}$$

One can get Maxwell equations from Lagrangian and Hamiltonian of electromagnetic fields.

For a single particle, if the forces exert on it is from potential $V(\vec{x})$, i.e. conservation force

$$\begin{aligned} H &= \mathrm{KE} + \mathrm{PE} \\ &= \frac{1}{2}\frac{\vec{p}^2}{m} + V(\vec{x}) \end{aligned}$$

We will see this gives strong motivation for QM.

In quantum mechanics, state of system is given by Ψ.

One can think $\Psi(x,t)$ as a wave function. More generally Ψ is a vector in an infinite dimensional space. We will elaborate more when we study linear algebra.

Recall a 3 dimensional vector $\vec{v}$ can be written in components

$$\vec{v} = v_x\hat{i} + v_y\hat{j} + v_z\hat{k}$$

or

$$(v_x, v_y, v_z) \text{ or even } (v_r, v_\theta, v_\phi)$$

A N dimensional vector $(v_1, v_2, ..., v_N)$; a ∞ dimensional vector $(v_1, v_2, ...)$.

1.2 Measurements

Question. *What does Ψ do?*

If the system is in state Ψ, what is position of particle? what is velocity of particle?

There are perfect English, but in QM they are meaningless. Because they assume particle has definite position and velocity?

The correct way to ask is that if one measures the position, what might he find?

Question. *How to determine Ψ?*

Do measurements? No, measurement changes the state. Instead, we prepare many identical system in state Ψ, then Ψ gives probability of result of experiment.

Question. *Does Ψ move?*

In classical mechanics, states change according to Newton's law. In QM Ψ changes according to Schrodinger equation

$$i\hbar\frac{d}{dt}(\text{state}) = (\text{Hamiltonian})(\text{state})$$

$$i\hbar\frac{d}{dt}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \tag{1.1}$$

Mathematically this is a partial differential equation first order in time. Given $\Psi(x,0)$, one can solve for $\Psi(x,t)$.

$$\begin{aligned}\text{RHS of (1.1)} &= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\Psi(x,t) \\ &= \left[\frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) + V(x)\right]\Psi(x,t)\end{aligned}$$

For the moment x, t are all exact, they are variables, no uncertainties yet.

1.3 Probability

Discrete variables

E.g. age of people in the room: 17,18,..,25,... Let

$$N(j) = \#\text{ with age } j$$

$$N = \sum_j N(j)$$

$$\text{Prob of picking one with age } j = P(j) = \frac{N(j)}{N}$$

Total probability is clearly

$$\sum_j P(j) = 1$$

and average age (in QM called expectation value)

$$\langle j\rangle = \sum_j jP(j)$$

Notice it is total possible that there is not a single person that has age comes close to the average if the data is divided into two extremes. So what does the expectation value really tell us?

We need to look at standard derivation to see how wide spread the data is. Let

$$\begin{aligned}
\Delta j &= j - \langle j \rangle \\
\langle \Delta j \rangle &= 0 \\
\left\langle (\Delta j)^2 \right\rangle &= \left\langle (j - \langle j \rangle)^2 \right\rangle = \left\langle j^2 - 2j \langle j \rangle + \langle j \rangle^2 \right\rangle = \left\langle j^2 \right\rangle - \langle j \rangle^2 \equiv \sigma^2
\end{aligned}$$

note: $\langle j^2 \rangle - \langle j \rangle^2$is always ≥ 0, so the definition of σ makes sense.

Continuous Variables

Greek rho

$$\rho(s) = \text{probability density}$$

s is the continuous variables.

$$\rho(s)ds = \text{prob of result in the range } s \text{ to } s + ds$$

Total probability is always 1, i.e. normalization

$$\int ds\rho(s) = 1$$

$$\langle s \rangle = \int dss\rho(s)$$

$$\langle f(s) \rangle = \int dsf(s)\rho(s)$$

for any function f, e.g. $f(s) = s^2$

$$\sigma^2 = \int ds(s - \langle s \rangle)^2 \rho(s) = \left\langle s^2 \right\rangle - \langle s \rangle^2$$

Gaussian Distribution

$$\rho(x) = Ae^{-\lambda(x-a)^2}$$

λ constant, A constant fixed by normalization. To find A, we first compute

$$I_0 = \int_{-\infty}^{\infty} dx e^{-\lambda x^2}$$

To do that, let's square our difficulty

$$\begin{aligned}
(I_0)^2 &= \int_{-\infty}^{\infty} dx e^{-\lambda x^2} \int_{-\infty}^{\infty} dy e^{-\lambda y^2} \\
&= \iint dx dy e^{-\lambda(x^2+y^2)} \\
&= \int_0^{\infty} dr r \int_0^{2\pi} d\theta e^{-\lambda r^2} \\
&= 2\pi \int_0^{\infty} dr r e^{-\lambda r^2} = \frac{\pi}{\lambda}
\end{aligned}$$

thus

$$I_0 = \sqrt{\frac{\pi}{\lambda}}$$

$$I_1 = \int_{-\infty}^{\infty} dx x e^{-\lambda x^2} = 0$$

because it is integration of an odd function.

$$I_2 = \int_{-\infty}^{\infty} dx x^2 e^{-\lambda x^2} = -\frac{dI_0}{d\lambda} = \frac{1}{2}\sqrt{\frac{\pi}{\lambda^3}}$$

$$I_3 = \int_{-\infty}^{\infty} dx x^3 e^{-\lambda x^2} = 0$$

and so on.

$$1 = \int_{-\infty}^{\infty} ds \rho(s) = A \int_{-\infty}^{\infty} dx e^{-\lambda(x-a)^2} = AI_0 \implies A = \sqrt{\frac{\lambda}{\pi}}$$

with substitution $u = x - a$.

$$\begin{aligned}
\langle x \rangle &= \int_{-\infty}^{\infty} \sqrt{\frac{\lambda}{\pi}} x e^{-\lambda(x-a)^2} \\
&= \int_{-\infty}^{\infty} \sqrt{\frac{\lambda}{\pi}} (x - a + a) e^{-\lambda(x-a)^2} \\
&= \sqrt{\frac{\lambda}{\pi}} I_1 + \sqrt{\frac{\lambda}{\pi}} a I_0 = a
\end{aligned}$$

$$\begin{aligned}
\langle x^2 \rangle &= \int_{-\infty}^{\infty} \sqrt{\frac{\lambda}{\pi}} [(x-a)^2 + 2(x-a)a + a^2] e^{-\lambda(x-a)^2} \\
&= \sqrt{\frac{\lambda}{\pi}} I_2 + a^2 \sqrt{\frac{\lambda}{\pi}} I_0 = \frac{1}{2\lambda} + a^2
\end{aligned}$$

Therefore we obtain

$$\sigma^2 = \frac{1}{2\lambda}$$

that is the larger λ is, the smaller σ is, so the distribution is narrower.

1.4 Wave Functions

Lecture 2 (9/5/13)

Let us cooperate probability density with wave function Ψ, we say

$$|\Psi(x,t)|^2 \, dx = \text{prob that measurement of position gives } x \text{to } x + dx$$

This kind of probabilistic deterministic view is different from thermal dynamics, whose probability is result of incomplete knowledge. In QM, Ψ does give complete story. Einstein was not happy about it, he believed there were hidden variables. He argued that if we had complete knowledge we would not resolve to probability, but he is wrong.

Another departure from classical view about this wave function is that measurement changes states. E.g. coin toss will give 50% heads and 50% tails, and keep tossing always 50/50. However, in QM, we preform “Stern-Gerlach” experiment, having some sliver atoms in state Ψ passing some magnet 50% beam comes out along up path and 50% comes out along down path. If we keep the upper path beam and let it pass another identical magnet apparatus, now not 50/50, but 100% beam comes out up.

The original Ψ before passing the first magnet is said to be superposition of up and down. Usually people think of QM, they think of atoms, but everything in the universe is QM. We know for normal objects, the wave functions are so peaked that there is no room for spreading, but it is not always the case: Schrodinger's cat.

A cat is placed in a box with some radioactive material, e.g. Uranium. A Geiger counter is in the box too. If the counter detects Uranium decays, it will release some poisonous substance and kill the cat. Since there is 50/50 chance that Uranium decays, we say the wave function of Uranium is superposition of decaying and not decaying. Since the consequence of decaying is directly linked to the life of the cat, applying QM philosophy to the cat, we have to conclude that for the time being the wave function of the cat is 50% life (front cover of Griffiths) and 50% dead (back cover of Griffiths).

This seemingly paradox doesn't carry any practical paradox, but still there are too many people trying to over mystify the story. Say that the cat is in the state between dead and life (i.e. ghost) or the action of opening the box collapses the wave function thus it forces the cat to choose a state, live or die. In fact after the detector detects decaying, the wave function has collapsed, and the cat dies. It doesn't relate to opening the box.

The formulation of superposition of contradicting states (up/down, decay/not decay) is more or less a mathematical trick. It is used to describe probability, and itself doesn't produce anything contradicting reality, e.g. a dead and life, ghost cat. In fact we are living in a dangerous world. One can get stuck by lightening right now, so according to QM doctrine, our wave functions should contain some probabilities of getting struck by lightning. After we place the cat in the box, the cat's probability of death goes up tremendously, and it is quantum mechanically calculable to be 50%, ignoring other factors may change the value, e.g. during that time earthquake happens, the cat is killed actually by the falling Geiger counter.

In most cases we should be able to normalize Ψ

$$\int_{-\infty}^{\infty} dx\, |\Psi(x,t)|^2 = 1 \tag{1.2}$$

The integrability of Ψ implies Ψ goes to 0 rapidly as $x \to \pm\infty$, which is a physical nature. Notice it is integral against x not t, Ψ involves in t. But for fixed x_0, it is possible that the particle may never and never will be there, i.e. $\Psi(x_0,t) = 0\ \forall t$, so

$$\int_{-\infty}^{\infty} dt\,|\Psi(x_0,t)|^2 = 0$$

This slows x and t are not exchangeable in non-relativistic QM.

Suppose at $t = t_0$, the wave function is normalized as (1.2), what happens at later time?

From Schrodinger equation (1.1), where $V(x)$ is always real. $V(x)$ is same in classical mechanics sense. Take complex conjugate of (1.1), obtaining

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

We compute

$$\begin{aligned}
\frac{\partial}{\partial t}|\Psi|^2 &= \frac{\partial}{\partial t}\Psi^*\Psi + \Psi^*\frac{\partial}{\partial t}\Psi \\
&= -\frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + V(x)\Psi^*\right]\Psi + \frac{1}{i\hbar}\Psi^*\left[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi\right] \\
&= \frac{1}{i\hbar}\left(\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \frac{\hbar^2}{2m}\Psi^*\frac{\partial^2\Psi}{\partial x^2}\right) \\
&= \frac{\hbar}{i2m}\frac{\partial}{\partial x}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right) \\
&= \frac{\partial}{\partial x}\left[\frac{1}{2m}\frac{\hbar}{i}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right)\right] \qquad (1.3)
\end{aligned}$$

The interpretation of above is

$$|\Psi|^2 = \text{prob density}$$

$$\frac{1}{2m}\frac{\hbar}{i}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right) = \text{prob current}$$

so (1.3) is continuity equation. Then

$$\frac{d}{dt}\int dx\,|\Psi|^2 = \int dx\frac{\partial}{\partial t}|\Psi|^2 = \frac{1}{2m}\frac{\hbar}{i}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right)\Bigg|_{x=-\infty}^{x=\infty} = 0$$

so normalization stays the same.

What else does the wave function tell us?

$$\langle x \rangle = \int_{-\infty}^{\infty} dx x \left|\Psi\right|^2$$

We guess

$$\langle v \rangle = \frac{d}{dt} \langle x \rangle$$

we will show this is in fact a good guess.

$$\begin{aligned} \langle v \rangle &= \int dx x \frac{\partial}{\partial x} \left[\frac{1}{2m} \frac{\hbar}{i} \left(\frac{\partial \Psi^*}{\partial x} \Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right) \right] \\ &= x \left[\frac{1}{2m} \frac{\hbar}{i} \left(\frac{\partial \Psi^*}{\partial x} \Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right) \right]_{x=-\infty}^{x=\infty} - \int dx \frac{1}{2m} \frac{\hbar}{i} \left(\frac{\partial \Psi^*}{\partial x} \Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right) \end{aligned}$$

assuming $\Psi x \to 0$ as $x \to \pm\infty$.

$$\langle v \rangle = \int dx \frac{1}{2m} \frac{\hbar}{i} \left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right)$$

integration by part on the second term on the right

$$\begin{aligned} \langle v \rangle &= \int dx \frac{1}{m} \frac{\hbar}{i} \Psi^* \frac{\partial \Psi}{\partial x} \\ &= \int dx \Psi^* \left(\frac{\hbar}{im} \frac{\partial}{\partial x} \right) \Psi \end{aligned}$$

momentum $\langle p = vm \rangle$, think in terms of operators, (we mean operator: send functions to functions.)

$$\langle x \rangle = \int dx \Psi^* x_{op} \Psi$$

$$\langle p \rangle = \int dx \Psi^* p_{op} \Psi$$

One can also check that, integration by parts

$$\langle p \rangle^* = \int dx \Psi \left(-\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi^* = \int dx \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi = \langle p \rangle$$

hence $\langle p \rangle$ is real.

It is possible to compute

$$\langle F(x,p) \rangle = \int dx \Psi^* F(x_{op}, p_{op}) \Psi$$

if the order ambiguity is resolved.

E.g.

$$\langle p^2 \rangle = \int dx \Psi^* \left(\frac{\hbar}{i} \frac{\partial}{\partial x} \right)^2 \Psi$$

Angular momentum, define in 3D

$$\langle L_z \rangle = \langle x p_y - y p_x \rangle = \int dx dy dz \Psi^* \frac{\hbar}{i} \left(x \frac{\partial \Psi}{\partial y} - y \frac{\partial \Psi}{\partial x} \right)$$

What about $\langle xp \rangle$ and $\langle px \rangle$?

$$\langle xp \rangle = \frac{\hbar}{i} \int dx \Psi^* x \frac{\partial \Psi}{\partial x}$$

$$\langle px \rangle = \frac{\hbar}{i} dx \Psi^* \left(x \frac{\partial \Psi}{\partial x} + \Psi \right)$$

Hence

$$\langle xp \rangle \neq \langle px \rangle \neq \left\langle \frac{1}{2}(xp + px) \right\rangle \neq \langle \sqrt{x} p \sqrt{x} \rangle \neq ...$$

Order matters.

What if change Ψ to $c\Psi$, for some multiple c?

$$\int dx \, |\Psi|^2 \to |c|^2 \int dx \, |\Psi|^2 = 1 \implies |c| = 1 \implies c = e^{i\alpha}, \alpha \text{ real}$$

what happens to expectation values?

$$\Psi \to e^{i\alpha} \Psi$$

$$\langle F(x,p) \rangle = \int dx e^{-i\alpha} \Psi^* F e^{i\alpha} \Psi$$

so no change. We conclude Ψ or $e^{i\alpha}\Psi$ describe same physical state.

1.5 Uncertainty Principle

Given Ψ we can measure $\langle x \rangle$, $\langle x^2 \rangle$, for some position x and calculate

$$\sigma_x^2 = \left\langle x^2 \right\rangle - \langle x \rangle^2$$

Similarly calculate

$$\sigma_p^2 = \left\langle p^2 \right\rangle - \langle p \rangle^2$$

Heisenberg says

$$\Delta x \Delta p \equiv \sigma_x \sigma_p \geq \frac{\hbar}{2} \text{ for any } \Psi \tag{1.4}$$

It is commonly interpreted (actually it's a corollary) as one can't simultaneously measure x and p, because when one probes the position more, the wave length of the apparatus gets shorter and the accuracy of measuring momentum gets worse. The direct way of thinking about Heisenberg's uncertainty principle is to think there are many identical systems, some are measured in positions and some are measured in momentum, then compute the standard derivation of the results of the measurement, it should satisfy (1.4).

Example. Suppose $\Psi = Ne^{-\lambda x^2/2}$,

$$1 = \int dx \, |\Psi|^2 = |N|^2 \sqrt{\frac{\pi}{\lambda}} \implies N = (\frac{\lambda}{\pi})^{1/4}$$

pick N real, since phase doesn't matter.

For that wave function

$$\langle x \rangle = N^2 \int dx x e^{-\lambda x^2} = 0$$

$$\left\langle x^2 \right\rangle = N^2 \int dx x^2 e^{-\lambda x^2} = \frac{1}{2\lambda}$$

$$\sigma_x^2 = \frac{1}{2\lambda}$$

check this has the correct dimension. Since the exponential is dimensionless

$$[\lambda] = \frac{1}{[\text{length}]^2}$$

so indeed

$$[\sigma_x] = [\text{length}]$$

Similarly compute

$$\langle p \rangle = \frac{d}{dt} \langle x \rangle = 0$$

or use brutal force

$$\langle p \rangle = \frac{\hbar}{i} \int dx \Psi^* \frac{\partial \Psi}{\partial x}$$

For $\langle p^2 \rangle$ use integration by parts

$$\begin{aligned} \langle p^2 \rangle &= (\frac{\hbar}{i})^2 \int dx \Psi^* \frac{\partial^2}{\partial x^2} \Psi = \hbar^2 \int dx \frac{\partial \Psi^*}{\partial x} \frac{\partial \Psi}{\partial x} \\ &= \hbar^2 \int dx \left(-\lambda x e^{-\lambda x^2/2} \right)^2 = \hbar^2 \lambda^2 \frac{1}{2\lambda} = \frac{\hbar^2 \lambda}{2} \end{aligned}$$

So

$$\sigma_p^2 = \hbar^2 \frac{\lambda}{2}$$

Graphically, as $\lambda \uparrow$, the width $\sigma_x \downarrow$, and the slope goes up $\sigma_p \uparrow$, because the total area under the curve is preserved. The width is $\sim \sigma_x \sim 1/\sqrt{\lambda}$, the peak is $\sim N \sim \sqrt[4]{\lambda}$.

Moreover we find

$$\sigma_x \sigma_p = \frac{\hbar}{2}$$

so this "randomly" chosen function gives the minimum uncertainty bound.

2 Time Independent Schrodinger Equation

Lecture 3 (9/10/13)

Consider single particle one dimension Schrodinger equation

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi \tag{2.1}$$

This is a linear equation, namely

1) If $\Psi(x,t)$ is a solution, $c\Psi$ is also a solution, with $\int |c|^2 |\Psi|^2 dx = 1$

2) If Ψ_1, Ψ_2 are solution, then $c_1\Psi_1 + c_2\Psi_2$ is also a solution.

(2.1) is first ode in time, so by existence and uniqueness of 1st order ODE, for given $\Psi(x, t=0)$, one can find $\Psi(x,t)$ for later t, by integrating steps and steps.

In classical mechanics, the absolutely scale of potential is irrelevant. What happen to wave function if $V(x) \to V(x) + V_0$?

Suppose $\Psi(x,t)$ solves (2.1). Consider

$$\Phi = e^{-iV_0t/\hbar}\Psi \tag{2.2}$$

then

$$\begin{aligned} i\hbar\frac{\partial\Phi}{\partial t} &= V_0\Phi + i\hbar e^{-iV_0t/\hbar}\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi\right) \\ &= V_0\Phi - \frac{\hbar^2}{2m}\frac{\partial^2\Phi}{\partial x^2} + V(x)\Phi \end{aligned}$$

Hence Φ solves

$$i\hbar\frac{\partial\Phi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Phi}{\partial x^2} + (V(x) + V_0)\,\Phi$$

note this added term $V_0\Phi$ is not an inhomogeneous term in the sense of ODE, so the solution from $\Psi \to \Phi$ is not just to add a particular solution.

Later we will see that (2.2) means the energy is increased by V_0 and no other physical observable difference.

One can also counting time at a different time, i.e. shift $t \to t + t_0$ in (2.1), then $\Phi(x,t) = \Psi(x, t+t_0)$ is a solution.

2.1 Separation of Variables

We want to solve (2.1), try

$$\Psi(x,t) = \phi(t)\psi(x) \tag{2.3}$$

This looks like a very special form of solutions, but it turns out all solutions if not in this form can be written as sum (possible ∞ sum) of (2.3).

Plug (2.3) in

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

dividing by $\phi\psi$,

$$i\hbar\frac{1}{\phi}\frac{\partial\phi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi\right)\frac{1}{\psi}$$

The LHS is only a function of t, while the RHS is only a function of x, so the two sides must equal to some constant E. Thus

$$\begin{cases} i\hbar\frac{\partial\phi}{\partial t} = E\phi \implies \phi = e^{-iEt/\hbar} \\ -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi \end{cases}$$

The second equation is called time independent Schrodinger equation.

What about normalization? From (2.3)

$$|\Psi|^2 = |\psi|^2 e^{-iEt/\hbar} e^{iE^* t/\hbar}$$

If E is real, then $|\Psi|^2 = |\psi|^2$.

If $E = \lambda + i\mu$ complex,

$$|\Psi(x,t)|^2 = |\psi(x)|^2 e^{-2\mu t/\hbar}$$

hence the overall normalization would be time dependent, which is not possible, so E must be real. (There are cases where people take E to be complex to describe unstable particles. That is very special.)

As we will see the letter E is chosen to be the constant means something, i.e. E is the energy

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = \left(\frac{1}{2m}p^2 + V\right)\psi = E\psi$$

$p = \frac{\hbar}{i}\frac{\partial}{\partial x}$.

Take complex conjugate of above. Since E is real

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + V\psi^* = E\psi^*$$

thus both ψ, ψ^* are solutions, so

$$\begin{cases} \psi + \psi^* \\ i(\psi - \psi^*) \end{cases}$$

are too solutions. In other words, we can always choose the solutions to time independent Schrodinger equation to be real.

