Quantum Mechanics I

Norman Christ

Transcribed by Ron Wu

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1 Fundamentals I

1.1 Fourier Trick

Lecture 1 (9/4/13)

In this course we deal with non-relativistic quantum mechanics. Despite its exclusion with resistivity, it is correct on its own right around the order of magnitudes we study

$$px \sim \hbar \qquad Et \sim \hbar \qquad L \sim \hbar$$

$$\hbar = \frac{h}{2\pi} = 1.05 \times 10^{-27} \mathrm{erg} \cdot \mathrm{sec}$$

One of the famous experiments that introduces quantum mechanics is diffraction grading. Suppose a beam of elections with momentum p incidents normally along x axis onto a thin sheet of atoms sitting in y axis with fixed separation d. Some beam are transmitted through causing bright background signals on the screen, and some gets scattered making diffraction patterns. Such phenomenon was successfully explained via wave mechanics. This was the starting point to associate scattered electrons with waves.

The observed diffraction agrees classical equation

$$d \sin\theta_n = n\lambda \tag{1.1}$$

with Brag's creative invention

$$\lambda = \frac{h}{p} \tag{1.2}$$

It becomes inevitable to assign a wave function to an electron. Try

$$|\psi(x)|^2 \Delta x = \text{prob of finding the electrons between } x \text{ and } x + \Delta x$$

and

$$\text{prob}(x_1 \leq x \leq x_2) = \int_{x_1}^{x_2} |\psi(x)|^2 dx$$

Since the election must be somewhere

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

This is conceptually different from EM wave. For EM waves, we take the amplitude

$$\frac{1}{8\pi}(E^2 + B^2) = \text{energy density}$$

which is a physical thing. QM wave amplitude

$$|\psi(x)|^2 = \text{prob density}$$

which is a distribution of knowledge much less physical. If later a measure find e^- near some place, then the wave function will collapse to the vicinity of that place, which is also very different from EM waves.

Recall Fourier transform

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

Inverse Fourier

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

this allows us to express $\psi(x)$ as superpositions of many waves, each with $k = 2\pi/\lambda$.

We now apply Fourier to the diffraction experiment.

Suppose there are N scatters ($N/2$ above the x axis and $N/2$ below the axis) and the scattered waves right passing the atoms have same amplitudes A. Fourier transform of them wrt to y is

$$\begin{aligned} F(k) &= \frac{1}{\sqrt{2\pi}} \sum_{j=-N/2}^{N/2} A e^{-ikdj} = \frac{A}{\sqrt{2\pi}} e^{ikd\frac{N}{2}} \sum_{j=0}^{N} e^{-ikdj} \\ &= \frac{A}{\sqrt{2\pi}} e^{ikd\frac{N}{2}} \frac{1 - e^{-ikd(N+1)}}{1 - e^{-ikd}} = \frac{A}{\sqrt{2\pi}} \frac{e^{ikd(\frac{N}{2}+\frac{1}{2})}}{e^{ik\frac{d}{2}}} \frac{1 - e^{-ikd(N+1)}}{1 - e^{-ikd}} \\ &= \frac{A}{\sqrt{2\pi}} \frac{\sin \frac{kd}{2}(N+1)}{\sin \frac{kd}{2}} \end{aligned} \tag{1.3}$$

One can graph (1.3), noticing it has minimal values at

$$\frac{kd}{2} = n\pi \tag{1.4}$$

We want to show this wave vector k is related to momentum.

y component of the momentum of the scattered e^-

$$p_y = p \sin\theta$$

By (1.1), (1.2), and (1.4)

$$p_y = p\frac{\lambda}{d}n = p\frac{2\pi\hbar}{pd}n = \frac{2n\pi}{d}\hbar = \hbar k$$

This correspondence between the wave number k of the Fourier transform and e^- momentum along with Parsvel's theorem suggest

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} |F(k)|^2 dk = \int_{-\infty}^{\infty} |F(\frac{p}{\hbar})|^2 \frac{dp}{\hbar}$$

so

$$\tilde{\psi}(p) = F(k = \frac{p}{\hbar})\frac{1}{\sqrt{\hbar}}$$

In classical mechanics position and momentum are not ultimately related. In QM Fourier links the two. This link becomes more apparent if we restrict x to a finite volume $0 \leq x \leq L$, which is equivalent to force $\psi(x)$ to live on a circle with circumference L.

$$\psi(0) = \psi(L) \quad \psi'(0) = \psi'(L)$$

Use e^{ikx} as a basis, we write

$$\psi(x) = \sum_{n=-\infty}^{\infty} \frac{e^{ik_n x}}{\sqrt{L}} \tilde{\psi}_n$$

$k_n = \frac{2\pi}{L}n$ quantized because of the periodic boundary conditions. $\tilde{\psi}_n$ is given by

$