Furthermore suppose potential is symmetric, $V(x) = V(-x)$. Then if $\psi = f(x)$ is solution, then $f(-x)$ is too a solution. Indeed

$$-\frac{\hbar^2}{2m}\frac{\partial^2 f(x)}{\partial x^2} + V(x)f(x) = Ef(x)$$

then

$$-\frac{\hbar^2}{2m}\frac{\partial^2 f(-x)}{\partial x^2} + V(-x)f(-x) = Ef(-x)$$

Hence

$$\begin{cases} f(x) + f(-x) \\ f(x) - f(-x) \end{cases}$$

are both solutions, and one is even, the other is odd.

Now we show E is indeed energy. Suppose

$$\Psi = \psi(x)e^{-iEt/\hbar} \tag{2.4}$$

then

$$\begin{aligned} \langle x \rangle &= \int dx x|\Psi|^2 = \int dx x|\psi|^2 \\ \langle p \rangle &= \int dx \Psi^* \frac{\hbar}{i}\frac{\partial}{\partial x}\Psi = \int dx \psi^* \frac{\hbar}{i}\frac{\partial}{\partial x}\psi \end{aligned} \tag{2.5}$$

Both $\langle x \rangle$,$\langle p \rangle$ are time independent. In fact for any $F(x,p)$, $\langle F(x,p) \rangle$ is time independent, so (2.4) is called stationary states of the Hamiltonian. Notice that stationary states are necessary physically stable. QM2 we will show stationary states can decay, so more realistic Hamiltonian should be taken into account.

Moreover take ψ real in (2.5),

$$\langle p\rangle = \frac{\hbar}{i}\int dx \frac{d}{dx}(\frac{1}{2}\psi^2) = \frac{\hbar}{i}\frac{1}{2}\left[\psi^2(\infty) - \psi^2(-\infty)\right] = 0$$

but $\langle p^2\rangle$ is not zero.

Find expectation value of Hamiltonian

$$\langle H\rangle = \int dx\psi^* \left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi\right) = \int dx\psi^* E\psi = E$$

so indeed E is the energy. What is $\langle H^2\rangle$?

$$\begin{aligned}\langle H^2\rangle &= \int dx\psi^* \left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\psi \\ &= \int dx\psi^* \left(\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right) E\psi = E^2\end{aligned}$$

so

$$\sigma_H^2 = 0$$

hence (2.4) stationary states have definite energy. It seems odd that stationary states have definite energy but $\langle p\rangle$ is always 0.

Next lecture we will show if Ψ is not stationary states, e.g. it is made of two stationary states with $E_1 \neq E_2$

$$\Psi = c_1\psi_1(x)e^{-iE_1t/\hbar} + c_2\psi_2(x)e^{-iE_2t/\hbar} \tag{2.6}$$

then many of the nice properties won't hold.

2.2 Infinite Square Well Potential

Suppose

$$V(x) = \begin{cases}\infty & x < 0 \\ 0 & 0 < x < a \\ \infty & x > a\end{cases}$$

hence there are impenetrable walls at $x = 0$ and a, so the particle (presumably with finite E) cannot go outside of the 1D box, i.e. $\psi = 0$ if $x < 0$ or $x > a$.

The wave function is continuous (otherwise the 2nd derivative in Schrodinger equation doesn't make much sense.) ψ' is finite (for most case ψ' is continuous, minimum requirement for ψ'' to exist, but here ψ' is not continuous at 0 and a. Because V is ∞ at 0 and a, by Schrodinger equation ψ'' is too ∞ at 0 and a) In the case of finite square well, we will see V is everywhere finite, so ψ and ψ' are continuous.

In $0 < x < a$, we solve

$$-\frac{\hbar^2}{2m}\psi'' = E\psi \tag{2.7}$$

If we rewrite it as

$$\frac{\psi''}{\psi} = -\frac{2m}{\hbar^2}E$$

it becomes clear that since $\psi(0) = \psi(a) = 0$, then $\psi \not\equiv 0$ should have a maximum or a minimum in $(0, a)$. If ψ has a maximum, then at that point $\psi > 0$ and $\psi'' < 0$, so $E > 0$. If ψ has a minimum, then at that point $\psi < 0$ and $\psi'' > 0$, so $E > 0$, hence to solve boundary value problem (2.7), we have to have $E > 0$.

Lecture 4 (9/12/13)

Since $E > 0$, define

$$E = \frac{\hbar^2 k^2}{2m}$$

so that we get rid of constants,

$$\psi'' = -k^2\psi$$

so

$$\psi = A\sin kx + B\cos kx \tag{2.8}$$

or

$$\psi = Ce^{ikx} + De^{-ikx}$$

Here (2.8) is more convenience. $\psi(0) = 0$, $B = 0$, $\psi(a) = 0$

$$ka = n\pi \implies k = \frac{n\pi}{a}\, n = 1, 2, ...$$

negative n represents the same state, with a different phase. Then

$$E = n^2 \frac{\hbar^2}{2m} \frac{\pi^2}{a^2}$$

Find A, choose A to be real

$$1 = \int_{-\infty}^{\infty} dx |\psi|^2 = \int_0^a dx A^2 \sin^2 kx = A^2 \frac{a}{2} \implies A = \sqrt{\frac{2}{a}}$$

using the track

$$\int_0^{2\pi} d\theta \sin^2\theta = \int_0^{2\pi} d\theta \cos^2\theta \qquad \int_0^{2\pi} d\theta (\sin^2\theta + \cos^2\theta) = 2\pi$$

so

$$\int_0^{\pi} d\theta \sin^2\theta = \frac{\pi}{2} \text{ or } \left\langle \sin^2\theta \right\rangle = \frac{1}{2}$$

Interestingly A is independent of n.

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x \qquad \text{with } E_n = n^2 \frac{\hbar^2}{2m} \frac{\pi^2}{a^2}$$

Plotting states ψ_1, ψ_2,.., we find that ψ_1 has 0 node (not counting 0 at end points), ψ_2 has 1 node, and ψ_3 has 2 nodes, etc. ψ_1 is even (thinking $x = \frac{a}{2}$ is the origin), ψ_2 is odd, and alternating. These two features of 1D energy states work in general.

Another interesting feature of $\{\psi_n\}$ is

$$\int dx \psi_m^* \psi_n = \delta_{mn} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases}$$

δ_{mn} called Kronecker delta. Indeed $m \neq n$

$$\begin{aligned}
\int dx \psi_m^* \psi_n &= \frac{2}{a}\int_0^a dx \sin\frac{m\pi x}{a}\sin\frac{n\pi x}{a} \\
&= \frac{2}{a}\int_0^a dx \frac{1}{2}\left(\cos\frac{(m-n)\pi x}{a} - \cos\frac{(m+n)\pi x}{a}\right) \\
&= \frac{\sin(m-n)\pi}{(m-n)\pi} - \frac{\sin(m+n)\pi}{(m+n)\pi} = 0
\end{aligned}$$

$\{\psi_n\}$ are orthonormal. This feature works in general too. In fact it works in 3D as well.

Suppose $E_1 \neq E_2$, and ψ_1, ψ_2 solve time independent Schrodinger equation. Consider

$$\int dx \psi_2^* \left(-\frac{\hbar^2}{2m}\psi_1'' + V\psi_1\right) = E_1 \int dx \psi_2^* \psi_1$$

on the other hand, use integration by parts twice

$$\int dx \psi_2^* \psi_1'' = -\int dx \psi_2^{*'} \psi_1' = \int dx \psi_2^{*''} \psi_1$$

so

$$\begin{aligned}
\int dx \psi_2^* \left(-\frac{\hbar^2}{2m}\psi_1'' + V\psi_1\right) &= \int dx \left(-\frac{\hbar^2}{2m}\psi_2^{*''} + V\psi_2^*\right)\psi_1 \\
&= E_2 \int dx \psi_2^* \psi_1
\end{aligned}$$

Then

$$E_1 \int dx \psi_2^* \psi_1 = E_2 \int dx \psi_2^* \psi_1 \implies \int dx \psi_2^* \psi_1 = 0$$

Now back to (2.6), we can easily check many things. For example

$$\begin{aligned}
\int dx \Psi^* \Psi &= |c_1|^2 \int dx |\psi_1| + |c_2|^2 \int dx |\psi_2| + c_1^* c_2 e^{i(E_1-E_2)t/\hbar} \int dx \psi_1^* \psi_2 \\
&\quad + c_1^* c_2 e^{i(E_1-E_2)t/\hbar} \int dx \psi_1^* \psi_2 + c_1 c_2^* e^{-i(E_1-E_2)t/\hbar} \int dx \psi_2^* \psi_1 \\
&= |c_1|^2 + |c_2|^2 \qquad (2.9)
\end{aligned}$$

Thanks to $\int dx \psi_m^* \psi_n = \delta_{mn}$, the last two terms on the right are 0, otherwise the normalization would be time dependent.

More

$$\langle H \rangle = |c_1|^2 E_1 + |c_2|^2 E_2 \tag{2.10}$$

2.3 Fourier Series

Given $f(x)$ periodic with period L, i.e.

$$f(x) = f(x+L)$$

assuming $f(x)$ is well behaved, continuous at most places.

One can write $f(x)$

$$f(x) = \sum_{n=1}^{\infty} a_n \sin\frac{2\pi n}{L}x + \sum_{n=1}^{\infty} b_n \cos\frac{2\pi n}{L}x + b_0$$

Find coefficients, pick $N = 1, 2, ...$

$$\begin{aligned}
\int_0^L dx \sin\frac{2\pi N x}{L} f(x) &= \sum_{n=1}^{\infty} a_n \int_0^L dx \sin\frac{2\pi N x}{L}\sin\frac{2\pi n}{L}x + \sum_{n=1}^{\infty} b_n \int_0^L dx \sin\frac{2\pi N x}{L}\cos\frac{2\pi n}{L}x \\
&\quad + \int_0^L dx \sin\frac{2\pi N x}{L} b_0 \\
&= a_N \frac{L}{2}
\end{aligned}$$

only one term survives, using the tracks

$$\int_0^{2\pi} d\theta \sin m\theta \cos n\theta \qquad \int_0^{2\pi} d\theta \sin m\theta \sin n\theta \qquad \int_0^{2\pi} d\theta \cos m\theta \cos n\theta \tag{2.11}$$

vanish unless $m = \pm n$, because

$$\cos m\theta = \frac{e^{im\theta} + e^{-im\theta}}{2} \qquad \sin m\theta = \frac{e^{im\theta} - e^{-im\theta}}{2i}$$

$$\int_0^{2\pi} d\theta e^{im\theta} e^{in\theta} = \frac{1}{i(m+n)}\, e^{i(m+n)\theta}\Big|_0^{2\pi} = 0 \text{ if } m+n \neq 0$$

but more $m = n$,

$$\int_0^{2\pi} d\theta \sin m\theta \cos n\theta = \frac{1}{m} \sin^2 m\theta \Big|_0^{2\pi} = 0$$

So the only non-zero terms in (2.11) are

$$\int_0^{2\pi} d\theta \sin^2 m\theta = \int_0^{2\pi} d\theta \cos^2 m\theta = \pi$$

So

$$a_N = \frac{2}{L} \int_0^L dx \sin \frac{2\pi N x}{L} f(x)$$

Similarly find

$$b_N = \frac{2}{L} \int_0^L dx \cos \frac{2\pi N x}{L} f(x)$$

$$b_0 = \frac{1}{L} \int_0^L dx f(x)$$

We now show the inside of Fourier series to solutions of Schrodinger equation.

We want to show the claim: any solution Ψ is made of sum of product (2.3). Let's use the ∞ square well as an example. (It is very hard to prove the claim directly for other cases.)

Suppose we have found a solution Ψ. Because $\Psi(x = 0, t) = \Psi(x = a, t) = 0$ $\forall t$, we can continuous extend Ψ to all x, i.e.

$$\tilde{\Psi}(x, t) = \Psi(x - Na, t)$$

for any N integers. Then $\tilde{\Psi}$ is periodic with period a (or say $2a$ doesn't matter), so $\tilde{\Psi}$ has a Fourier representation

$$\tilde{\Psi} = \sum(\sin, \cos)$$

Because it vanishes at $x = 0$,

$$\tilde{\Psi} = \sum_n a_n(t) \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

Since it solves the Schrodinger equation, so $a_n(t)$ has to be

$$\begin{aligned}\tilde{\Psi} &= \sum_n c_n e^{-iE_n t/\hbar} \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \\ &= \sum_n c_n e^{-iE_n t/\hbar} \psi_n(x) \qquad (2.12)\end{aligned}$$

proving the claim.

What is the meaning of c_n's? cf (2.9), (2.10) or more generally

$$\begin{aligned}1 &= \int_{-\infty}^{\infty} dx |\Psi|^2 = \int_0^a dx |\tilde{\Psi}|^2 \\ &= \sum_n c_n^* e^{iE_n t/\hbar} \sum_m c_m e^{-iE_m t/\hbar} \underbrace{\int_0^a dx \psi_n^* \psi_m}_{\delta_{mn}} = \sum_n |c_n|^2\end{aligned}$$

In summary:

$$|\Psi(x,t)|^2 \, dx = \text{prob that position measurement, results } x \text{to } x + dx$$

$$|c_n|^2 = \text{prob that energy measurement gives } E_n$$

so we have seen both continuous and discrete probabilities.

2.4 Infinite Square Well Potential (continued)

Lecture 5 (9/17/13)

Check uncertainty principle of the solution (2.12), for convenience, choosing n odd,

$$\langle x \rangle = \frac{a}{2} \qquad \langle x^2 \rangle = \int_0^a dx x^2 |\psi_n|^2 = a^2 (\frac{1}{3} - \frac{1}{2n^2\pi^2})$$

$$\sigma_x^2 = a(\frac{1}{12} - \frac{1}{2n^2\pi^2})$$

$$\langle p \rangle = 0 \qquad \langle p^2 \rangle = \left\langle \frac{p^2}{2m} \right\rangle 2m = 2mE_n$$

$$\sigma_p^2 = \frac{\hbar^2\pi^2}{a^2} n^2$$

then

$$\sigma_x \sigma_p = \frac{\hbar}{2}\sqrt{\frac{\pi^2 n^2}{3} - 2}$$

which is minimal when $n = 1$, still $\sigma_x \sigma_p > \hbar/2$.

Ground state energy $n = 1$

$$E_1 = \frac{\pi^2}{2}\frac{\hbar^2}{ma^2} = \frac{\pi^2}{2}\left(\frac{\hbar}{mc}\right)^2 \frac{mc^2}{a^2} = \frac{\pi^2}{2}\left(\frac{\lambda_c}{a}\right)^2 mc^2 \tag{2.13}$$

where $\lambda_c = \hbar/mc$ called Compton wavelength.

This shows that if the box is too small, so that $\lambda_c \approx a \implies E \approx mc^2$. Thus kinematic energy $\approx$ rest energy. We shall expect to see relativistic effects, such as $e^- e^+$ creation, so Schrodinger equation is no longer correct.

How small a is too small?

$$\hbar = 1.05 \times 10^{-34} \text{J} \cdot \text{sec}$$

$$m_{proton} = 1.67 \times 10^{-27} \text{kg}$$

$$m_{elec} = 9.11 \times 10^{-31} \text{kg}$$

$$1 \text{eV} = 1.60 \times 10^{-19} \text{J}$$

If we assume energy of particles in 3D box is on the same order as in 1D box, then putting H atom in 1meter box

$$E_1 \sim \frac{(10^{-34})^2}{(10^{-27})(1)} \sim 10^{-41} \text{J} \sim 10^{-22} \text{eV}$$

so not too much relativistic effects. Question: Can wave function be 1m long? In principle yes. But there may complications due to random effects, fluctuations.

Typical $E_H \sim 3$ or 4eV at room temperature. Put e^- in a 10^{-10}m $= 1\overset{\text{o}}{\text{A}}$rmstrong box

$$E_1 \sim \frac{(10^{-34})^2}{(10^{-30})(10^{-10})^2} \sim 10^{-18} \text{J} \sim 10 \text{eV}$$

Lastly let us suppose we start the wave function

$$\Psi(x,0) = Ne^{-b(x-\frac{a}{2})^2} \text{ with } N = \sqrt{\frac{b}{\pi}} \tag{2.14}$$

in the ∞ square well. We want to see its evolution.

Actually (2.14) is not totally correct solution, because it does not vanish at the walls. But if we have the width Δx small, or

$$\sqrt{b} \sim 1/\Delta x \tag{2.15}$$

large, then it is approximately okay. Find c_n

$$\begin{aligned} c_n &= \int_0^a dx \sqrt{\frac{2}{a}} \sin\frac{n\pi}{a}x \sqrt{\frac{b}{\pi}} e^{-b(x-\frac{a}{2})^2} \\ &= \sqrt{\frac{2}{a}}\sqrt{\frac{b}{\pi}} \int_0^a dx \sin(\frac{n\pi(x-\frac{a}{2})}{a} + \frac{n\pi}{2}) e^{-b(x-\frac{a}{2})^2} \end{aligned}$$

For n even

$$c_n \sim \int dx \sin\frac{n\pi x}{a} e^{-bx^2} = 0$$

because shift $x - a/2 \to x$, two integrands are odd and even function.

For n odd

$$c_n = \sqrt{\frac{2b}{a\pi}} \int dx \cos\frac{n\pi x}{a} e^{-bx^2} = \sqrt{\frac{2}{a}} \left(\frac{\pi}{b}\right)^{\frac{1}{4}} e^{-\frac{n^2\pi^2}{4ba^2}}$$

indeed the Fourier transform of Gaussian is a Gaussian.

$$|c_n|^2 = \frac{2}{a}\sqrt{\frac{\pi}{b}} e^{-\frac{n^2\pi^2}{2ba^2}} \qquad n = 1,3,5...$$

Think this as a function of n, and when n is large, c_n becomes roughly continuous. Then we can talk about the width of c_n, i.e. the typical N, the average of the probability

$$N \sim \frac{\sqrt{2b}a}{\pi} \sim \frac{a}{\Delta x}$$

where Δx is the initial width of the wave function, cf (2.15). And by the typical

$$E_N \sim N^2 \left(\frac{\lambda_c}{a}\right)^2 mc^2 \sim \left(\frac{\lambda_c}{\Delta x}\right)^2 mc^2$$

showing Δx cannot be too small.

2.5 Bounded States Solutions

Suppose $V(x) \to \infty$ as $x \to \pm\infty$. For finite E, there will be regions of x where $V(x) > E$, called classically forbidden regions, and regions where $V(x) < E$, called classically allowed.

Clearly the two ends of the x axis are forbidden regions, we want to solve

$$-\frac{\hbar^2}{2m}\psi'' = (E - V)\psi \tag{2.16}$$

In the forbidden regions, ψ'' and ψ have same signs, so if $\psi > 0$, no maximum there. If $\psi < 0$, no minimum there. In the right most forbidden regions, for the wave function to be normalizable, we need to have

1) If $\psi > 0$ at x_0, ψ' has to be $< 0 \; \forall x \geq x_0$. Because otherwise if ψ' is positive then $\psi'' > 0$ makes ψ' growing so ψ is growing.

2) If $\psi < 0$, then ψ' has to be $> 0 \; \forall x \geq x_0$.

3) Since the overall sign is irrelevant, we assume $\psi > 0$ at x_0 in the right most forbidden regions, then ψ will stay positive. Because if it happens for some $x > x_0$ cross x axis, then at point after crossing $\psi < 0$, $\psi' < 0$, $\psi'' < 0$ then it will keep going down, bad. This also shows $\psi > 0$ for all $x < x_0$ in the right most forbidden regions.

Hence ψ is always > 0 in the right most forbidden regions, and approaches x axis asymptotically. The good candidate for ψ is of course exponential decay.

The above argument is good for solving (2.16) numerically. We have to pick the right E to make it work. It turns out that to make (2.16) work in the right most forbidden regions and in the left most forbidden regions. There are limits on E for which normalizable solutions exist, but in 3D there are cases where no E for which normalizable solutions exist.

2.6 Simple Harmonic Potential (ODE Way)

$$V = \frac{1}{2}kx^2 = \frac{1}{2}mw^2x^2 \qquad w = \sqrt{\frac{k}{m}}$$

Time-independent Schrodinger

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}mw^2\psi = E\psi \tag{2.17}$$

Redefine things, so that constants go away.

$$E = \frac{\hbar w}{2}K \qquad x = \sqrt{\frac{\hbar}{mw}}\xi$$

Then (2.17) becomes

$$-\frac{d^2\psi}{d\xi^2} + \xi^2\psi = K\psi$$

Or

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi \tag{2.18}$$

Lecture 6 (9/19/13)

We tackle (2.18) by two methods: one always works, the other works only for few cases.

Solve the differential equation

Fix K, for large $|\xi|$

$$\psi'' \approx \xi^2\psi$$

try $\psi = e^{f(\xi)}$

$$\psi' = f'e^f \qquad \psi'' = (f'' + f'^2)e^f = \xi^2 e^f$$

thus

$$f'' + f'^2 = \xi^2$$

suppose $f'' \ll f'^2 \implies f' = \pm\xi$,

$$f = \pm\frac{1}{2}\xi^2$$

check indeed $f'' = \pm 1 \ll f'^2 = \xi^2$.

At large ξ,

$$\psi = Ae^{-\xi^2/2} + Be^{\xi^2/2} \text{ with } B = 0$$

After figuring out the asymmetrical behavior, we try

$$\psi = h(\xi)e^{-\xi^2/2} \tag{2.19}$$

for ξ may be not too large.

$$\psi' = (h' - \xi h)e^{-\xi^2/2}$$

$$\psi'' = [h'' - 2\xi h' + (\xi^2 - 1)h]e^{-\xi^2/2} = (\xi^2 - K)he^{-\xi^2/2}$$

So

$$h'' - 2\xi h' + (K - 1)h = 0 \tag{2.20}$$

Try series solution

$$h = \sum_{j=0}^{\infty} a_j \xi^j = a_0 + a_1\xi + a_2\xi^2 + ... \tag{2.21}$$

$$h' = \sum_{j=1}^{\infty} a_j j \xi^{j-1}$$

$$h'' = \sum_{j=2}^{\infty} a_j j(j-1)\xi^{j-2} = \sum_{j=0}^{\infty} a_{j+2}(j+2)(j+1)\xi^j$$

Plugging into (2.20)

$$\sum_{j=0}^{\infty}[a_{j+2}(j+2)(j+1) - 2a_j j + a_j(K-1)]\xi^j = 0$$

for all ξ, thus for every j

$$a_{j+2} = \frac{2j + 1 - K}{(j+2)(j+1)}a_j \tag{2.22}$$

Since (2.20) is a 2nd order ODE, we want 2 initial conditions: a_0, a_1. They will specify all other a's.

Suppose $j \gg 1$, and suppose $j = 2l$ even (hence choosing $a_1 = 0$ kills all odd terms.)

$$a_{2(l+1)} = a_{j+2} \approx \frac{2j}{j^2} a_j = \frac{1}{l} a_{2l}$$

$$a_{2l} \approx \frac{1}{l-1} a_{2(l-1)}$$

By induction,

$$a_{2(j+1)} = \frac{\text{const}}{l!}$$

Consider ξ large, then in (2.19), the high order term (i.e. large j's term) in h are important.

$$h = \sum_{j=0}^{\infty} a_j \xi^j \approx \sum_{l=0}^{\infty} a_{2l} \xi^{2l} = \text{const} \sum_{l=0}^{\infty} \frac{1}{l!} (\xi^2)^l \propto e^{\xi^2}$$

Therefore for ξ large

$$\psi \sim e^{\xi^2} e^{-\xi^2/2} = e^{\xi^2/2}$$

not good.

Here the higher term in (2.21) doesn't decrease fast enough, so we need artificially to force (2.21) to terminate. So we have to do

(1) pick a

$$K = 2n + 1 \tag{2.23}$$

for some $n = 0, 1, 2, ...$, so that

$$a_{j+2} = 0 \text{ if } j = n$$

and all successions a_{j+4}, a_{j+6},.. are 0.

And (2) we need the series a_{j+1}, a_{j+3}, ... to terminate as well, this can done only by imposing one of terms to be 0, then by (2.21) all of them will be 0.

In summary

If n in (2.23) is chosen to be even,

$$\begin{cases} a_{n+2} \text{ and all higher even } = 0 \\ \text{all odd } a\text{'s } = 0 \end{cases}$$

If n in (2.23) is chosen to be odd,

$$\begin{cases} a_{n+2} \text{ and all higher odd=0} \\ \text{all even } a\text{'s } = 0 \end{cases}$$

This says as we discussed before for symmetric potential the eigenstates are alternating between even and odd functions.

In summary, the solution to simple harmonic potential

$$E_n = (n + \frac{1}{2})\hbar w$$

For $n = 0$, $h = a_0$, $n = 1$, $h = a_1\xi$. $n = 2$, $h = a_0 - 2a_0\xi^2$.

$$\psi_n(\xi) = \text{const}H_n(\xi)e^{-\xi^2/2}$$

H_n Hermite polynomials.

$$\begin{aligned} H_0 &= 1 \\ H_1 &= 2\xi \\ H_2 &= 4\xi^2 - 2 \\ H_3 &= 8\xi^3 - 12\xi \\ H_n &= 2^n\xi^n + ... \end{aligned} \tag{2.24}$$

In the final form

$$\psi_n(x) = \left(\frac{mw}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{mw}{\hbar}}x\right) e^{-\frac{mwx^2}{2\hbar}}$$

Some properties of Hermit polynomials

1) $H_n' = 2nH_{n-1}$

2) $H_{n+1} - 2\xi H_n + 2nH_{n-1} = 0$

3) $H_n = (-1)^n e^{\xi^2} \frac{d^n}{dx^n} e^{-\xi^2}$

4) $e^{-z^2+2z\xi} = \sum \frac{z^n}{n!} H_n(\xi)$

The next two are more important

5) Orthogonality

$$\int d\xi \left(e^{-\xi^2/2}H_n(\xi)\right)\left(e^{-\xi^2/2}H_m(\xi)\right) \propto \delta_{mn}$$

6) Completeness, "any" function can be written as

$$\psi = \sum c_n e^{-\xi^2/2}H_n(\xi)$$

2.7 Simple Harmonic Potential (Ladder Way)

Lecture 7 (9/24/13)

From last time we know energy is in unit $\hbar w$, we take

$$\frac{H}{\hbar w} = \frac{1}{2m\hbar w}(p^2 + (mwx)^2)$$

We try to decompose it. Let

$$a_+ = \frac{1}{\sqrt{2m\hbar w}}(-ip + mwx) = \frac{1}{\sqrt{2m\hbar w}}(-\hbar\frac{d}{dx} + mwx)$$

$$a_- = \frac{1}{\sqrt{2m\hbar w}}(ip + mwx) = \frac{1}{\sqrt{2m\hbar w}}(\hbar\frac{d}{dx} + mwx)$$

Or in our dimensionless units

$$a_+ = \frac{1}{\sqrt{2}}(-\frac{d}{d\xi} + \xi)$$

$$a_- = \frac{1}{\sqrt{2}}(\frac{d}{d\xi} + \xi)$$

If we compute

$$\begin{aligned}
a_+a_- &= \frac{1}{2m\hbar w}(-ip + mwx)(ip + mwx) \\
&= \frac{1}{2m\hbar w}[p^2 + (mwx)^2 + imw(xp - px)] \\
a_-a_+ &= \frac{1}{2m\hbar w}[p^2 + (mwx)^2 - imw(xp - px)]
\end{aligned}$$

Recall

$$[x,p]f = (xp - px)f = \frac{\hbar}{i}[x\frac{d}{dx}f - \frac{d}{dx}(xf)] = i\hbar f$$

Thus

$$\begin{aligned}
a_+a_- &= \frac{1}{2m\hbar w}[p^2 + (mwx)^2] - \frac{1}{2} = \frac{H}{\hbar w} - \frac{1}{2} \\
a_-a_+ &= \frac{H}{\hbar w} + \frac{1}{2}
\end{aligned}$$

With little manipulations,

$$H = \hbar w(a_+a_- + \frac{1}{2}) = \hbar w(a_-a_+ - \frac{1}{2})$$

and

$$[a_+, a_-] = a_+a_- - a_-a_+ = -1$$

Now suppose we have some stationary state

$$H\psi_E = E\psi_E$$

Let $\phi(x) = a_+\psi(x)$

$$\begin{aligned}
H\phi &= Ha_+\psi_E = \hbar w(a_+a_- + \frac{1}{2})a_+\psi_E \\
&= \hbar w(a_+a_-a_+ + \frac{1}{2}a_+)\psi_E = \hbar w[a_+(a_+a_- + 1) + \frac{1}{2}a_+]\psi_E \\
&= \hbar w a_+(a_+a_- + 1 + \frac{1}{2})\psi_E \\
&= a_+[\hbar w(a_+a_- + \frac{1}{2})\psi_E + \hbar w\psi_E] = a_+H\psi_E + a_+\hbar w\psi_E \\
&= (E + \hbar w)\phi
\end{aligned}$$

Hence if ψ_E is an eigenfunction with energy E, then $a_+\psi$ is an eigenstate with energy $E + \hbar w$. By induction $a_+^2\psi$ is an eigenstate with energy $E + 2\hbar w$, etc. We call a_+ raising operator.

Going through the algebra for a_-, one can show $a_-\psi$ is an eigenstate with energy $E - \hbar w$, so call a_- lowing operator.

Similar as before

$$-\frac{\hbar^2}{2m}\psi'' = (E-V)\psi$$

to have non-zero normalizable solutions. $\psi \to 0$ as $x \to \pm\infty$, then there exists some finite x such that ψ has maximum or minimum there, so $\psi > 0$, $\psi'' < 0$ or $\psi < 0$, $\psi'' > 0$. In other words, there exists some finite x such that

$$E - V(x) > 0$$

so at least

$$E \geq 0$$

Therefore we need to have some ψ_0 such that

$$a_-\psi_0 = 0$$

then

$$H\psi_0 = \hbar w(a_+a_- + \frac{1}{2})\psi_0 = \frac{1}{2}\hbar w\psi_0$$

so $\hbar w/2$ is the lowest energy eigenvalue.

Suppose we use $(a_+)^n\psi_0$ to get normalized ψ_n, clearly

$$H\psi_n = \hbar w(n + \frac{1}{2})\psi_n$$

Since $H\psi_n = \hbar w(a_+a_- + \frac{1}{2})\psi_n$, we obtain

$$a_+a_-\psi_n = n\psi_n$$

and

$$a_-a_+\psi_n = (a_+a_- + 1)\psi_n = (n+1)\psi_n \tag{2.25}$$

To find the form of ψ_n's, we start from ψ_0.

$$a_-\psi_0 = \frac{1}{\sqrt{2m\hbar w}}(\hbar\frac{d}{dx} + mwx)\psi_0 = 0$$

so

$$\psi_0 = ce^{-\frac{mw}{2\hbar}x^2} = ce^{-\frac{\xi^2}{2}}$$

This indeed agrees what we found last time, with $c = H_0$ Hermite 0 order. cf (2.24).

To find ψ_1, we say

$$\begin{aligned}
\psi_1 &= (\text{const})a_+\psi_0 && (2.26)\\
&= (\text{const})\frac{1}{\sqrt{2m\hbar w}}(-\hbar\frac{d}{dx} + mwx)e^{-\frac{mw}{2\hbar}x^2}\\
&= (\text{const})\frac{1}{\sqrt{2m\hbar w}}(mwx + mwx)e^{-\frac{mw}{2\hbar}x^2}\\
&= (\text{const})\frac{1}{\sqrt{2m\hbar w}}(2mwx)e^{-\frac{mw}{2\hbar}x^2}
\end{aligned}$$

The factor indeed agrees H_1 Hermite 1 order.

We want to know the proportionality in (2.26). Suppose $f(x)$, $g(x)$ vanish at $x = \pm\infty$,

$$\begin{aligned}
\int dx f^*(a_+g) &= \int dx f^*\frac{1}{\sqrt{2m\hbar w}}(-\hbar\frac{d}{dx} + mwx)g\\
&= \frac{1}{\sqrt{2m\hbar w}}\int dx \hbar g\frac{df^*}{dx} + mwxf^*g\\
&= \int dx(a_-f^*)g
\end{aligned}$$

showing a_- is the adjoint of a_+.

Let $f = a_+\psi_n$, $g = \psi_n$

$$\int dx(a_+\psi_n)^*(a_+\psi_n) = \int dx(a_-a_+\psi_n)^*\psi_n$$

By (2.25),

$$RHS = (n+1)\int dx\psi_n^*\psi_n = n+1$$

while

$$LHS = \int dx|a_+\psi_n|^2 = \int dx|(\text{const})\psi_{n+1}|^2$$

so choose const $= \sqrt{n+1}$. In summary

$$a_+\psi_n = \sqrt{n+1}\psi_{n+1}$$

and by (2.25),

$$a_-\psi_n = \sqrt{n}\psi_{n-1}$$

One big advantage of $a_\pm$ operators is that they simplify calculations. If we write

$$\begin{aligned} x &= \sqrt{\frac{\hbar}{2mw}}(a_+ + a_-) \\ p &= i\sqrt{\frac{m\hbar w}{2}}(a_+ - a_-) \end{aligned}$$

for example compute expectation value of state ψ_n,

$$\langle x \rangle = \sqrt{\frac{\hbar}{2mw}} \int dx \psi_n^*(a_+ + a_-)\psi_n = 0$$

$$\begin{aligned} \left\langle x^2 \right\rangle &= \frac{\hbar}{2mw} \int dx \psi_n^*(a_+ + a_-)^2\psi_n \\ &= \frac{\hbar}{2mw} \int dx \psi_n^*(a_+^2 + a_-^2 + a_+a_- + a_-a_+)\psi_n \\ &= \frac{\hbar}{2mw}[n + (n+1)] \end{aligned}$$

$$\begin{aligned} \left\langle p^2 \right\rangle &= -\frac{m\hbar w}{2} \int dx \psi_n^*(a_+^2 + a_-^2 - a_+a_- - a_-a_+)\psi_n \\ &= \frac{m\hbar w}{2}[n + (n+1)] \end{aligned}$$

Then we find average potential and kinetic energies

$$\langle U \rangle = \left\langle \frac{1}{2}mw^2x^2 \right\rangle = \frac{1}{2}\hbar w(n + \frac{1}{2}) = \frac{1}{2}E_n$$

$$\langle KE \rangle = \left\langle \frac{p^2}{2m} \right\rangle = \frac{1}{2} E_n$$

agreeing classical results.

Simple harmonic oscillators are useful in many different areas. If we forget about gravity, EM field in a box can be quantized using SHO. In solid state, SHO analogous vibration modes, phonon, are used to calculate specific heat.

2.8 1D Free Particle

Lecture 8 (9/26/13)

$V = 0$, as before $E \geq 0$, so let $E = \frac{\hbar^2 k^2}{2m}$, then

$$H\psi = E\psi$$

becomes

$$-\frac{d^2\psi}{dx^2} = k^2\psi$$

Solutions

$$\psi_k = Ae^{ikx} + Be^{-ikx}$$

Putting in time,

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar} = Ae^{i(kx - \frac{k^2\hbar}{2m}t)} + Be^{-i(kx + \frac{k^2\hbar}{2m}t)}$$

and assume $k > 0$, then $e^{i(kx - \frac{k^2\hbar}{2m}t)}$ is right moving wave with phase velocity $k\hbar/2m$. $e^{-i(kx + \frac{k^2\hbar}{2m}t)}$ is left moving.

Clearly

$$\int_{-\infty}^{\infty} dx |\psi_k|^2 = \infty$$

not normalizable. This turns out to be important. Recall for harmonic oscillator if E is not properly chosen, ψ grows to ∞. Here ψ doesn't grow. So not too bad.

Previously we had discrete E_n and corresponding complete orthogonal stationary states ψ_n. For any $\Psi(x, t = 0)$, we find c_n s.t.

$$\Psi(x, t = 0) = \sum_n c_n \psi_n(x)$$

then

$$\Psi(x,t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar}$$

Now E_n are continuous. We try

$$\Psi(x, t=0) = \int_{-\infty}^{\infty} dk \frac{\phi(k)}{\sqrt{2\pi}} \psi_k$$

where $\psi_k = e^{ikx}$ is the basis, and $dk\frac{\phi(k)}{\sqrt{2\pi}} \leftrightarrow c_n$.

$$\Psi(x,t) = \int_{-\infty}^{\infty} dk \frac{\phi(k)}{\sqrt{2\pi}} e^{-iE_n t/\hbar} \psi_k$$

2.9 Fourier Transform

Suppose f is square integrable, i.e.

$$\int_{-\infty}^{\infty} |f|^2 dx < \infty$$

Let $F(k)$ be the Fourier transform of $f(x)$,

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) e^{-ikx}$$

Inverse transform

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk F(k) e^{ikx}$$

Parseval says

$$\int_{-\infty}^{\infty} dk |F(k)|^2 = \int_{-\infty}^{\infty} dx |f(x)|^2$$

The physical interpretation is that

$$|\psi(x)|dx \text{ prob of finding particle at } x \text{ to } x+dx$$

$|\phi(k)|dE$ prob of finding particle with enegry E to $E+dE$ or momentum k to $k+dk$

Bessel says

$$\text{As } k \to \infty,\ F(k) \to 0$$

That is before as $k \to \infty$, e^{ikx} oscillates much more rapidly than f, so in the integral

$$F(k) = \int dx f(x) e^{ikx}$$

f acts like an envelope, the total area is close to 0.

Recall for discrete E_n

$$\int dx \psi_m^* \psi_n = \delta_{mn}$$

and c_m in $\psi = \sum c_n \psi_n$ is given by

$$c_m = \int dx \psi_m^* \psi = \sum c_n \int dx \psi_m^* \psi_n = \sum c_n \delta_{mn} = c_m \tag{2.27}$$

Dirac says let's do this continuously

$$\int dx \psi_k^* \psi_q = \begin{cases} 0 & k \neq q \\ \infty & k = q \end{cases} \propto \delta(k-q)$$

where $\delta(k-q)$ is Dirac delta function. It is actually a distribution.

Let $\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$ be the basis

$$\psi(x) = \int dk \phi(k) \frac{1}{\sqrt{2\pi}} e^{ikx}$$

and inverse Fourier

$$\phi(q) = \int dx \psi(x) \frac{1}{\sqrt{2\pi}} e^{-iqx}$$

Motivated by (2.27), we want

$$\phi(q) = \int dx \psi_q^* \psi(x)$$

Indeed

$$\begin{aligned} \phi(q) &= \int dx \frac{1}{\sqrt{2\pi}} e^{-iqx} \int dk \phi(k) \frac{1}{\sqrt{2\pi}} e^{ikx} \\ &= \int dk [\int \frac{dx}{2\pi} e^{i(k-q)x}] \phi(k) \end{aligned}$$

is true if we identify

$$\int \frac{dx}{2\pi} e^{i(k-q)x} = \delta(k-q)$$

Why? Because

$$\int dk\delta(k-q)\phi(k) \quad \approx \quad \lim_{\Delta k \to 0} \sum \Delta k \delta(k-q)\phi(k)$$

Since $\delta(k-q) \to \infty$ at $k \to q$, the sum collapses to

$$RHS = \lim_{\Delta k \to 0} \Delta k(k \approx q)\delta(k-q)\phi(q) = \phi(q)$$

because

$$\lim_{\Delta k \to 0} \Delta k \delta(k-q) = 1$$

this is $\delta(k-q) \to \infty$ at $k \to q$ and the integral of $\int dk\delta(k-q) = 1$ if the interval of integration contains q.

Some representations of δ.

We have seen

$$\delta(x) = \frac{1}{2\pi} \int dk e^{ikx}$$

$$\delta(k) = \frac{1}{2\pi} \int dx e^{ikx}$$

A new one

$$\delta(x) = \lim_{a \to 0} \frac{1}{\pi} \frac{a}{a^2 + x^2}$$

Indeed

$$\int f(x)\delta(x)dx = \lim_{a \to 0} \int dx f(x) \frac{1}{\pi} \frac{a}{a^2 + x^2} = \lim_{a \to 0} f(0) \int dx \frac{1}{\pi} \frac{a}{a^2 + x^2} = f(0)$$

Another good one

$$\delta(x) = \lim_{b \to \infty} \frac{b}{\sqrt{\pi}} e^{-b^2 x^2}$$

What is $\delta(-x)$?

$$\int_{-\infty}^{\infty} dxf(x)\delta(-x) = \int_{-\infty}^{\infty}(-1)d(-x)f(-x)\delta(x) = f(-0) = \int_{-\infty}^{\infty} dxf(x)\delta(x)$$

Hence

$$\delta(x) = \delta(-x)$$

What is $\delta(cx)$? From above we can assume $c > 0$

$$\int_{-\infty}^{\infty} dxf(x)\delta(cx) = \int_{-\infty}^{\infty} \frac{1}{c}dxf(\frac{x}{c})\delta(x) = \frac{1}{c}f(0) = \int_{-\infty}^{\infty} dxf(x)\frac{1}{c}\delta(x)$$

Hence

$$\delta(cx) = \frac{\delta(x)}{|c|}$$

2.10 1D Free Particle (continued)

Recall we mentioned that the phase velocity of $\Psi(x,t) = Ae^{ik(x-\frac{\hbar k}{2m}t)}$ with energy $\frac{\hbar^2 k^2}{2m}$ and momentum $\hbar k$ was $\frac{\hbar k}{2m}$. But we know classical particle velocity is

$$v = \frac{p}{m} = \frac{\hbar k}{m}$$

is twice of the phase velocity.

Why? From uncertainty principal, definite energy state of a continuum energy system is unachievable. Instead we should form wave packet, which is made of waves with similar momentum.

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\phi(k)e^{i(kx-\frac{E_k t}{\hbar})}$$

where $\phi(k)$ refers to the momentum amplitude or before we called it the Fourier transform of $\psi(x)$ with momentum k. We know the wave packet has similar momentum, so $\phi(k)$ is peaked near k_0.

In more traditional form let $w(k) = E_k/\hbar$, then

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\phi(k)e^{i(kx-wt)}$$

Denote $w_0 = w(k_0)$ and $w'_0 = \left(\frac{dw}{dk}\right)_{k_0}$. For k near k_0, we can expend

$$w(k) = w(k_0) + \left(\frac{dw}{dk}\right)_{k_0} (k - k_0) + ... = w_0 + w'_0(k - k_0)$$

then

$$\begin{aligned}
\Psi(x,t) &= \frac{1}{\sqrt{2\pi}} \int dk \phi(k) e^{i(kx - w_0 t - w'_0 kt + w'_0 k_0 t)} \\
&= \frac{1}{\sqrt{2\pi}} e^{i(-w_0 t + w'_0 k_0 t)} \int dk \phi(k) e^{ik(x - w'_0 t)}
\end{aligned}$$

For finding $|\Psi(x,t)|^2 dx$ or other physical observables, they are functions of $x - w'_0 t$, i.e. the observable value moves at velocity

$$v_g = \left(\frac{dw}{dk}\right)_{k_0}$$

in this case $v_g = \hbar k_0 / m$ agrees the classical value.

Lecture 9 (10/1/13)

We look at how wave functions evolve. We recall

$$\int_{-\infty}^{\infty} dx e^{-Ax^2} = \sqrt{\frac{\pi}{A}}$$

$$\int_{-\infty}^{\infty} dx e^{-Ax^2 - Bx} = \int_{-\infty}^{\infty} dx e^{-A(x + \frac{B}{2A})^2} e^{\frac{B^2}{4A}} = \sqrt{\frac{\pi}{A}} e^{\frac{B^2}{4A}}$$

A, B can be complex.

Say we start the wave function

$$\Psi(x, t = 0) = N e^{-ax^2} \text{ with } N = \left(\frac{2a}{\pi}\right)^{1/4} \tag{2.28}$$

then

$$\phi(k) = \frac{1}{\sqrt{2\pi}} N \int dx e^{-ax^2} e^{-ikx} = \frac{N}{\sqrt{2a}} e^{-\frac{k^2}{4a}}$$

So at $t = 0$

$$\langle x \rangle = 0 \qquad \langle x^2 \rangle = \frac{1}{4a}$$

$$\langle k \rangle = 0 \qquad \left\langle k^2 \right\rangle = a$$

We now have two ways to find $\langle k \rangle$ and $\langle k^2 \rangle$

$$\left\langle k^2 \right\rangle = \int dx \psi^*(x) \left(\frac{\hbar}{i} \frac{d}{dx} \right)^2 \psi(x) \text{ or } \left\langle k^2 \right\rangle = \int dk k^2 |\phi(k)|^2$$

As we saw before

$$\sigma_x = \sqrt{\frac{1}{4a}} \qquad \sigma_p = \hbar\sqrt{a}$$

so

$$\sigma_x \sigma_p = \frac{\hbar}{2}$$

Now consider time evolution,

$$\begin{aligned} \Psi(x,t) &= \frac{1}{\sqrt{2\pi}} \int dk \frac{N}{\sqrt{2a}} e^{-\frac{k^2}{4a}} e^{ikx} e^{-iE_k t/\hbar} \\ &= \frac{1}{\sqrt{2\pi}} \frac{N}{\sqrt{2a}} \int dk e^{-\left(\frac{1}{4a} + i\frac{\hbar}{2m}t\right)k^2} e^{ikx} \\ &= N\left(1 + \frac{2i\hbar a t}{m}\right)^{-\frac{1}{2}} e^{-ax^2\left(1+\frac{2i\hbar a t}{m}\right)^{-1}} \end{aligned} \tag{2.29}$$

consistency check $t = 0$, $\Psi = Ne^{-ax^2}$.

We have a complex Gaussian (2.29). Don't know what it means, take absolute value

$$\begin{aligned} |\Psi|^2 &= N^2 \left[\left(1 + \frac{2i\hbar a t}{m}\right)\left(1 - \frac{2i\hbar a t}{m}\right) \right]^{-\frac{1}{2}} \exp\left[-ax^2\left(\frac{1}{1 + \frac{2i\hbar a t}{m}} + \frac{1}{1 - \frac{2i\hbar a t}{m}}\right)\right] \\ &= N^2\left(1 + \frac{4\hbar^2 a^2 t^2}{m^2}\right)^{-\frac{1}{2}} \exp\left[-2ax^2\left(1 + \frac{4\hbar^2 a^2 t^2}{m^2}\right)^{-1}\right] \end{aligned}$$

Let $T = \frac{m}{2\hbar a}$, then

$$|\Psi|^2 = N^2\left(1 + \frac{t^2}{T^2}\right)^{-\frac{1}{2}} \exp\left[-2a\left(1 + \frac{t^2}{T^2}\right)^{-1} x^2\right]$$

Then

$$\sigma_x = \sqrt{\frac{1}{4a}\left(1 + \frac{t^2}{T^2}\right)}$$

σ_x initially grows slowly for $t < T$, then σ_x grows fast $t > T$. However σ_p is the same because of absence of potential.

The growth of σ_x seems to be disturbing. What happen to a large object? Does its wave packet spread as time goes by? For election mass 10^{-31}kg. At $t = 0$, take $\Delta x \sim 10^{-10}$m.

$$a \sim \frac{1}{4(\Delta x)^2} \sim 10^{19}\text{m}^{-2} \quad \hbar \sim 10^{-34}\text{J} \cdot \text{sec}$$

$$T = \frac{(10^{-31})}{(10^{-34})(10^{19})} \sim 10^{-15}\text{sec}$$

For ordinary object mass 10^2kg. At $t = 0$, $\Delta x \sim 10^{-6}$m

$$T \sim 10^{25}\text{sec}$$

longer than the age of the universe 10^{17}sec. One memorizing trick 1yr $= \pi \times 10^7$ sec and $\pi \sim \sqrt{10}$.

We could have chosen a more general expansion than (2.28) to start with

$$\Psi(x, t = 0) = Ne^{-a(x-x_0)^2}e^{ik_0x}$$

so that Ψ is centered at x_0 and its momentum is centered at k_0. That is because

$$\begin{aligned}
\phi(k) &= \frac{1}{\sqrt{2\pi}}\int dx N e^{-a(x-x_0)^2}e^{ik_0x}e^{-ikx} \\
&= \frac{N}{\sqrt{2\pi}}\int dx e^{-ax^2}e^{ik_0(x+x_0)}e^{-ik(x+x_0)} \\
&= \frac{N}{\sqrt{2\pi}}e^{i(k_0-k)x_0}\sqrt{\frac{\pi}{a}}e^{-(k-k_0)^2/4a}
\end{aligned}$$

2.11 Finite Square Well

$$V = \begin{cases} 0 & I : x < -a \\ -V_0 & II : -a < x < a \\ 0 & III : x > a \end{cases}$$

$V_0 > 0$. As before $E > -V_0$. If $E > 0$, we will see the solutions are related to free particles. If $-V_0 < E < 0$, we will see that wave functions with discrete energy and are concentrated in/near well.

First consider $-V_0 < E < 0$.

For region $x < -a$ or $x > a$, let

$$E = -\frac{\hbar^2 k^2}{2m}$$

then Schrodinger gives

$$\psi'' = k^2 \psi$$

region $x < -a$

$$\psi_I = Ae^{-kx} + Be^{kx} \quad A = 0$$

region $x > a$

$$\psi_{III} = Fe^{-kx} + Ge^{kx} \quad G = 0$$

For region $-a < x < a$, let

$$E + V_0 = \frac{\hbar^2 l^2}{2m}$$

then Schrodinger gives

$$\psi'' = -l^2 \psi$$

so

$$\psi_{II} = C \sin lx + D \cos lx$$

Want ψ and ψ' continuous, at $x = a$,

$$C \sin la + D \cos la = Fe^{-ka}$$

$$lC \cos la - lD \sin la = -kFe^{-ka}$$

at $x = -a$

$$Be^{-ka} = -C \sin la + D \cos la$$

$$kBe^{-ka} = lC \cos la + lD \sin la$$

Lecture 10 (10/8/13)

Suppose ψ is even, $B = F$, $C = 0$, so

$$l \tan la = k \text{ or } la \tan la = ka$$

Let $z = la$. $z_0 = a\sqrt{2mV_0}/\hbar$, so $z_0^2 - z^2 = k^2a^2$, hence

$$z \tan z = \sqrt{z_0^2 - z^2}$$

or

$$\tan z = \sqrt{\frac{z_0^2}{z^2} - 1} \tag{2.30}$$

The solutions for z, which are the intersections, give allowed l, hence allowed E. The bigger $z_0$is, i.e. bigger V_0 (deeper well) or bigger a (wider well), more solutions exist. Notice for any well, by the graph of (2.30), there is always at f least one even solution.

If ψ is odd, $B = -F$, $D = 0$, similarly solve

$$la \cot la = -ka$$

showing not necessarily always have odd solution.

Now do $E > 0$ scattering solution, $l = \sqrt{2m(E + V_0)}/\hbar$ is the same,

$$\begin{aligned}
\psi_I &= Ae^{ikx} + Be^{-ikx} \\
\psi_{II} &= C \sin lx + D \cos lx \\
\psi_{III} &= Fe^{ikx} + Ge^{-ikx}
\end{aligned}$$

This can be thought of replacing k by ik from bound case, and

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Solution is not normalizable, just like free particle, the final solution can be obtained from wave packet. Boundary conditions give 4 equations. We have 6 unknowns: A, B, C, D, E, F. One constant is overall factor, don't care. The other extra constant $G = 0$ is set by the initial condition: assume particles come in from the left, i.e. no left moving wave in region $x > a$. Notice that if we assume starting the particle in the well, i.e. $A = G = 0$, and assume the solution to have parity.

We will end up being

$$la\tan la = ika$$

Thus no real solutions. Starting the particle in the well doesn't yield any stationary state.

At $x = -a$

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= -C\sin la + D\cos la \\ ik(Ae^{-ika} - Be^{ika}) &= l(C\cos la + D\sin la) \end{aligned}$$

At $x = a$

$$\begin{aligned} C\sin la + D\cos la &= Fe^{ika} \\ l(C\cos la - D\sin la) &= ikFe^{ika} \end{aligned}$$

From here, we can solve for B, C, D, F in terms of free parameter A. Although the wave function is not normalizable, we can still talk about reflection coefficient

$$\frac{|B|^2}{|A|^2} = R$$

transmission coefficient

$$\frac{|F|^2}{|A|^2} = T$$

Lecture 11 (10/10/13)

Suppose we do this kind of experiment, sometimes we see particle passing through, sometimes bouncing back. Reflection is classically non-sense for particles. Is it possible to have no reflection? Possible if $\sin 2la = 0$, then $la = n\pi/2$, $n = 1, 2, 3, \ldots$ The experiment with inert gas and sending e^- confirms such effect (Ramsauer-Townsend). The exact expression for T

$$T = \left(1 + \frac{V_0^2}{4E(E+V_0)}\sin^2 2la\right)^{-1}$$

Tunneling

Suppose we are interested in finite square barrier with $0 < E < V_0$

$$V = \begin{cases} 0 & x < -a \\ V_0 & -a < x < a \\ 0 & x > a \end{cases}$$

Follow the same step. First argue no stationary solution for particle starting in the barrier, because no real solution

$$ika = la \tanh la$$

Hence the solution looks like

$$\begin{cases} \psi_I = Ae^{ikx} + Be^{-ikx} \\ \psi_{II} = Ce^{lx} + De^{-lx} \\ \psi_{III} = Fe^{ikx} \end{cases}$$

then solve for B, C, D, F.

2.12 Dirac-Delta Well

$$V = -\alpha\delta(x)$$

think this as a limiting case of $a \to 0$, $V_0 \to \infty$. One can argue that as $a \to 0$, it becomes harder and harder to get to excited states, because excited states have many nodes and antinodes, i.e. the wave function oscillates within the well. As we will show there is only one bound state.

$$\psi'' = -\frac{2m}{\hbar^2}(E + \alpha\delta(x))\psi \tag{2.31}$$

$E < 0$. For $x < 0$

$$\psi_L = Ae^{kx} + Be^{-kx}$$

For $x > 0$

$$\psi_R = Ce^{kx} + De^{-kx}$$

clearly $B = C = 0$. Assuming ψ is continuous at $x = 0$, $A = D$.

At $x = 0$, what about

$$\psi_L' = \psi_R'?$$

Integrate (2.31),

$$\int_{-\epsilon}^{\epsilon} \psi''(x)dx = -\frac{2m}{\hbar^2}(\int_{-\epsilon}^{\epsilon} E\psi dx + \alpha \int_{-\epsilon}^{\epsilon} \delta(x)\psi)$$

$$\psi'(0+) - \psi'(0-) = 0 - \frac{2m}{\hbar^2}\alpha\psi(0)$$

so

$$k(-D - A) = -\frac{2m}{\hbar^2}\alpha A \implies k = \frac{m\alpha}{\hbar^2}$$

$$E = -\frac{m\alpha^2}{2\hbar^2}$$

one and only one bound state.

The solution may seem surprising. Why not is the solution $\delta(x)$, i.e. the particle is fixed in the $\delta(x)$ potential? Because delta potential has 0 outside the well, to get delta solution, we use ∞ square well of 0 width.

The graph of solution shows that near $x = 0$ the function is continuous, and the slope, ψ', is a step function, and here ψ'' is indeed a delta function as in (2.31).

Scattering Case $E > 0$

Let $E = \frac{\hbar^2 k^2}{2m}$

$$\begin{aligned} \psi_L &= Ae^{ikx} + Be^{-ikx} \\ \psi_R &= Fe^{ikx} + Ge^{-ikx} \end{aligned}$$

$G = 0$ for particle entering from the left. Continuity at $x = 0$

$$A + B = F$$

Derivative

$$\psi_R'(0+) - \psi_L'(0-) = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

so

$$ik(F - A + B) = -\frac{2m\alpha}{\hbar^2}(A + B)$$

Solve for

$$B = \frac{i\beta}{1 - i\beta}A \qquad F = \frac{1}{1 - i\beta}A$$

$\beta = \frac{m\alpha}{\hbar^2 k}$, compute transmission, reflection coefficients

$$T = \frac{1}{1 + \beta^2} \qquad R = \frac{\beta^2}{1 + \beta^2}$$

Delta Function Barrier

$E > 0$ no bound state, change $\alpha \to -\alpha$, but T, R are the same, so things can go through ∞ barrier, provided the width of barrier is 0.

3 Formalism

3.1 Vector Space

Lecture 12 (10/15/13)

A quantum state corespondents to a vector. We first study some general properties of vectors.

Definition. Vector space (finite dimensional)

1) set of vectors $|a\rangle$, $|5\rangle$, $|\text{George}\rangle$ and scalars, complex numbers

2) operations: addition $|a\rangle + |b\rangle = |c\rangle$ such that

$$\begin{aligned} |a\rangle + |b\rangle &= |b\rangle + |a\rangle \\ |a\rangle + (|b\rangle + |c\rangle) &= (|a\rangle + |b\rangle) + |c\rangle \end{aligned}$$

3) There exists a null vector $|\text{null}\rangle$ s.t.

$$|\text{null}\rangle + |a\rangle = |a\rangle$$

Griffiths uses $|0\rangle$, we should never do so, e.g. SHO $|0\rangle$ is ground state.

4) Each vector has additive inverse

$$|a\rangle + |a \text{ inverse}\rangle = |\text{null}\rangle$$

Griffiths uses $|-a\rangle$, we should never do so, e.g. $|p\rangle$ and $|-p\rangle$ mean two waves moving in opposite direction. They are never inverse to each other.

5) operation: scalar multiplication $r\,|a\rangle = |f\rangle$ such that

$$\begin{aligned}
a(b\,|c\rangle) &= (ab)\,|c\rangle \\
a(|b\rangle + |c\rangle) &= a\,|b\rangle + a\,|c\rangle \\
(a+b)\,|f\rangle &= a\,|f\rangle + b\,|f\rangle \\
0\,|a\rangle &= |\text{null}\rangle \\
1\,|a\rangle &= |a\rangle
\end{aligned}$$

Use definition we see that since $-\,|a\rangle + |a\rangle = (-1+1)\,|a\rangle = 0\,|a\rangle = |\text{null}\rangle$, inverse of $|a\rangle$ is $-\,|a\rangle$.

Example of vectors:

3 dimensional spatial vector, $dim = 3$

Polynomial of degree $\leq N$, $dim = N+1$

$$|a\rangle = a_0 + a_1 x + a_2 x^2 + ... + a_N a^N$$

Definition. If $a\,|\alpha\rangle + b\,|\beta\rangle + c\,|\gamma\rangle + ... = 0$, iff $a = b = c = ... = 0$, then $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, ...$ are linearly independent.

The set of dependent if it's not linearly independent.

Definition. Basis of a vector space is linearly independent set that spans the space.

Dimension of space = number of vector in basis = maximum number of linearly independent vectors.

Suppose basis $|e_1\rangle$, $|e_2\rangle$, ..., $|e_N\rangle = \{|e_j\rangle\}$, any vector

$$|\alpha\rangle \;=\; \sum_{i=1}^{N} a_i\,|e_i\rangle = (a_1, a_2, .., a_N) \quad |\beta\rangle = \sum_{i=1}^{N} b_i\,|e_i\rangle$$

so

$$\begin{aligned} |\alpha\rangle + |\beta\rangle &= \sum_{i=1}^{N}(a_i + b_i)\,|e_i\rangle \\ \lambda\,|\alpha\rangle &= \sum_{i=1}^{N}\lambda a_i\,|e_i\rangle \\ |\text{null}\rangle &= \sum_{i=1}^{N} 0\,|e_i\rangle \end{aligned}$$

i.e.

$$\begin{aligned} |\text{null}\rangle &= (0, 0, ..., 0) \\ |\alpha \text{ inverse}\rangle &= (-a, -a, ..., -a) \end{aligned}$$

Generalize inner product.

Definition. Given $|\alpha\rangle$,$|\beta\rangle$, $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$ =complex number such that

$$\langle\alpha|\alpha\rangle = \|\alpha\|^2 > 0, {=}0 \text{ iff } |\alpha\rangle = |\text{null}\rangle$$

($\|\alpha\|$ denotes norm of $|\alpha\rangle$), and

$$\langle\alpha|\,(b\,|\beta\rangle + c\,|\gamma\rangle) = b\,\langle\alpha|\beta\rangle + c\,\langle\alpha|\beta\rangle$$

Example: 3-dim complex spatial vector

$$\langle\vec{v}|\vec{w}\rangle = (\vec{v}^*)\cdot(\vec{w}) = v_x^* w_x + v_y^* w_y + v_z^* w_z = \langle\vec{w}|\vec{v}\rangle^*$$

For polynomial of degree $\leq N$, possible inner products

1) $\langle f|g\rangle = f_0^* g_0 + f_1^* g_1 + ... + f_N^* g_N$

2) $\langle f|g\rangle = \int_{-1}^{1} dx f^*(x) g(x)$

3) $\langle f|g\rangle = \int_{-\infty}^{\infty} dx f^*(x)g(x)e^{-x^2}$, this guarantees to converge, the form relates to Hermite polynomial.

Suppose $\{|e_i\rangle\}$ is a basis

Definition. If $\langle a|b\rangle = 0$, $|a\rangle$ and $|b\rangle$ are orthogonal. If $\langle e_i|e_j\rangle = \delta_{ij}$, the basis is orthonormal.

In this basis

$$\begin{aligned} |\alpha\rangle &= a_1 |e_1\rangle + a_2 |e_2\rangle + ... + a_N |e_N\rangle \\ |\beta\rangle &= b_1 |e_1\rangle + b_2 |e_2\rangle + ... + b_N |e_N\rangle \end{aligned}$$

$$\begin{aligned} \langle\alpha|\beta\rangle &= a_1^* b_1 + ... + a_N^* b_N \\ \langle e_j|\alpha\rangle &= a_j \\ \langle\alpha|e_j\rangle^* &= a_j^* \end{aligned}$$

and

$$|\alpha\rangle = \sum_j |e_j\rangle \langle e_j|\alpha\rangle$$

Think $\langle\alpha|$ as dual vector of $|\alpha\rangle$

$$\langle\alpha| = \sum a_j^* \langle e_j|$$

Example of orthonormal basis

1) 3 dim spatial vectors

$$\{|e_i\rangle\} = \hat{i}, \hat{j}, \hat{k}; \quad \hat{e}_r, \hat{e}_\theta, \hat{e}_\phi$$

2) Polynomial

Take $\{1, x, x^2, ..., x^N\}$ a basis.

(a) If inner product is $\langle f|g\rangle = f_0^* g_0 + ... + f_N^* g_N$, and associate

$$\begin{aligned} 1 &= (1,0,0,...) \\ x &= (0,1,0,...) \\ &... \end{aligned}$$

then $\{1, x, x^2, ..., x^N\}$ is an orthonormal basis.

(b) If inner product is $\langle f|g\rangle = \int_{-\infty}^{\infty} dx f^*(x) g(x) e^{-x^2}$, then Hermite polynomial is an orthogonal basis.

(c) If inner product is defined as $\langle f|g\rangle = \int_{-1}^{1} dx f^*(x) g(x)$, then Legendre polynomials is an orthogonal basis. They are found by Gram-Schmidt

$$|e_0'\rangle = N_0 |e_0\rangle$$

$$\langle e_0'|e_0'\rangle = \int_{-1}^{1} dx |N_0|^2 = 2|N_0|^2 = 1 \implies |e_0'\rangle = \frac{1}{\sqrt{2}}$$

To ensure $\langle e_1'|e_0'\rangle = 0$, we put

$$\begin{aligned} |e_1'\rangle &= N_1 \left(|e_1\rangle - |e_0'\rangle \langle e_0'|e_1\rangle\right) \\ &= N_1 \left(|e_1\rangle - |e_0'\rangle \int_{-1}^{1} dx \frac{1}{\sqrt{2}} x\right) = N_1 |e_1\rangle \end{aligned}$$

$$\langle e_1'|e_1'\rangle = |N_1|^2 \int_{-1}^{1} dx x^2 = 1 \implies |e_1'\rangle = \sqrt{\frac{3}{2}} x$$

$$\begin{aligned} |e_2'\rangle &= N_2 \left(|e_2\rangle - |e_0'\rangle \langle e_0'|e_2\rangle - |e_1'\rangle \langle e_1'|e_2\rangle\right) \\ &= N_2 [x^2 - \frac{1}{\sqrt{2}} \frac{\sqrt{2}}{3} - \sqrt{\frac{3}{2}} x(0)] \end{aligned}$$

$$\langle e_2'|e_2'\rangle = |N_2|^2 \int_{-1}^{1} dx (x^2 - \frac{1}{3})^2 = |N_2|^2 (\frac{2}{5} - \frac{4}{9} + \frac{2}{9}) \implies |e_2'\rangle = 3\sqrt{\frac{5}{8}} (x^2 - \frac{1}{3})$$

We show Schwartz Inequality,

Let

$$|\gamma\rangle = |\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle} |\alpha\rangle$$

$$
\begin{aligned}
0 \leq \langle\gamma|\gamma\rangle &= \langle\beta|\gamma\rangle - \left(\frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\right)^* \langle\alpha|\gamma\rangle \\
&= \langle\beta|\beta\rangle - \frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\langle\beta|\alpha\rangle - \left(\frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\right)^* \langle\alpha|\beta\rangle + \left|\frac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}\right|^2 \langle\alpha|\alpha\rangle \\
&= \|\beta\|^2 - \frac{|\langle\alpha|\beta\rangle|^2}{\|\alpha\|^2}
\end{aligned}
$$

Therefore

$$\|\alpha\|\,\|\beta\| \geq |\langle\alpha|\beta\rangle|$$

For the 3 dim spatial vector, it says

$$|\vec{v}||\vec{w}| \geq |\vec{v}\cdot\vec{w}|$$

or meaning $|\cos\theta| \leq 1$.

Equality is obtained if $|\gamma\rangle = 0$, so $|\beta\rangle \parallel |\alpha\rangle$.

Lecture 13 (10/17/13)

3.2 Linear Transformation

$$\hat{T} : |\alpha\rangle \to |\alpha'\rangle = \hat{T}|\alpha\rangle = |T\alpha\rangle$$

such that

$$\hat{T}\,(a|\alpha\rangle + b|\beta\rangle) = a\hat{T}|\alpha\rangle + b\hat{T}|\beta\rangle$$

Examples:

1) rotation of 3D spatial vector

2) differentiation on degree $\leq N$ polynomials. However integration on degree $\leq N$ poly is not, because it is not closed. Squaring degree

e $\leq N$ poly is not, because it isn't closed and not linear.

Choose an orthonormal basis $\{|e_j\rangle\}$. Specify $\hat{T}$'s action on the basis

$$\hat{T}|e_n\rangle = \sum_j T_{jn}|e_j\rangle = T_{1n}|e_1\rangle + T_{2n}|e_2\rangle + \ldots \tag{3.1}$$

If $|\alpha\rangle = \sum_n a_n |e_n\rangle$, i.e. components of $|\alpha\rangle$ are a_n's,

$$\hat{T}|\alpha\rangle = \sum_n \sum_j a_n T_{jn} |e_j\rangle = \sum_j \left(\sum_n T_{jn} a_n \right) |e_j\rangle$$

where $\sum_n T_{jn} a_n$ can be thought as matrix multiplication, matrix $\hat{T}$ multiplies column vector $|\alpha\rangle$. Put

$$|\alpha'\rangle = \hat{T}|\alpha\rangle = \sum_k a'_k |e_k\rangle$$

then

$$a'_k = \sum_l T_{lk} a_k$$

That is why in (3.1) we use T_{jn} not T_{nj}. Same awkwardness happens in (3.2).

Naturally we call T_{lk} the matrix elements of T, which are given by first fixing a basis

$$\langle e_i| \left(\hat{T}|e_j\rangle \right) = \left\langle e_i \middle| \hat{T} \middle| e_j \right\rangle = \langle e_i| \left(\sum_k T_{kj} |e_k\rangle \right) = \sum_k T_{kj} \langle e_i|e_k\rangle = T_{ij}$$

Consider composition of linear transformations

$$|v\rangle \xrightarrow{\hat{T}} \hat{T}|v\rangle \xrightarrow{\hat{S}} \hat{S}\left(\hat{T}|v\rangle\right) = \hat{S}\hat{T}|v\rangle$$

Put $R = ST$, let's see what matrix elements of R look like? Write $|v\rangle = \sum_k v_k |e_k\rangle$, then

$$\begin{aligned} T|v\rangle &= \sum_{jk} T_{jk} v_k |e_j\rangle \\ ST|v\rangle &= \sum_{ijk} S_{ij} T_{jk} v_k |e_i\rangle \end{aligned}$$

Since

$$R|v\rangle = \sum_i R_{ik} v_k |e_i\rangle$$

we get R to be the product of matrix multiplication.

3.3 Properties of Square Matrix

Transpose of Matrix

$$(T^t)_{ij} = T_{ji}$$

If $T = T^t$, T is symmetric. If $T = -T^t$, T is antisymmetric. Show

$$(ST)^t = T^t S^t$$

Indeed

$$(ST)^t_{ki} = (ST)_{ik} \quad = \quad \sum_j S_{ij} T_{jk} = \sum_j S^t_{ji} T^t_{kj} = \sum_j T^t_{kj} S^t_{ji} = (T^t S^t)_{ki}$$

Hermitian Conjugate

$$T^\dagger = (T^*)^t = (T^t)^*$$

$$(ST)^\dagger = T^\dagger S^\dagger$$

If $S = S^\dagger$, S is hermitian. If $S = -S^\dagger$, S is anti hermitian.

Product of two symmetric or hermitian matrices may not be symmetric or hermitian

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

this is due to the fact that matrix multiplication is not commutative, so we define commutator

Commutator

$$ST - TS = [S, T] = -[T, S]$$

Unit Matrix

$$I_{ij} = \delta_{ij}$$

Inverse Matrix

$$T^{-1}T = TT^{-1} = I$$

T^{-1} exists iff $\det T \neq 0$. If $\det T = 0$, T is singular.

$$(ST)^{-1} = T^{-1}S^{-1}$$

Unitary Matrix

$$U^{-1} = U^\dagger$$

or

$$UU^\dagger = U^\dagger U = I$$

We show unitary transformation preserve dot product
Let $|w'\rangle = U|w\rangle$, $|v'\rangle = U|v\rangle$

$$\begin{aligned} \langle w'|v'\rangle &= \sum_i (w')_i^* v_i' = \sum_i \left(\sum_k U_{ik} w_k\right)^* \left(\sum_j U_{ij} v_j\right) \\ &= \sum_{ijk} U_{ik}^* U_{ij} w_k^* v_j = \sum_{jk} \underbrace{\sum_i (U^\dagger)_{ki} U_{ij}}_{\delta_{kj}} w_k^* v_j = \sum_j w_j^* v_j = \langle w|v\rangle \end{aligned}$$

Base Change Matrix

Two base (not necessary orthonormal) $\{|e_i\rangle\}$, $\{|f_j\rangle\}$. Suppose two are connected by S

$$|e_i\rangle = \sum S_{ji} |f_j\rangle \tag{3.2}$$

For any vector $|\alpha\rangle$, there are two representations

$$|\alpha\rangle = \sum_i a_i^e |e_i\rangle = \sum_i a_i^f |f_i\rangle$$

then

$$a_i^f = \sum_j S_{ij} a_j^e$$

or

$$a^f = Sa^e \tag{3.3}$$

Let us now examine the effect of base change on linear transformations. Suppose

$$|\alpha\rangle \xrightarrow{\hat{T}} |\alpha'\rangle$$

suppose we know the matrix elements of T in both base

$$\begin{aligned}(a')^e &= T^e a^e \\ (a')^f &= T^f a^f\end{aligned}$$

then by (3.3)

$$T^f = S T^e S^{-1}$$

we call T^f & T^e are similar.

If $\{|e_i\rangle\}$, $\{|f_j\rangle\}$ are orthonormal, then S in (3.2) is unitary.

Trace and Determinant

They are invariant under change of basis.

$$\det T^f = \det(S T^e S^{-1}) = \det S \det T^e \det S^{-1} = \det T^e$$

Trace

$$\mathrm{Tr} T = \sum T_{kk}$$

First show

$$\mathrm{Tr} AB = \mathrm{Tr} BA \tag{3.4}$$

Indeed

$$\sum_k (AB)_{kk} = \sum_{kj} A_{kj} B_{jk} = \sum_{jk} B_{jk} A_{kj} = \sum_j (BA)_{jj}$$

now

$$\mathrm{Tr} T^f = \mathrm{Tr} S T^e S^{-1} = \mathrm{Tr} T^e S^{-1} S = \mathrm{Tr} T^e$$

Lecture 14 (10/22/13)

(3.4) is only true for finite dimensional matrix. Consider ∞ matrices

$$A = \begin{pmatrix} 0 & \sqrt{1} & & & \\ & 0 & \sqrt{2} & & \\ & & 0 & \sqrt{3} & \\ & & & 0 & \ddots \\ & & & & \ddots \end{pmatrix} \quad B = \begin{pmatrix} 0 & & & & \\ \sqrt{1} & 0 & & & \\ & \sqrt{2} & 0 & & \\ & & \sqrt{3} & 0 & \\ & & & \ddots & \ddots \end{pmatrix}$$

[the physical models of A and B are a_- and a_+, lowing and raising operators. Because

$$\begin{aligned} |\psi\rangle &= c_0 |0\rangle + c_1 |1\rangle + ... = \begin{pmatrix} c_0 \\ c_1 \\ \vdots \end{pmatrix} \\ a_- |\psi\rangle &= c_1\sqrt{1}\,|0\rangle + c_2\sqrt{2}\,|1\rangle + ... = \begin{pmatrix} c_1\sqrt{1} \\ c_2\sqrt{2} \\ \vdots \end{pmatrix} \end{aligned}$$

] then

$$AB = \begin{pmatrix} 1 & & & & \\ & 2 & & & \\ & & 3 & & \\ & & & 4 & \\ & & & & \ddots \end{pmatrix} \quad BA = \begin{pmatrix} 0 & & & & \\ & 1 & & & \\ & & 2 & & \\ & & & 3 & \\ & & & & \ddots \end{pmatrix}$$

$$\mathrm{Tr}AB - \mathrm{Tr}BA = \mathrm{Tr}(AB - BA) = \infty$$

Hence $\mathrm{Tr}AB \neq \mathrm{Tr}BA$.

Eigenvectors & Eigenvalues

$$\hat{T}\,|\alpha\rangle = \lambda\,|\alpha\rangle \iff Ta = \lambda a \iff (T - \lambda)a = 0 \tag{3.5}$$

where a is the component vector of $|\alpha\rangle$ in some chosen basis.

For nontrivial a to satisfy (3.5), iff $\det|T-\lambda|=0$, i.e.

$$\det\begin{vmatrix} T_{11}-\lambda & T_{12} & \\ T_{21} & T_{22}-\lambda & \\ & & \ddots \end{vmatrix}=0$$

which gives a polynomial in λ of degree N

$$(-\lambda)^N+(\mathrm{Tr}T)(-\lambda)^{N-1}+...+\det T=0$$

There will be N complex roots, and some may be degenerated.

Example 1

$$T=\begin{pmatrix} 0 & 3 \\ -3 & 0 \end{pmatrix}$$

$$\det|T-\lambda|=\begin{vmatrix} -\lambda & 3 \\ -3 & -\lambda \end{vmatrix}=\lambda^2+9=0 \implies \lambda=\pm 3i$$

$\lambda^{(1)}=3i$,

$$Ta=3ia \implies \begin{pmatrix} 0 & 3 \\ -3 & 0 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}=3i\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \implies ia_1=a_2 \implies a^{(1)}=\mathrm{const}\begin{pmatrix} 1 \\ i \end{pmatrix}$$

$\lambda^{(2)}=-3i$,

$$a^{(2)}=\mathrm{const}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

and we have in general that antisymmetric matrix has pure imaginary eigenvalues, and we check

$$\left\langle \alpha^{(1)} \middle| \alpha^{(2)} \right\rangle = 1+i^2=0$$

Example 2

$$T=\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

only one eigenvalue $\lambda=1$ and only one eigenvector $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Example 3

$$T = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

eigenvalue $\lambda = 1, 1, -1$, and there are three independent eigenvectors

$$a^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad a^{(2)} = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \quad a^{(3)} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

we can check they are mutually orthogonal, and can be made to be orthonormal.

If we choose these orthonormal eigenvectors $\{|f_i\rangle\}$ to be the basis, then T is diagonal. Indeed

$$T_{ij} = \langle f_i|T|f_j\rangle = \lambda_j \langle f_i|f_j\rangle = \lambda_j \delta_{ij}$$

In our previous notation that S is denoted to be the basis change matrix

$$|e_i\rangle = S_{ji}\,|f_j\rangle \text{ and } |f_j\rangle = a_i^{(j)}\,|e_i\rangle$$

then

$$a_i^{(j)} = (S^{-1})_{ij}$$

ith component of the jth eigenvector, i.e. $S^{-1} = S^\dagger$, unitary matrix, has $a^{(j)}$ as its columns.

So in that notation, we have

$$(ST^eS^{-1})_{il} = \sum_{jk} S_{ij}T_{jk}(S^{-1})_{kl} = \sum_{jk} S_{ij}T_{jk}a_k^{(l)} = \lambda^{(l)} \sum_j S_{ij}a_j^{(l)} = \lambda^{(l)} \sum_j S_{ij}(S^{-1})_{jl} = \lambda^{(l)}\delta_{il}$$

Hence indeed in the basis of $\{|f\rangle\}$,

$$T^f = ST^eS^{-1} = \begin{pmatrix} \lambda^{(1)} & & \\ & \lambda^{(2)} & \\ & & \ddots \end{pmatrix}$$

From above we conclude that $n \times n$ matrix M is diagonalizable iff there are

n linear independent eigenvectors.

By the spectral theorem, referring to the case of orthonormal basis, M is diagonalizable iff M is normal, i.e. $[M, M^\dagger] = 0$. So Hermitian matrix or unitary matrix is diagonalizable.

Question: given two normal matrices A and B, in what situation there exists S diagonalizes both simultaneously? It is possible if

$$0 = [SAS^{-1}, SBS^{-1}] = SAS^{-1}SBS^{-1} - SBS^{-1}SAS^{-1} = S[A,B]S^{-1} \iff [A,B] = 0$$

This is part of the general statement that A and B are simultaneously diagonalizable if and only if they commute. Hence they share the same eigenvectors.

Hermitian Matrix & Hermitian Transformation

$$\hat{T}\,|\beta\rangle = |T\beta\rangle$$

Define Hermitian conjugate transformation

$$\hat{T}^\dagger\,|\alpha\rangle = \left|T^\dagger\alpha\right\rangle$$

s.t.

$$\left\langle T^\dagger\alpha\middle|\beta\right\rangle = \langle\alpha|T\beta\rangle$$

or

$$\left\langle\beta\middle|T^\dagger\alpha\right\rangle = \langle\alpha|T\beta\rangle^*$$

Let us see the matrix associated with $\hat{T}^\dagger$.

$$\begin{aligned}
\left\langle\beta\middle|T^\dagger\alpha\right\rangle &= \sum_j \beta_j^*(T^\dagger\alpha)_j = \sum_{jk}\beta_j^*(T^\dagger)_{jk}\alpha_k \\
\langle\alpha|T\beta\rangle^* &= \left(\sum_k \alpha_k^*(T\beta)_k\right)^* = \left(\sum_{kj}\alpha_k^*(T_{kj}\beta_j)\right)^* = \sum_{jk}\alpha_k T_{kj}^*\beta_j^*
\end{aligned}$$

Hence

$$(T^\dagger)_{jk} = T_{kj}^*$$

the matrix associated with $\hat{T}^\dagger$ is Hermitian conjugate matrix. If T is Hermitian

$$\langle T\alpha|\beta\rangle = \langle\alpha|T\beta\rangle$$

Some properties about Hermitian transformations

Lecture 15 (10/24/13)

1) Eigenvalues are real.

Proof 1

$$\left\langle\alpha\middle|\hat{T}\alpha\right\rangle = \left\langle\hat{T}^\dagger\alpha\middle|\alpha\right\rangle = \left\langle\hat{T}\alpha\middle|\alpha\right\rangle = \left\langle\alpha\middle|\hat{T}\alpha\right\rangle^*$$

$\left\langle\alpha\middle|\hat{T}\alpha\right\rangle$ is real for any $|\alpha\rangle$. Say $\hat{T}\,|\beta\rangle = \lambda\,|\beta\rangle$,

$$\underbrace{\langle\beta|T\beta\rangle}_{\text{real}} = \lambda\underbrace{\langle\beta|\beta\rangle}_{\text{real}}$$

so λ has to be real.

Proof 2

$$\sum_j T_{ij}b_j = \lambda b_i \tag{3.6}$$

Take complex conjugate

$$\sum_j T^*_{ij}b^*_j = \lambda^* b^*_i$$

Since $T^*_{ij} = T^\dagger_{ji} = T_{ji}$,

$$\sum_j T_{ji}b^*_j = \lambda^* b^*_i \tag{3.7}$$

Take dot product of (3.6), (3.7)

$$\begin{aligned}\sum_{ij} b^*_i T_{ij} b_j &= \lambda\sum_i b^*_i b_i \\ \sum_{ij} b_i T_{ji} b^*_j &= \lambda^*\sum_i b_i b^*_i\end{aligned}$$

Therefore

$$\lambda = \lambda^*$$

2) Eigenvectors with different λ's are orthogonal

$$\begin{aligned} \hat{T}\,|\alpha\rangle &= \lambda\,|\alpha\rangle \\ \hat{T}\,|\beta\rangle &= \lambda'\,|\beta\rangle \end{aligned}$$

$$\left\langle \beta \middle| \hat{T} \middle| \alpha \right\rangle = \lambda\,\langle \beta|\alpha\rangle = \left\langle T^\dagger \beta \middle| \alpha \right\rangle = \langle T\beta|\alpha\rangle = \lambda'\,\langle \beta|\alpha\rangle$$

$$(\lambda - \lambda')\,\langle \alpha|\beta\rangle = 0 \implies \langle \alpha|\beta\rangle = 0$$

3) Eigenvectors span space. (without proof) So can be made an orthonormal basis.

3.4 Use of Linear Algebra in QM

Dual Space

$$|\alpha\rangle \leftrightarrow \langle\alpha|$$

Kets: vector space. Bras: dual vector space.

$$a\,|\alpha\rangle + b\,|\beta\rangle \leftrightarrow a^*\,\langle\alpha| + b^*\,\langle\beta|$$

Suppose $\langle e_i|e_j\rangle = \delta_{ij}$

$$\begin{aligned} |\alpha\rangle &= \sum_i a_i\,|e_i\rangle \implies a_i = \langle e_i|\alpha\rangle \\ &= \sum_i \langle e_i|\alpha\rangle\,|e_i\rangle \\ &= \sum_i |e_i\rangle\,\langle e_i|\,|\alpha\rangle \implies \sum_i |e_i\rangle\,\langle e_i| = I \end{aligned}$$

Spectral Decomposition of $\hat{T}$

Suppose $\hat{T}\left|e_j\right\rangle = \lambda_j \left|e_j\right\rangle$

$$\hat{T} = \sum_j \lambda_j \left|e_j\right\rangle \left\langle e_j\right| = \sum_j \left|e_j\right\rangle \lambda_j \left\langle e_j\right|$$

If $\left|\alpha\right\rangle = \sum a_i \left|e_i\right\rangle$, $\hat{T}\left|\alpha\right\rangle = \sum a_i \lambda_i \left|e_i\right\rangle$

$$\hat{T} = \sum_{ij} \left|e_i\right\rangle T_{ij} \left\langle e_j\right|$$

$$\mathrm{Tr}\hat{T} = \sum_k \left\langle e_k \middle| \hat{T} \middle| e_k \right\rangle = \sum_{ij} \underbrace{\langle e_j | e_i \rangle}_{\delta_{ij}} T_{ij} = \sum T_{ii}$$

Hilbert Space

If Ψ_1, Ψ_2 are solutions, so is $a\Psi_1(x,t) + b\Psi_2(x,t) = \Psi_3(x,t)$. This suggests to treat $\left|\Psi\right\rangle$, QM physical state, as some vector in what space?

Want square integrable function, i.e.

$$\int dx \left|f(x)\right|^2 \text{ finite}$$

and dot product

$$\langle f|g\rangle = \int dx f^*(x) g(x)$$

If f, g are square integrable, so is $f+g$.

$$\begin{aligned} \int |f+g|^2 &= \int |f|^2 + \int |g|^2 + \int fg^* + \int f^* g \\ \left| \int fg^* \right| &\leq \left(\int |f|^2 \right)^{1/2} \left(\int |g|^2 \right)^{1/2} \text{ by Holder} \end{aligned}$$

We arrive the definition of Hilbert space, which is an infinite dimensional vector space. We say

$$\text{QM Physcial State } \left|\Psi\right\rangle \longleftrightarrow \text{Vectors in Hilbert space } \left|\Psi\right\rangle \text{ or } e^{i\beta}\left|\Psi\right\rangle$$

Note $|\Psi\rangle$ and $e^{i\beta}|\Psi\rangle$ give the same physical state, but $|\Psi\rangle + e^{i\beta}|\Phi\rangle \neq |\Psi\rangle + |\Phi\rangle$.

Hermitian Transformation: Operators

$$f(x) \xrightarrow{Q} (Qf)(x)$$

is linear s.t.

$$Q(af + bg) = a(Qf) + b(Qg)$$

Examples of operators

1) Multiply by functions $F(x)$

2) Differentiation

3) $(Qf)(x) = \int dx' Q(x, x') f(x')$

Could have problems of closure.

For example, f square integrable, but xf is not in Hilbert. One way to resolve this issue is to extend to Fock space.

Sometimes we have to restrict Hilbert to functions that vanish at end points

Consider $Q = \frac{\hbar}{i}\frac{\partial}{\partial x}$ to make it Hermitian

$$\int_a^b dx g^*(x) \frac{\hbar}{i}\frac{df(x)}{dx} = \frac{\hbar}{i}\int_a^b dx \left(\frac{d}{dx}(g^* f) - \frac{dg^*}{dx} f\right) = \frac{\hbar}{i}\cancel{g^* f|_a^b} + \int_a^b dx \underbrace{-\frac{\hbar}{i}\frac{dg^*}{dx}}_{\left(\frac{\hbar}{i}\frac{dg}{dx}\right)^*} f$$

Sometimes we have to change the operator. E.g. for $x\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)$ to be Hermitian, use

$$x\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) + \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) x$$

Eigenfunctions, Eigenvalues

$$Q f_\lambda(x) = \lambda f_\lambda(x)$$

λ eigenvalue, $f_\lambda(x)$ eigenfunction. We have seen when Q =Hamiltonian, λ =energy.

1) SHO $\rightarrow$ discrete spectrum

2) free particles $\rightarrow$continuous spectrum

3) finite square well $\rightarrow$both bounded and unbounded states

Another example take $Q = \frac{\hbar}{i}\frac{\partial}{\partial x}$

$$\text{eignefunctions const} e^{ikx}, \quad \text{eigenvalues } \hbar k$$

There are two common ways to define the domain of the function space.

1) To define the wave functions on circle of circumference L, then $f(x) = f(x+L)$, so

$$\hbar k = \frac{2\pi n\hbar}{L} \text{ discrete}$$

2) To define the wave functions on real line $-\infty < x < \infty$. Then $\hbar k$ is continuously real number.

$$f = e^{ikx}$$

is not square integrable. It oscillates at $\pm\infty$. To form wave packet will be good. This also reconfirms that eigenvalue is real. If $\hbar k$ were complex, e^{ikx} blew up, so not good.

Lecture 16 (10/29/13)

Hermitian Operator

$$Q\left|f_\lambda\right\rangle = \lambda f_\lambda$$

	Discrete Spectrum	Continuous Spectrum
	λ real, λdiscrete variable	λ real, λcontinuous variable
orthogonality	$\langle f_\lambda \mid f_{\lambda'}\rangle = \delta_{\lambda\lambda'}$	$\langle f_\lambda \mid f_{\lambda'}\rangle = \delta(\lambda - \lambda')$
completeness	If $\left|\Psi\right\rangle = \sum_\lambda a_\lambda \left|f_\lambda\right\rangle$, $I = \sum_\lambda \left|f_\lambda\right\rangle \left\langle f_\lambda\right|$ $a_\lambda = \langle f_\lambda \mid \Psi\rangle$	If $\left|\Psi\right\rangle = \int d\lambda a(\lambda)\left|f_\lambda\right\rangle$, $I = \int d\lambda \left|f_\lambda\right\rangle \left\langle f_\lambda\right|$ $a(\lambda) = \langle f_\lambda \mid \Psi\rangle$
	If $\left|\Phi\right\rangle = \sum_\lambda b_\lambda \left|f_\lambda\right\rangle$, $\left\langle\Phi\right| = \sum_\lambda b_\lambda^* \left\langle f_\lambda\right|$ $\langle\Phi\mid\Psi\rangle = \sum b_\lambda^* a_\lambda$	If $\left|\Phi\right\rangle = \int d\lambda b(\lambda)\left|f_\lambda\right\rangle$, $\left\langle\Phi\right| = \int d\lambda b^*(\lambda)\left\langle f_\lambda\right|$ $\langle\Phi\mid\Psi\rangle = \int d\lambda b^*(\lambda) a(\lambda)$

Summary

$$
\begin{aligned}
\text{QM states} &\iff \text{vectors in Hilbert space}\\
\text{Physical Observables} &\iff \text{Hermitian operators (transformation)}\\
\text{Possble variables} &\iff \text{eigenvalues}\\
\text{Expectation value} &\iff \langle\Psi|Q|\Psi\rangle \ \text{ if } \ \langle\Psi|\Psi\rangle = 1\\
\text{Eigenstates of } Q &\iff \langle f_\lambda|Q|f_\lambda\rangle = \lambda \langle f_\lambda|f_\lambda\rangle = \lambda\\
& \qquad \left\langle f_\lambda \middle| Q^2 \middle| f_\lambda \right\rangle = \lambda^2\\
& \qquad \Delta Q = \left\langle Q^2 \right\rangle_{f_\lambda} - \langle Q\rangle_{f_\lambda}^2 = \lambda^2 - \lambda^2 = 0
\end{aligned}
$$

The last statement says the measurement on eigenfunction has definite value.

To utilize the properties of measurement, for given Q, we found the set of eigenfunctions $\{|f_\lambda\rangle\}$, use them as basis, then write each state in this basis

$$
|\Psi\rangle = \sum c_\lambda |f_\lambda\rangle
$$

then the probability that measurement gives λ as a result is $|c_\lambda|^2$. For different Q, use different $\{|f_\lambda\rangle\}$ to write $|\Psi\rangle$.

If it is continuous variable or mixed variables, use

$$
|\Psi\rangle = \int d\lambda c(\lambda) |f_\lambda\rangle \qquad |\Psi\rangle = \sum c_\lambda |f_\lambda\rangle + \int d\lambda c(\lambda) |f_\lambda\rangle
$$

There is one issue time average is not the same as space average, i.e. measure many identical systems, the result is the probability of getting λ, but measure one system many times will return the same value. Then the wave function has collapsed, which extra imposition out captured in Schrodinger equation

$$
i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle
$$

States with Definite Momentum

We want eigenstate of momentum operator

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

with eigenvalue p. This is

$$\psi_p = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

x is defined on the real. And such ψ_p is called eigenstate of momentum operator in the position space. We can check

$$\langle \psi_p | \psi_{p'} \rangle = \int dx \psi_p^* \psi_{P'} = \frac{1}{2\pi} \int d\left(\frac{x}{\hbar}\right) e^{-i(p'-p)x/\hbar} = \delta(p'-p)$$

States with Definite Position

We want eigenstate of position operator

$$x_{op}\psi_y(x) = y\psi_y(x) \implies \psi_y = \delta(x-y)$$

such ψ_y is called eigenstate of position operator in the position space. We check

$$\langle \psi_y | \psi_{y'} \rangle = \int dx \delta(x-y)\delta(x-y') = \delta(y-y')$$

We can also write things in term of momentum space. First recognize

$$|\psi\rangle = \underbrace{\int dx \, |x\rangle \langle x|}_{I} \, |\psi\rangle = \int dx \, \langle x|\psi\rangle \, |x\rangle$$

compare this to table on page 68, we infer that $|x\rangle$ means states with definite position x and

$$\langle x|\psi\rangle = \psi(x)$$

gives probability of finding particle at position x. So in this new language x_{op}, p_{op}

in x basis are denoted

$$\begin{aligned}\langle x|\hat{x}|\psi\rangle &= x\langle x|\psi\rangle = x\psi(x)\\ \langle x|\hat{p}|\psi\rangle &= \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle = \frac{\hbar}{i}\frac{\partial\psi(x)}{\partial x}\end{aligned}$$

Therefore in the momentum space

$$\begin{aligned}\psi(p) &= \langle p|\psi\rangle = \left\langle p\middle|\left(\int dx\,|x\rangle\langle x|\right)\middle|\psi\right\rangle\\ &= \int dx\,\langle p|x\rangle\langle x|\psi\rangle\end{aligned}$$

$$\langle p|x\rangle = \langle x|p\rangle^* = (\psi_p(x))^* = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}$$

so the conversion with momentum space and position space is

$$\psi(p) = \int\frac{dx}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}\psi(x)$$

We can now convert

$$\psi_{x_0}(x) = \delta(x-x_0) \rightarrow \psi(p) = \frac{1}{\sqrt{2\pi\hbar}}e^{-ipy/\hbar}$$

This shows convert into momentum space

$$x_{op} = x \rightarrow x_{op} = i\hbar\frac{\partial}{\partial p} \tag{3.8}$$

An alternative confirmation to above

Suppose

$$|F\rangle = x_{op}|\psi\rangle \longleftrightarrow \langle x|F\rangle = x\psi(x)$$

then

$$\begin{aligned}\langle p|F\rangle &= \int dx\,\langle p|x\rangle\langle x|F\rangle\\ &= \frac{1}{\sqrt{2\pi\hbar}}\int dxe^{-ipx/\hbar}x\psi(x)\end{aligned} \tag{3.9}$$

On the other hand suppose (3.8) is right, then

$$\langle p|F\rangle = i\hbar\frac{\partial}{\partial p}\langle p|\psi\rangle = i\hbar\frac{\partial}{\partial p}\int\frac{dx}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}\psi(x) = \frac{1}{\sqrt{2\pi\hbar}}\int dx e^{-ipx/\hbar}x\psi(x)$$

agrees (3.9).

We can also convert

$$\psi_{p_0}(x) = \frac{1}{\sqrt{2\pi\hbar}}e^{ip_0x/\hbar} \to \psi(p) = \delta(p-p_0)$$

This shows in momentum space

$$p_{op} = p$$

Example: SHO

$$H = \frac{p^2}{2m} + \frac{1}{2}mw^2x^2$$

In x basis

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}mw^2x^2$$

In p basis

$$H = \frac{p^2}{2m} - \frac{1}{2}mw^2\hbar^2\frac{\partial^2}{\partial p^2}$$

We solve the problem in terms of energy eigenstates $|0\rangle, |1\rangle, ...$

$$|\psi\rangle = \sum c_n|n\rangle$$

We can now compute the component in x or p basis

$$\psi(x) = \langle x|\psi\rangle \text{ and } \psi(p) = \langle p|\psi\rangle$$

Lecture 17 (10/31/13)

We can check all three representations give three ways to compute the same norm of $|\psi\rangle$

$$\langle\psi|\psi\rangle = \int dx\,\langle\psi|x\rangle\langle x|\psi\rangle = \int dx\,|\psi(x)|^2$$

$$\langle\psi|\psi\rangle = \int dp\,\langle\psi|p\rangle\langle p|\psi\rangle = \int dp\,|\psi(p)|^2$$

$$\langle\psi|\psi\rangle = \langle\psi|\left(\sum |E_n\rangle\langle E_n|\right)|\psi\rangle = \sum |\langle E_n|\psi\rangle|^2 = \sum |c_n|^2$$

Is still true in x or p basis,

$$[\hat{x},\hat{p}] = i\hbar?$$

In x basis

$$[x,p]\psi(x) = \frac{\hbar}{i}\left(x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right)\psi = \frac{\hbar}{i}\left(x\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial x} - \psi\right) = i\hbar\psi$$

In p basis

$$[x,p]\psi(p) = i\hbar\left(\frac{\partial}{\partial p}p - p\frac{\partial}{\partial p}\right)\psi = i\hbar\psi$$

In 3 dimensional it becomes

$$[r_j^A, p_k^B] = i\hbar\delta_{jk}\delta_{AB}$$

A, B label particles.

Uncertainty Principle

One consequence of non-commutativity of x and p is the uncertainty principle. Suppose A, B Hermitian operator, $|\psi\rangle$ normalized state. Define

$$|f\rangle = (A - \langle A\rangle)|\psi\rangle \qquad |g\rangle = (B - \langle B\rangle)|\psi\rangle$$

then

$$\begin{aligned}\langle f|f\rangle &= \{\langle\psi|(A-\langle A\rangle)\}\{(A-\langle A\rangle)|\psi\rangle\}\\ &= \langle\psi|A^2|\psi\rangle - 2\langle A\rangle\langle\psi|A|\psi\rangle + \langle A\rangle^2\langle\psi|\psi\rangle = \langle A^2\rangle - \langle A\rangle^2 = \sigma_A^2\end{aligned}$$

Similarly

$$\langle g|g\rangle = \sigma_B^2$$

By Schwartz inequality

$$\langle f|f\rangle \langle g|g\rangle \geq |\langle f|g\rangle|^2$$

= obtained if $|g\rangle \propto |f\rangle$. Since for any complex number $|z|^2 \geq (\Im z)^2$,= obtained if $\Re z = 0$. Thus

$$\begin{aligned} \langle f|f\rangle \langle g|g\rangle \geq |\langle f|g\rangle|^2 &\geq (\Im \langle f|g\rangle)^2 \\ &= \left(\frac{\langle f|g\rangle - \langle g|f\rangle}{2i}\right)^2 = \left(\frac{\langle\psi|(AB-BA)|\psi\rangle}{2i}\right)^2 \end{aligned}$$

because $\langle f|g\rangle = \langle\psi|AB|\psi\rangle - \langle A\rangle\langle B\rangle$ and $\langle g|f\rangle = \langle\psi|BA|\psi\rangle - \langle A\rangle\langle B\rangle$. Put $A = x$, $B = p$,

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \tag{3.10}$$

= obtained (i.e. minimum uncertainty) when $|g\rangle = ib\,|f\rangle$, b real. Hence in x basis

$$\left(\frac{\hbar}{i}\frac{d}{dx} - \langle p\rangle\right)\psi(x) = ib\,(x - \langle x\rangle)\,\psi(x)$$

therefore Gaussian wave function saturates uncertainty

$$\psi(x) = \text{const}e^{-\frac{b}{2\hbar}(x-\langle x\rangle)^2} e^{\frac{i}{\hbar}\langle p\rangle x}$$

E.g. photons $p = \hbar/\lambda$, (3.10) gives

$$\Delta x \geq \lambda \quad \Delta p \geq \frac{\hbar}{\lambda}$$

E.g. SHO

$$E = \frac{p^2}{2m} + \frac{1}{2}mw^2x^2$$

Heisenberg

$$x \gtrsim \Delta x \quad p \gtrsim \Delta p \text{ and } \Delta x \gtrsim \frac{\hbar}{2\Delta p}$$

we get

$$\langle E\rangle \geq \frac{(\Delta p)^2}{2m} + \frac{1}{2}mw^2\frac{\hbar^2}{(2\Delta p)^2}$$

which attains minimum at $(\Delta p)^2 = \frac{m\hbar w}{2}$, so

$$E \geq \frac{1}{2}\hbar w$$

E.g. Hydrogen Atom

$$E = \frac{\vec{p}^2}{2m} - \frac{e^2}{r}$$

Seems like as $r \to 0$, $E \downarrow$. But by uncertainty $r \to 0$, $x \to 0$ so $p \to \infty$. The energy time uncertainty

$$(\Delta E)(\Delta t) \sim \hbar \tag{3.11}$$

because

$$\begin{aligned}
\Delta E &\approx \Delta\left(\frac{p^2}{2m}\right) = \frac{p}{m}\Delta p \\
\Delta t &\approx \frac{\Delta x}{v} = \frac{m}{p}\Delta x
\end{aligned}$$

(3.11) has application e.g. in α decay.

Time dependent Observable

Lecture 18 (11/7/13)

As one last application of uncertainty principle, we look at Q with time dependence, e.g. $Q = p^2 t^2$.

$$\langle Q \rangle = \langle \psi | Q | \psi \rangle = \int dx \psi^*(x) \hat{Q} \psi(x)$$

$$\frac{d}{dt}\langle Q \rangle = \frac{d}{dt}\langle \psi | Q | \psi \rangle = \frac{\partial \langle \psi |}{\partial t} Q |\psi\rangle + \left\langle \psi \middle| \frac{\partial Q}{\partial t} \middle| \psi \right\rangle + \left\langle \psi \middle| Q \frac{\partial}{\partial t} \middle| \psi \right\rangle$$

passing the t derivative into the integral changes to partial t derivative.

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

$$i\hbar \frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle \qquad -i\hbar \frac{\partial}{\partial t}\langle \psi | = \langle \psi | H$$

Hence

$$i\hbar\frac{d}{dt}\langle Q\rangle = -\langle\psi|HQ|\psi\rangle + i\hbar\langle\psi|Q|\psi\rangle + \langle\psi|QH|\psi\rangle = \left\langle\psi\middle|[Q,H] + i\hbar\frac{\partial Q}{\partial t}\middle|\psi\right\rangle$$

Or

$$\frac{d}{dt}\langle Q\rangle = \frac{1}{i\hbar}\langle[Q,H]\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle \tag{3.12}$$

Plugging in $H = p^2/2m + V(x)$, putting $Q = x$

$$\frac{d}{dt}\langle x\rangle = \frac{1}{i\hbar}\left\langle[x,\frac{p^2}{2m}]\right\rangle = \frac{1}{i\hbar}\frac{1}{2m}\langle[x,p]p + p[x,p]\rangle = \frac{\langle p\rangle}{m}$$

Similarly

$$\frac{d}{dt}\langle p\rangle = \left\langle-\frac{\partial V}{\partial x}\right\rangle$$

By (3.12), if $[Q,H] = 0$ and $\partial Q/\partial t = 0$, then Q is a conserved quantity.

4 Three Dimensional QM

The separation of variable is the same

$$\Psi(x,y,z,t) = e^{-iEt/\hbar}\psi(x,y,z)$$

$$H = -\frac{\hbar^2}{2m}\underbrace{\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}}_{\nabla^2} + V(x,y,z)$$

∇^2 =Laplace. In spherical coordinate

$$\begin{cases} x = r\sin\theta\cos\phi \\ y = r\sin\theta\sin\phi \\ z = r\cos\theta \end{cases}$$

and $d^3x = dxdydz = r^2\sin\theta drd\theta d\phi = r^2 drd\phi d(\cos\theta)$ provided absorbing the negative sign by flipping the integration limit, i.e.

$$\int dr \int d\phi \int_0^\pi d\theta \to \int dr \int d\phi \int_{-1}^1 d(\cos\theta)$$

We need to figure out angular momentum operator. From classical mechanics

$$\begin{aligned}
\vec{L} &= \vec{r} \times \vec{p} \\
L^2 &= \vec{r}^2\vec{p}^2 \sin^2\angle(\vec{r},\vec{p}) = \vec{r}^2\vec{p}^2 - (\vec{r}\cdot\vec{p})^2
\end{aligned}$$

So we get

$$p^2 = \frac{(\vec{r}\cdot\vec{p})^2}{r^2} + \frac{\vec{L}^2}{r^2} = (\hat{r}\cdot\vec{p})^2 + \frac{\vec{L}^2}{r^2}$$

In spherical coordinate

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\underbrace{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]}_{:=-L_{op}^2/\hbar^2}$$

We guess $\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}$ resembles $p_r^2 = (\hat{r}\cdot\vec{p})^2$, so what is p_r? Guess

$$p_r = \frac{\hbar}{i}\left(\frac{\partial}{\partial r} + f(r)\right)$$

want to satisfy 1) p_r Hermitian; 2) $[p_r, r] = -i\hbar$

$$\begin{aligned}
\int d^3x\psi^*\hat{p}_r\varphi &= \int drr^2 d\theta\sin\theta d\phi\psi^*\frac{\hbar}{i}\left(\frac{\partial\psi}{\partial r} + f\varphi\right) \\
&= \int drd\theta\sin\theta d\phi\left(-\frac{\hbar}{i}\frac{\partial}{\partial r}(r^2\psi^*)\varphi + \frac{\hbar}{i}fr^2\psi^*\varphi\right) \text{ (integration by parts)} \\
&= \int drr^2 d\theta\sin\theta d\phi\left[\frac{\hbar}{i}\left(-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\psi^*\right)\varphi + \frac{\hbar}{i}f\psi^*\varphi\right] \\
&= \int drr^2 d\theta\sin\theta d\phi\left[-\frac{\hbar}{i}\frac{\partial\psi^*}{\partial r} - \frac{\hbar}{i}\left(\frac{2}{r}\right)\psi^* + \frac{\hbar}{i}f\psi^*\right]\varphi
\end{aligned}$$

We want RHS $= \int d^3x(\hat{p}_r\psi)^*\varphi$, so

$$-\frac{\hbar}{i}\frac{\partial}{\partial r} - \frac{\hbar}{i}\left(\frac{2}{r}\right) + \frac{\hbar}{i}f = -\frac{\hbar}{i}\frac{\partial}{\partial r} - \frac{\hbar}{i}f \implies f = \frac{1}{r}$$

Does $p_r^2 \sim \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}$?

$$\begin{aligned} p_r^2 F(r) &= \left(\frac{\hbar}{i}\right)^2 \left(\frac{\partial}{\partial r} + f(r)\right)\left(\frac{\partial}{\partial r} + f(r)\right) F(r) \\ &= -\hbar^2 \left(\frac{\partial^2 F}{\partial r^2} + \frac{1}{r}\frac{\partial F}{\partial r} + \frac{\partial}{\partial r}\frac{1}{r}F + \frac{F}{r^2}\right) = -\hbar^2\left(\frac{\partial^2 F}{\partial r^2} + \frac{2}{r}\frac{\partial F}{\partial r}\right) \end{aligned}$$

Check

$$[p_r, r]F = \frac{\hbar}{i}\left(\frac{d}{dr}rF + F - r\frac{d}{dr}F - F\right) = \frac{\hbar}{i}F$$

4.1 Angular Momentum Operator (Ladder Way)

Classical mechanics says

$$L_x = yp_z - zp_y = p_z y - p_y z$$

We find

$$[L_x, x] = 0, \quad [L_x, y] = i\hbar z$$

or

$$[L_j, r_k] = i\hbar\epsilon_{jkl}r_l$$

where Einstein summing is assumed and

$$\epsilon_{ijk} = \begin{cases} 1 & 123, 231, 312 \\ -1 & 132, 321, 213 \\ 0 & \text{otherwise} \end{cases}$$

useful identity

$$\epsilon_{ijk}\epsilon_{ilm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}$$

Similar find

$$\begin{aligned}
[L_j, p_k] &= i\hbar\epsilon_{jkl}p_l \\
[L_j, L_k] &= i\hbar\epsilon_{jkl}L_l
\end{aligned}$$

and

$$[L_j, r^2] = \sum_k [L_j, r_k r_k] = \sum \left([L_j, r_k]r_k + r_k[L_j, r_k]\right) = \sum_{kl} 2i\hbar\epsilon_{jkl}r_l r_k = 0$$

sum of antisymmetric tensor is 0. Moreover

$$[L_j, f(r^2)] = 0$$

In particular

$$[L_j, |\vec{r}|] = 0$$

Similar

$$[L_j, p^2] = 0$$

So if $V(\vec{r}) = V(|\vec{r}|)$ spherical symmetric potential, then $[L_j, H] = 0$, so $\vec{L}$ is conserved.

Lecture 19 (11/12/13)

Similarly if $V(\vec{r}) = V(|\vec{r}|)$

$$[L^2, H] = 0$$

therefore one can find simultaneous eigenstate of H, L^2, L_z. Why z? because later expressions will be simpler in light of spherical coordinate.

Define

$$L_\pm = L_x \pm iL_y$$

then

$$\begin{aligned}
[L_z, L_+] &= [L_z, L_x + iL_y] = i\hbar L_y - i(i\hbar L_x) = \hbar L_+ \\
[L_z, L_-] &= -\hbar L_-
\end{aligned}$$

Suppose

$$L^2 |\psi\rangle = \lambda |\psi\rangle \text{ and } L_z |\psi\rangle = \mu |\psi\rangle$$

call $|\psi\rangle = |\lambda, \mu\rangle$

$$\begin{aligned} L^2(L_\pm |\lambda, \mu\rangle) &= L_\pm L^2 |\lambda, \mu\rangle = \lambda L_\pm |\lambda, \mu\rangle \\ L_z(L_\pm |\lambda, \mu\rangle) &= (L_\pm L_z \pm \hbar L_\pm) |\lambda, \mu\rangle = (\mu \pm \hbar) L_\pm |\lambda, \mu\rangle \end{aligned}$$

Hence

$$L_\pm |\lambda, \mu\rangle \text{ is an eigenstate of } L^2,\ L_z \text{with eigenvalue } \lambda,\ \mu \pm \hbar$$

One can apply $L_\pm$ consecutively to permute L_z's eigenstates from one to the next.

Since $L^2 = L_x^2 + L_y^2 + L_z^2$,

$$\langle L^2 \rangle \geq \langle L_z^2 \rangle \implies \lambda \geq \mu^2$$

and the ladder operation much terminate at some point.

$$L_+L_- = (L_x + iL_y)(L_x - iL_y) = L_x^2 + L_y^2 - i[L_x, L_y] = L^2 - L_z^2 + \hbar L_z$$

and

$$L_-L_+ = L^2 - L_z^2 - \hbar L_z$$

So

$$L^2 = L_+L_- + L_z^2 - \hbar L_z = L_-L_+ + L_z^2 + \hbar L_z$$

Suppose that $\hbar l$ =maximal value of μ for a given λ and $\hbar \bar{l}$ is then minimal value,

$$L_+ |\lambda, l\rangle = 0$$

$$\begin{aligned} \lambda |\lambda, l\rangle &= L^2 |\lambda, l\rangle = (L_-L_+ + L_z^2 + \hbar L_z) |\lambda, l\rangle \\ &= (0 + \hbar^2 l^2 + \hbar^2 l) |\lambda, l\rangle = \hbar^2 l(l+1) |\lambda, l\rangle \end{aligned}$$

$$L_- \left|\lambda, \bar{l}\right\rangle = 0$$

$$\begin{aligned}\lambda\left|\lambda,\bar{l}\right\rangle &= L^2\left|\lambda,\bar{l}\right\rangle = (L_+L_- + L_z^2 - \hbar L_z)\left|\lambda,\bar{l}\right\rangle \\ &= (0+\hbar^2 l^2 - \hbar^2 l)\left|\lambda,\bar{l}\right\rangle = \hbar^2 l(l-1)\left|\lambda,\bar{l}\right\rangle\end{aligned}$$

Hence

$$l(l+1) = \lambda = \bar{l}(\bar{l}-1) \implies \bar{l} = -l \text{ or } \bar{l} = l+1(\text{drop})$$

Thus starting from highest $\langle L_z\rangle = \hbar l$, with $\langle L^2\rangle = \hbar^2 l(l+1)$ apply lowering operator $2l$ times, so $2l$ =integer,

$$\hbar l \to \hbar(l-1) \to \hbar(l-2) \to ... \to \hbar(-l)$$

with total $2l+1$ states with same $\langle L^2\rangle$,

$$l = \text{integer or integer} + \frac{1}{2} \tag{4.1}$$

and

$$\left\langle L^2\right\rangle = \hbar^2 l(l+1) \geq \left\langle L_z^2\right\rangle$$

$=$ obtained if $l=0$.

Later we will show for Hydrogen, orbit

$$\begin{aligned} s \to l &= 0 \\ p \to l &= 1 \\ d \to l &= 2 \\ &... \end{aligned}$$

s orbit has $l=0$ which shows Bohr was not totally correct. He predicted $L = n\hbar$, so no $l=0$.

In (4.1), l =integer $+1/2$ is not possible. First show

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi} \tag{4.2}$$

because

$$\begin{aligned}
\frac{\hbar}{i}\frac{\partial}{\partial \phi}\psi &= \frac{\hbar}{i}\left(\frac{\partial \psi}{\partial x}\frac{\partial x}{\partial \phi}+\frac{\partial \psi}{\partial y}\frac{\partial y}{\partial \phi}+\frac{\partial \psi}{\partial z}\frac{\partial z}{\partial \phi}\right)=\frac{\hbar}{i}\left(\frac{\partial \psi}{\partial x}(-y)+\frac{\partial \psi}{\partial y}(x)+0\right)\\
&= \frac{\hbar}{i}\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\psi = L_z\psi
\end{aligned}$$

If $L_z\left|\psi\right\rangle=\hbar m\left|\psi\right\rangle$

$$\psi(r,\theta,\phi)=e^{im\phi}F(r,\theta)$$

Since $\psi(r,\theta,\phi+2\pi)=\psi(r,\theta,\phi)$

$$e^{2\pi i m}=1 \implies m=\text{integer}$$

so is l in (4.1), maximum value of m.

Lecture 20 (11/19/13)

We will write down similar expressions to (4.2) without proof

$$\begin{aligned}
L_x &= \frac{\hbar}{i}\left(-\sin\phi\frac{\partial}{\partial\theta}-\cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)\\
L_y &= \frac{\hbar}{i}\left(\cos\phi\frac{\partial}{\partial\theta}-\sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)
\end{aligned}$$

Then

$$\begin{aligned}
L_\pm &= \hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta}\pm i\cot\theta\frac{\partial}{\partial\phi}\right)\\
L^2 &= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]
\end{aligned}$$

4.2 Spherical Harmonics

We have

$$L_\pm\left|l,m\right\rangle \propto \left|l,m\pm 1\right\rangle$$

From there we want to find

$$\psi_{lm}(\theta,\phi)=\langle\theta,\phi|l,m\rangle \qquad \psi_{lm}=e^{im\phi}f(\theta)$$

Since $L_+ |l,l\rangle = 0$,

$$\begin{aligned} 0 = L_+\psi_{ll}(\theta,\phi) &= L_+ \langle\theta,\phi|l,l\rangle \\ &= \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\psi_{ll}(\theta,\phi) = \hbar e^{i(l+1)\phi}\left(\frac{\partial}{\partial\theta} + l\cot\theta\right)f(\theta) \end{aligned}$$

So

$$f = \text{const}(\sin\theta)^l$$

Standard choice

$$\psi_{lm}(\theta,\phi) = Y_{lm}(\theta,\phi)$$

spherical harmonics

$$Y_{lm}(\theta,\phi) = \epsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta)$$

$$\epsilon = \begin{cases}(-1)^m & m \geq 0\\ 1 & m < 0\end{cases}$$

P_l^m associated Legendre polynomial, $m = 0$ Legendre polynomial. Orthogonality

$$\langle lm|l'm'\rangle = \delta_{ll'}\delta_{mm'} = \int_0^{2\pi} d\phi\int_0^{\pi} d\theta\sin\theta Y_{lm}^*(\theta,\phi)Y_{l'm'}(\theta,\phi)$$

Although the total wave functions of different energy are orthogonal due to the Hermiticity of the Hamilton, it doesn't imply the radial wave function will be orthogonality by itself, as one can check explicit for the case of hydrogen, only this is true for hydrogen $\psi_{nlm} = R_{nl}Y_{lm}$

$$\int_0^\infty R_{nl}^* R_{n'l} r^2 dr = \delta_{nn'}$$

and

$$\int r^2 dr\int\sin\theta d\theta\int d\phi\psi_{nlm}^*\psi_{n'l'm'} = \delta_{nn'}\delta_{ll'}\delta_{mm'}$$

Legendre polynomial

$$
\begin{aligned}
P_0(\cos\theta) &= 1 \\
P_1(\cos\theta) &= \cos\theta \\
P_2(\cos\theta) &= \frac{1}{2}(3\cos^2\theta - 1)
\end{aligned}
$$

Spherical Harmonics

$$
\begin{aligned}
l=0 \quad Y_{00} &= \frac{1}{\sqrt{4\pi}} \\
l=1 \quad Y_{11} &= -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi} \sim \frac{x+iy}{r} \\
Y_{10} &= \sqrt{\frac{3}{4\pi}}\cos\theta \sim \frac{z}{r} \\
Y_{1-1} &= \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi} \sim \frac{x-iy}{r} \\
l=2 \quad Y_{22} &= \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{2i\phi} \sim \frac{(x+iy)^2}{r^2} \\
Y_{21} &= \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi} \sim \frac{(x+iy)z}{r^2} \\
Y_{20} &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) \sim \frac{3z^2 - r^2}{r^2} \\
Y_{2-1} &= -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{-i\phi} \sim \frac{(x-iy)z}{r^2} \\
Y_{2-2} &= -\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{-2i\phi} \sim \frac{(x-iy)^2}{r^2}
\end{aligned}
$$

4.3 Full Wave Function

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r)$$

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{1}{\hbar^2}\frac{L^2}{r^2}$$

For fixed l, m

$$\psi(r,\theta,\phi) = R(r)Y_{lm}(\theta,\psi)$$

Solving time independent Schrodinger equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{L^2}{2mr^2}+V(r)\right]RY_{lm}=ERY_{lm}$$

Treating $\frac{L^2}{2mr^2}+V(r)$ as effective potential.

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+\frac{\hbar^2 l(l+1)}{2mr^2}+V(r)\right]R\cancel{Y_{lm}}=ER\cancel{Y_{lm}} \tag{4.3}$$

The equation above is independent of m, which is saying that the choice of z axis should be arbitrary.

Use $u(r)=rR(r)$ then the normalization for $R(r)$ becomes

$$1=\int_0^\infty r^2|R(r)|^2dr=\int_0^\infty dr|u|^2$$

The normalization of $R(r)$ requires $u(0)=0$ and $u(\infty)=0$.

To solve for $u(r)$, (4.3) gives

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2}+\left(\frac{\hbar^2 l(l+1)}{2mr^2}+V(r)\right)u(r)=Eu(r) \tag{4.4}$$

and we need to know $V(r)$.

Lecture 21 (11/21/13)

If we're only interested in $u(r)$, r near the origin. We can neglect $V(r)u(r)$, because $u\to 0$.

Suppose near the origin $u(r)\sim r^n$, solve (4.4)

$$n(n-1)r^{n-2}=l(l+1)r^{n-2} \implies n=-l \text{ or } n=l+1$$

Since l, maximum value of m, ≥ 0, $n=-l$ gives r^{-l} divergent. Not good, therefore near origin

$$\psi\sim r^l Y_{lm}$$

4.4 Two Examples

Infinite well potential

$$V(r) = \begin{cases} 0 & r \leq a \\ \infty & r > a \end{cases}$$

Put $E = \frac{\hbar^2 k^2}{2m}$, then (4.4) for $0 < r < a$

$$-u'' + \frac{l(l+1)}{r^2} u = k^2 u$$

and $u(0) = 0$,$u(a) = 0$.

$l = 0$

$$u'' + k^2 u = 0 \implies u = A \sin kr + B \cos kr$$

$$\begin{aligned} u(0) &= 0 \implies B = 0 \\ u(a) &= 0 \implies k = \frac{n\pi}{a} \end{aligned}$$

$$E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

$$\psi_{nlm} = \psi_{n00} = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} r \sqrt{\frac{1}{4\pi}} \frac{1}{r}$$

$l > 0$

$$u'' + \left[k^2 - \frac{l(l+1)}{r^2}\right] u = 0$$

$$u = Arj_l(kr) + Brn_l(kr)$$

j_l spherical Bessel function. n_l spherical Neumann function.

$$\begin{aligned} j_l(s) &= (-s)^l \left(\frac{1}{s}\frac{d}{ds}\right)^l \frac{\sin s}{s} \\ n_l(s) &= -(-s)^l \left(\frac{1}{s}\frac{d}{ds}\right)^l \frac{\cos s}{s} \end{aligned}$$

j_l is good at origin

$$
\begin{aligned}
j_0 &= \frac{\sin s}{s} \to 1 \\
j_1 &= \frac{\sin s}{s^2} - \frac{\cos s}{s} \to 0 \\
j_2 &= (-s)^2 \left(\frac{1}{s}\frac{d}{ds}\right)\left(\frac{1}{s}\frac{d}{ds}\right)\frac{\sin s}{s} = \frac{1}{s^3}(3\sin s - 3s\cos s - s^2 \sin s) \to \text{const}
\end{aligned}
$$

while n_l is bad at origin

$$
\begin{aligned}
n_0 &= -\frac{\cos s}{s} \\
n_1 &= -\frac{\cos s}{s^2} - \frac{\sin s}{s}
\end{aligned}
$$

One can show $s \to 0$

$$
\begin{aligned}
j_l(s) &\to \text{const} s^l \\
n_l(s) &\to \text{const}\frac{1}{s^{l+1}}
\end{aligned}
$$

For our case

$$
\begin{aligned}
u(0) &= 0 \implies B = 0 \\
u(a) &= 0 \implies j_l(ka) = 0 \implies k_n a = \beta_{nl}
\end{aligned}
$$

$\beta_{nl} = n$th zero of the lth spherical Bessel function. $l > 0$

$$
\begin{aligned}
E_{nl} &= \frac{\hbar^2}{2ma^2}\beta_{nl}^2 \\
\psi_{nlm} &= A j_l\left(\frac{\beta_{nl}}{a}r\right) Y_{lm}(\theta, \phi)
\end{aligned}
$$

Numerical calculation shows the energy levels

$l=0$	$l=1$	$l=2$	$l=3$
	118.9 (3)		
			108.5 (7)
88.9 (1)			
		82.6 (5)	
	59.2 (3)		
			48.8 (7)
39.5 (1)			
		33.2 (5)	
	20.2 (3)		
9.9 (1)			

number in the parentheses indicates the number of degenerated states.

Second Example: Simple Harmonic Oscillation

$$V = \frac{mw^2}{2}(x^2 + y^2 + z^2) = \frac{mw^2}{2} r^2$$

It can be solved in Cartesian and spherical coordinate.

Lecture 22 (11/26/13)

$$H = \left(\frac{p_x^2}{2m} + \frac{mw^2x^2}{2}\right) + \left(\frac{p_y^2}{2m} + \frac{mw^2y^2}{2}\right) + \left(\frac{p_z^2}{2m} + \frac{mw^2z^2}{2}\right)$$

So

$$\psi(x,y,z) = A(x)B(y)C(z)$$

$$E = \left(n_x + \frac{1}{2}\right)\hbar w + \left(n_y + \frac{1}{2}\right)\hbar w + \left(n_z + \frac{1}{2}\right)\hbar w$$

Ground state

$$n_x = n_y = n_z = 0 \qquad E = \frac{3}{2}\hbar w$$

1st excited state

$$(1,0,0)\ (0,1,0)\ (0,0,1) \qquad E = \frac{5}{2}\hbar w$$

2nd excited state

$$\begin{matrix} (2,0,0)\ (0,2,0)\ (0,0,2) \\ (1,1,0)\ (0,1,1)\ (1,0,1) \end{matrix} \qquad E = \frac{7}{2}\hbar w$$

$$\psi^C \propto H_{n_x}\left(\sqrt{\frac{mw}{\hbar}}x\right) H_{n_y}\left(\sqrt{\frac{mw}{\hbar}}y\right) H_{n_z}\left(\sqrt{\frac{mw}{\hbar}}z\right) e^{-\frac{mw}{2\hbar}(x^2+y^2+z^2)} \tag{4.5}$$

What about spherical way?

$$\psi^S_{nlm}(r,\theta,\psi) = R_{nl}(r)Y_{lm}(\theta,\psi) \tag{4.6}$$

R_{nl} (n is the energy label) solves

$$-\frac{\hbar^2}{2m}\left(\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr}\right) + \left(\frac{1}{2}mw^2r^2 + \frac{\hbar^2 l(l+1)}{2mr^2}\right)R = ER$$

(4.6) is solution, eigenstate of the spherical Hamiltonian, while (4.5) is solution, eigenstate of the Cartesian Hamiltonian.

Since we already know the expression of the solutions (4.5), we can work backwards to find R_{nl}.

The ground state in $|n_x, n_y, n_z\rangle$ is

$$\sim e^{-(\dots)r^2}$$

no angle dependence so $l = m = 0$,

$$\psi^S_{000} \sim e^{-(\dots)r^2} Y_{00} = R_{00} Y_{00}$$

from there one can find R_{00} easily.

1st excited states,

$$\psi^C_{100} \sim x e^{-(\dots)r^2} = \left[r e^{-(\dots)r^2}\right] \frac{x}{r} \sim R_{11} \frac{-Y_{11} + Y_{1-1}}{\sqrt{2}}$$

from there one can find R_{11}

$$R_{11} \sim r e^{-(\dots)r^2}$$

with proper normalization. Alternatively we can use

$$\psi^C_{010} \sim y e^{-(\dots)r^2} = \left[r e^{-(\dots)r^2}\right] \frac{y}{r} \sim R_{11} \frac{iY_{11} + iY_{1-1}}{\sqrt{2}}$$

or

$$\psi^C_{001} \sim z e^{-(\dots)r^2} = \left[r e^{-(\dots)r^2}\right] \frac{z}{r} \sim R_{11} Y_{10}$$

to find R_{11}. Hence we found three solutions $R_{11}Y_{11}$, $R_{11}Y_{1-1}$, and $R_{11}Y_{10}$.

2nd excited states

$$\psi^C_{110} \sim xy e^{-(\dots)r^2} \sim R_{22} \frac{Y_{22} - Y_{2-2}}{\sqrt{2}}$$

$$\psi^C_{101} \sim xz e^{-(\dots)r^2} \sim R_{22} \frac{-Y_{21} + Y_{2-1}}{\sqrt{2}}$$

$$\psi^C_{011} \sim yz e^{-(\dots)r^2} \sim R_{22} \frac{iY_{21} + iY_{2-1}}{\sqrt{2}}$$

any of them will give R_{22}, hence we found five solutions, $R_{22}Y_{2m}$, $m = -2, -1, 0, 1, 2$. The last solution is by considering the sum of

$$\begin{aligned} \psi^C_{200} + \psi^C_{020} + \psi^C_{002} &\sim \left(2\frac{mw}{\hbar}x^2 - 1\right) e^{-(\dots)r^2} + \left(2\frac{mw}{\hbar}y^2 - 1\right) e^{-(\dots)r^2} + \left(2\frac{mw}{\hbar}z^2 - 1\right) e^{-(\dots)r^2} \\ &= \left(2\frac{mw}{\hbar}r^2 - 3\right) e^{-(\dots)r^2} \sim R_{20} Y_{00} \end{aligned}$$

because has no angular dependence.

3rd excited states, 10 states: 7 in $l = 3$ and 3 in $l = 1$.

$E = \frac{11}{2}\hbar w$	$\overline{(1)}$		$\overline{(5)}$		$\overline{(9)}$
$E = \frac{9}{2}\hbar w$		$\overline{(3)}$		$\overline{(7)}$	
$E = \frac{7}{2}\hbar w$	$\overline{(1)}$		$\overline{(5)}$		
$E = \frac{5}{2}\hbar w$		$\overline{(3)}$			
$E = \frac{3}{2}\hbar w$	$\overline{(1)}$				
	$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$

thus $n_x + n_y + n_z = \text{even} \implies l = $even. $n_x + n_y + n_z = \text{odd} \implies l = $odd. Why?

Suppose $(x, y, z) \to (-x, -y, -z)$. Because $n_x + n_y + n_z = \text{even} \implies$ must be $+--$ or $+++$so the product of the three Hermite polynomial is even, so ψ^C is even. And when $l = $even, Y_{lm} is even.

What's special about Harmonic potential? It is one of the only two potentials that have closed orbits. There is another conserved quantity Runge-Lenz vector. Its magnitude is about eccentricity of the ellipse orbit.

$$\frac{\vec{L} \times \vec{p} + \vec{p} \times \vec{L}}{2} - k\hat{r}$$

The other closed orbit potential is

$$V \sim \frac{1}{r}$$

4.5 Hydrogen

One could use Runge-Lenz vector, combining commutative relation with H, L. One can define ladder operators and solve Hydrogen energy spectrum in that way. But we will follow ODE way.

We use Gaussian unit, popular unit in atomic physics

$$4\pi\epsilon_0 \leftrightarrow 1$$

$$V_{eff} = -\frac{e^2}{r} + \frac{\hbar^2 l(l+1)}{r^2}$$

Graph of V_{eff} when $l \neq 0$, at the origin $V_{eff} \to \infty$. For all l, $V_{eff} \to 0^-$, as $r \to \infty$, so

$$\begin{aligned} E &> 0 \text{ Scattering states} \implies \text{continuum eigenstates (uninteresting)} \\ E &< 0 \text{ Bound states} \end{aligned}$$

$$\psi = \frac{u(r)}{r} Y_{lm}(\theta, \phi)$$

$$-\frac{\hbar^2}{2m} u'' + V_{eff} u = Eu$$

$u(0) = u(\infty) = 0$.

Solve $E < 0$, define ρ dimensionless

$$\kappa = \sqrt{\frac{-2mE}{\hbar^2}} \; \rho = \kappa r \; \rho_0 = \frac{2me^2}{\hbar^2 \kappa} \tag{4.7}$$

then

$$u'' - \frac{l(l+1)}{r^2} u + \frac{2me^2}{\hbar^2} \frac{1}{r} u = -\frac{2m}{\hbar^2} Eu$$

Substitute in ρ

$$\kappa^2 \frac{d^2 u}{d\rho^2} - \kappa^2 \frac{l(l+1)}{\rho^2} u + \frac{2me^2}{h^2} \kappa \frac{u}{\rho} = \kappa^2 u$$

or

$$\frac{d^2 u}{d\rho^2} - \frac{l(l+1)}{\rho^2} u + \frac{\rho_0}{\rho} u = u \tag{4.8}$$

For very large ρ, $V_{eff} \approx 0$

$$\frac{d^2 u}{d\rho^2} = u$$

$$u \approx Ae^{-\rho} + Be^{\rho}$$

$B = 0$, because $u(\infty) = 0$

Lecture 23 (12/3/13)

For very small ρ, and $l \neq 0$,

$$\frac{d^2 u}{d\rho^2} - \frac{l(l+1)}{\rho^2} u = 0$$

$$u \approx C\rho^{l+1} + D\rho^{-l}$$

$D = 0$, because $u(0) = 0$.

So we guess

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho) \tag{4.9}$$

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j$$

We didn't absorb ρ^{l+1} in $v(\rho)$ so that the algebra is cleaner. We notice that (4.9) is very good at the origin. $\rho \ll 1$, (4.9)$\to \rho^{l+1}$. But it turns out to be bad at ∞. We need to control the power series.

Plug (4.9) in (4.8), simplify

$$\rho \frac{d^2 v}{d\rho^2} + 2(l + 1 - \rho)\frac{dv}{d\rho} + [\rho_0 - 2(l + 1)]v = 0$$

With the help of reindex, we can equate coefficients

$$\begin{aligned} v' &= \sum_{j=0}^{\infty} j c_j \rho^{j-1} = \sum_{j=0}^{\infty} (j + 1)c_{j+1}\rho^j \\ \rho v'' &= \sum_{j=0}^{\infty} j(j + 1)c_{j+1}\rho^j \end{aligned}$$

we get

$$\sum j(j+1)c_{j+1}\rho^j + \sum 2(l+1)(j+1)c_{j+1}\rho^j - \sum 2jc_j\rho^j + \sum [\rho_0 - 2(l+1)]c_j\rho^j = 0$$

so

$$[j(j + 1) + 2(l + 1)(j + 1)]c_{j+1} + [-2j + \rho_0 - 2(l + 1)]c_j = 0$$

or

$$c_{j+1} = \frac{2(j + l + 1) - \rho_0}{(j + 1)(j + 2l + 2)} c_j$$

Large j

$$c_{j+1} \approx \frac{2}{j} c_j$$

or

$$c_j \approx \frac{2^j}{j!}$$

so

$$v \sim e^{2\rho}$$

or

$$u \sim \rho^{l+1} e^{\rho}$$

bad, so the series must terminate

$$\rho_0 = 2(j + l + 1) = 2n$$

for some integer $n = 1, 2, 3, ...$

Then by (4.7)

$$E_n = -\frac{\hbar^2 \kappa^2}{2m} = -\frac{\hbar^2}{2m} \frac{m^2 e^4}{\hbar^4 n^2} = -\frac{me^4}{2\hbar^2 n^2} \qquad n \geq l + 1$$

Ground state energy

$$\begin{aligned} E_1 &= -\frac{me^4}{2\hbar^2} = -13.6\text{eV} \\ 1\text{eV} &= 1.6 \times 10^{-19}\text{J} \end{aligned}$$

$n = 4$	$\frac{E_1}{16}$	$\underline{4s}$		$\underline{4p}$	$\underline{4d}$	$\underline{4f}$
$n = 3$	$\frac{E_1}{9}$	$\underline{3s}$		$\underline{3p}$	$\underline{3d}$	
$n = 2$	$\frac{E_1}{4}$	$\underline{2s}$ $\downarrow$	$\swarrow$	$\underline{2p}$		
$n = 1$	E_1	$\underline{1s}$	$\swarrow$			

	$l = 0$	$l = 1$	$l = 2$	$l = 3$	$l = 4$	$l = 5$
Spectrum names	*s*harp	*p*inciple	*d*iffuse	*f*ine	g	h

One can also study the transitions, e.g.

$$2p \to 1s + \text{photon}$$

photon carries energy $E = \hbar w = \frac{hc}{\lambda}$

$$E = E_{2p} - E_{1s} = \frac{me^4}{2\hbar^2}\left(\frac{1}{2^2} - \frac{1}{2}\right)$$

$$n \to 1 \quad \text{Lyman series}$$

$$n \to 2 \quad \text{Balmer series}$$

Define

$$\text{Bohr radius} = a = \frac{\hbar^2}{me^2} = .529 \times 10^{-10} m$$

then

$$\kappa = \frac{me^2}{\hbar^2 n} = \frac{1}{an} \quad \rho = \frac{r}{an}$$

Hence

$$R_{nl}(r) = \frac{1}{r}u(r) = \frac{1}{r}\left(\frac{r}{an}\right)^{l+1} e^{-\frac{r}{an}} v_{nl}\left(\frac{r}{an}\right)$$

Let us figure out what radial component of Hydrogen looks like. From

$$c_{j+1} = \frac{2(j+l+1) - 2n}{(j+1)(j+2l+2)} c_j$$

$n = 1,\ l = 0$

$$c_1 = 0 \implies c_2 = c_3 = ... = 0$$

$$v_{10} = c_0$$

so

$$R_{10}(r) = \text{const}\frac{1}{a}e^{-r/a}$$

$n = 2,\ l = 0$

$$c_1 = -c_0,\ c_2 = 0$$

$$
\begin{aligned}
l=0 \qquad & R_{10} = (\text{const}) e^{-r/a} \text{ no node} \\
& R_{20} = (\text{const}) \left(1 - \frac{r}{2a}\right) e^{-r/2a} \text{ one node} \\
& R_{30} = (\text{const}) \left[1 - \frac{2r}{3a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right] e^{-r/3a} \text{ two nodes} \\
l=1 \qquad & R_{21} = (\text{const}) \frac{r}{a} e^{-r/2a} \text{ no node exclude origin} \\
& R_{31} = (\text{const}) \frac{r}{a} \left(1 - \frac{r}{6a}\right) e^{-r/a} \text{ one node exclude origin}
\end{aligned}
$$

The pattern is

$$R_{nl} \text{ has } n-l-1 \text{ nodes away from the origin}$$

Normalized hydrogen wave function

$$
\begin{aligned}
\psi_{nlm} &= R_{nl}(r) Y_{lm}(\theta, \phi) \\
&= \left(\frac{2}{na}\right)^{3/2} \sqrt{\frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-r/na} \left(\frac{2r}{na}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na}\right) Y_{lm}(\theta, \phi) \qquad (4.10)
\end{aligned}
$$

L_{n-l-1}^{2l+1}, associated Laguerre polynomials, they are not orthogonal alone. They are orthogonal in the sense that (see Abramowitz and Stegun, Handbook of Mathematical Functions. Chapter 22)

$$\int dx e^{-x} x^{\alpha} L_m^{\alpha} L_n^{\alpha} \propto \delta_{mn}$$

Lecture 24 -Last Lec- (12/5/13)

Graph of $|\psi|^2$ of (4.10) shows that larger n, it extends out further because $e^{-r/na}$ decreases slower and higher energy; same n, larger l, it concentrated further out because to achieve higher angular momentum while maintaining same energy is to distribute mass further out.

Graph of $|\psi|^2$ of (4.10) is independent of ϕ because $Y \sim e^{im\phi}$, so it is possible to draw 2D density plots with the understanding that the full plots are obtained by rotating about z axis. E.g. we draw contour plot for $|\psi_{210}|^2 =$ some constant. Set $a = 1$

$$r^2 e^{-r} \cos^2 \theta = 0.01$$

Solve numerically for various θ

θ(degrees)	r
0	8.99
15	8.91
30	8.63
45	8.09
60	7.15
70	6.06
75	5.20
80	3.74
82	2.47
85	-0.77
89	-2.05

$-$ value means no valid solution for r for the chosen level curve. Use these valid values and $\cos^2\theta = \cos^2(\pi - \theta)$, we should get a graph that looks like a figure 8 aligned with the z axis.

One can study the maximum point of the probability density function $\psi_{nlm}(r,\theta,\phi)$. E.g. for ψ_{100} maximum is attained at $\vec{r} = 0$.

One may also be interested in the radial distribution function

$$\psi(r) = \int d\Omega \psi_{nlm}(r,\theta,\phi) = R_{nl}(r)$$

For ψ_{100} it is very simple

$$|R_{nl}(r)|^2 r^2 = (\text{const}) r^2 e^{-2r/a}$$

it has maximum at $r = a$, i.e. the most probable radial distance to find e^- of hydrogen. While the expectation value of r is not a

$$\langle r \rangle = \int r |\psi_{100}|^2 d^3x = 4a \int e^{-2r/a} \left(\frac{r}{a}\right)^3 d\left(\frac{r}{a}\right) = \frac{3}{2}a$$

4.6 Spin

Spin accounts any momentum other than orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$. Spin is an intrinsic angular momentum, may have nothing to do with the idea of spin in classical mechanics, or even stupid to think it is same as in classical mechanics, as Pauli suggested. But why is it still called "spin"? Because the notion of spin in QM compatible with conservation of angular momentum, because spin of particles dictates particle behavior in magnetic field; and because spin gives arise to fine structure of atomic spectra. All of three effects can be interpreted as classical spinning objects as analogous in classical mechanics. The idea of spin, like a classical planet with orbital motion and spin motion, was first put forward by Kronig (1924), but he was discouraged by Pauli so that he didn't publish the paper. 1925 Goudsmtt and Uhlenbeck published paper on spin.

Why did Pauli say the idea of spin was stupid? (Griffiths problem 4.25) Suppose e^- spin around its axis. Let R be the radius of e^-, then the Coulomb potential of e^- is

$$\frac{e^2}{R} \sim mc^2$$

assuming the intrinsic potential energy is at the same order with rest energy. This gives $R \sim 10^{-15}m$ much bigger than what should be, but a smaller R would just make the situation worse. Suppose angular momentum associated with the spinning is

$$mRv$$

and it is at the order of $\hbar$, then

$$mRv \sim \frac{e^2 v}{c^2} \sim \hbar \implies \frac{v}{c} \sim \frac{\hbar c}{e^2} = 137$$

Hence a point on the equator of the e^- surface moves at speed 100 times than c.

So the best way to reconcile the contradiction is to think of spin as a new degree of freedom, which has rotational symmetry. It is intrinsic so that it commutes with

$$[S_j, r_k] = [S_j, p_k] = [S_j, L_k] = 0 \tag{4.11}$$

and its rotational symmetry gives

$$\left.\begin{array}{c}[S_j, S_k] = i\hbar\epsilon_{jkl}S_l \\ [S^2, S_k] = 0\end{array}\right\} \implies \begin{array}{c}\vec{S}^2 = S_x^2 + S_y^2 + S_z^2 \to \hbar^2 s(s+1) \quad s = 0, \frac{1}{2}, 1, \frac{3}{2}, ... \\ S_z \to \hbar m_s \quad m_s = s, s-1, ..., -s\end{array} \tag{4.12}$$

Spin is not classically rotation, so no requirement for

$$\psi(\phi) = \psi(\phi + 2\pi)$$

so we cannot get rid of $\frac{1}{2}, \frac{3}{2}, ...$

For any elementary particle, s is fixed, unlike l, for e^{-1} of hydrogen orbit angular momentum can be any value $l = 0, 1, 2, ..., n-1$, while s is always $\frac{1}{2}$. This gives another reason why we shouldn't think spin as classical spinning motion.

$$\begin{aligned} s = \frac{1}{2} \quad &\to \quad \text{electrons,quarks,neutrinos} \\ &\qquad \text{protons, nentrons (they are composite)} \\ s = 1 \quad &\to \quad \text{photons, } W^{\pm}, Z\text{bosons} \\ s = 0 \quad &\to \quad \text{Higgs (only known particle with } s = 0) \\ &\qquad \text{pions (composite)} \end{aligned}$$

Spin of composite particles is not determined solely by the constituents: proton $uud \to s = \frac{1}{2}$, Δ^+ $uud \to s = \frac{3}{2}$

Relativistic QM gives answer why s is fixed, but the argument is absurd.

Electron Spin

Because of intrinsic nature of spin (4.11), we can study spin wave function or wave vector independent of $\psi(\vec{x})$ of the particles

Before we studied $\psi(\vec{x})$ and $\psi(\vec{p})$ in $|x\rangle$ and $|p\rangle$ base we showed the conversion between functional forms and vector forms.

$$\psi(\vec{x}) = \langle\vec{x}|\psi\rangle$$

since $|x\rangle$ and $|p\rangle$ base are continuous, functional forms have some advantage. For spin, the basis is discrete. 2 dimensional for electron spin. So vector form has some edge.

Denote

$$\begin{aligned} \left| s=\frac{1}{2}, m=\frac{1}{2} \right\rangle &= |\uparrow\rangle \text{ spin up} \\ \left| s=\frac{1}{2}, m=-\frac{1}{2} \right\rangle &= |\downarrow\rangle \text{ spin up} \end{aligned}$$

as a set of basis, and they are eigenvector of S_z

$$\begin{aligned} S_z |\uparrow\rangle &= \frac{\hbar}{2} |\uparrow\rangle \\ S_z |\downarrow\rangle &= -\frac{\hbar}{2} |\downarrow\rangle \end{aligned}$$

For an arbitrary spin

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} \text{ with } |a|^2 + |b|^2 = 1$$

χ of $|\uparrow\rangle$ is $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, χ of $|\downarrow\rangle$ is $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$, in this basis

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

Define $S_+ = S_x + iS_y$

$$S_+ |\uparrow\rangle = 0$$

$$S_+ |\downarrow\rangle = \hbar\sqrt{s(s+1) - m_s(m_s+1)}\, |\uparrow\rangle = \hbar\sqrt{\frac{1}{2}(\frac{1}{2}+1) + \frac{1}{2}(-\frac{1}{2}+1)}\, |\uparrow\rangle = \hbar\, |\uparrow\rangle$$

Hence

$$S_+ = \frac{\hbar}{2} \begin{pmatrix} & 1 \\ 0 & \end{pmatrix}$$

Similarly define $S_- = S_x - iS_y$

$$S_- = \frac{\hbar}{2}\begin{pmatrix} & 0 \\ 1 & \end{pmatrix}$$

then

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2}\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$$

$$S_y = \frac{1}{2i}(S_+ - S_-) = \frac{\hbar}{2}\begin{pmatrix} & -i \\ i & \end{pmatrix}$$

Define Pauli matrices

$$\sigma_x = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} \quad \sigma_y = \begin{pmatrix} & -i \\ i & \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

$$S_j = \frac{\hbar}{2}\sigma_j$$

One can easily check Pauli matrices satisfy the commutative relations in (4.12).

As an exercise what is eigenstate of S_x? In the $|\uparrow\rangle, |\downarrow\rangle$ basis

$$\left|S_x = \frac{\hbar}{2}\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{4.13}$$

$$\left|S_x = -\frac{\hbar}{2}\right\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

More general for any direction

$$\hat{n} = \sin\theta\cos\phi\hat{i} + \sin\theta\sin\phi\hat{j} + \cos\theta\hat{k}$$

the eigenstate of $\hat{n} \cdot \vec{S}$

$$\hat{n} \cdot \vec{S} = \frac{\hbar}{2} \quad \longrightarrow \quad \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix}$$
$$\hat{n} \cdot \vec{S} = -\frac{\hbar}{2} \quad \longrightarrow \quad \begin{pmatrix} e^{-i\phi}\sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}$$

check it works for the special cases S_x,

$$\hat{x}: \ \phi = 0, \theta = \frac{\pi}{2}$$

and S_y

$$\hat{y}: \ \phi = \frac{\pi}{2}, \theta = \frac{\pi}{2}$$

Back to (4.13) if the particle is in $S_x = \frac{\hbar}{2}$ state, then if we measure S_z

$$\text{the prob of getting } \frac{\hbar}{2} \text{ is } \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2} \tag{4.14}$$

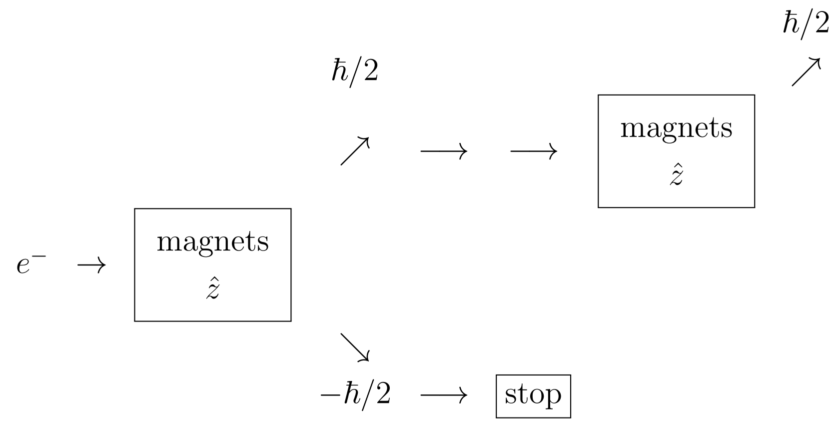
$$\text{the prob of getting } -\frac{\hbar}{2} \text{ is } \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2} \tag{4.15}$$

Similarly if the particle is in $S_x = -\frac{\hbar}{2}$ state, then if we measure S_z

$$\text{the prob of getting } \tfrac{\hbar}{2} \text{ or } -\tfrac{\hbar}{2} \text{is } \tfrac{1}{2} \tag{4.16}$$

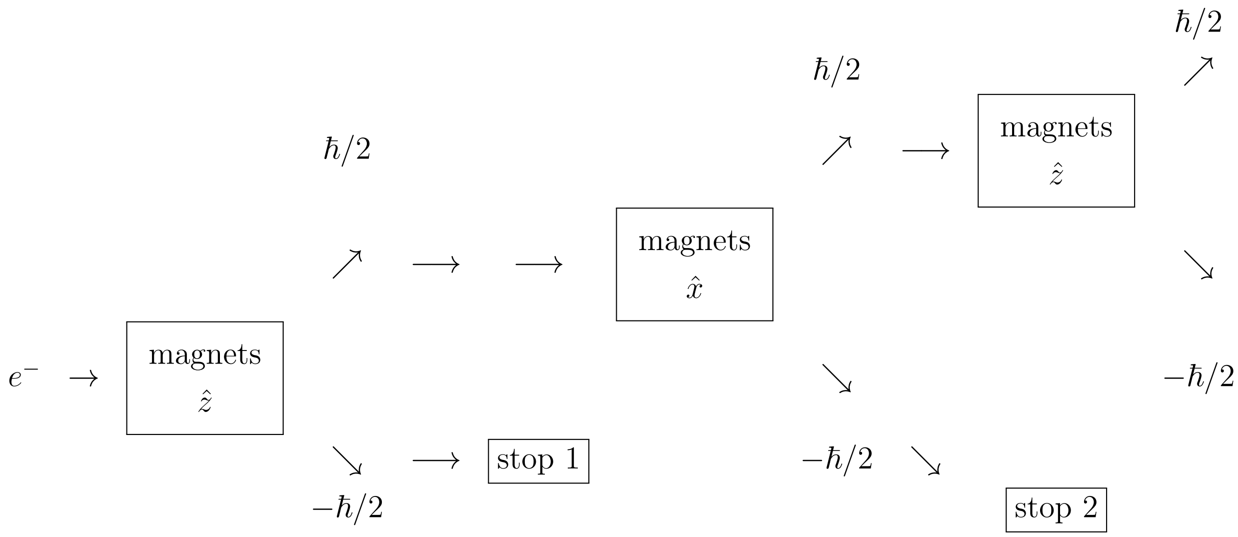
The situation becomes peculiar when one performs series of Stern-Gerlach experiments.

Exp 1



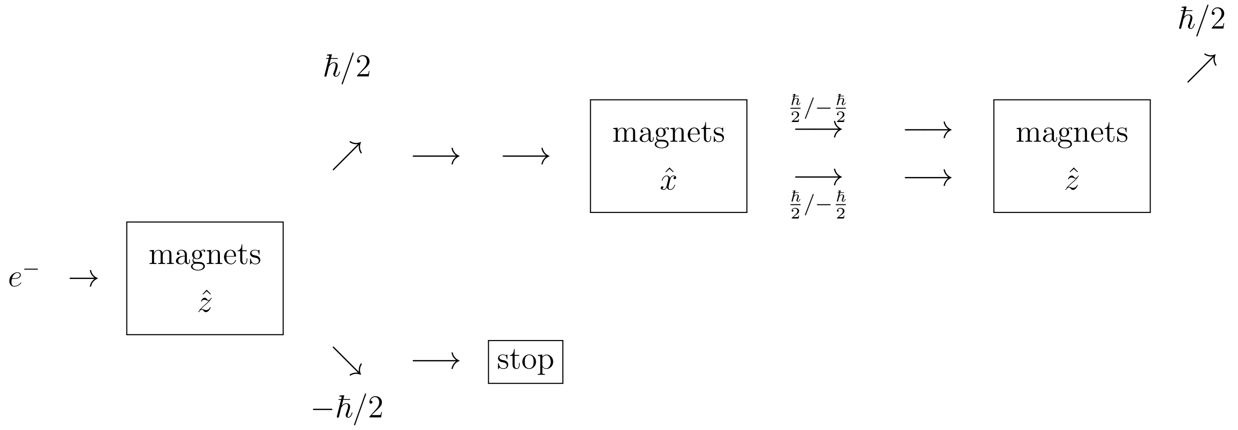
shows continuing measurements return same value.

Exp 2



shows the measurement of $\hat{x}$ on $S_z = \frac{\hbar}{2}$ states alter the states.

Exp 3



shows that without stop2 from Exp 2 the measurement of $\hat{x}$ on $S_z = \frac{\hbar}{2}$ states doesn't alter the states. More precisely if we don't know the S_x value of the particle coming out of the magnets $\hat{x}$ then its S_z will not change. If we do look at the S_x value of the particle coming out of the magnets $\hat{x}$ then its S_z, as in the diagram below, by (4.14), (4.15), (4.16), will change. This is similar to the double slit experiment. Knowing which slit particles pass through will change the interference pattern.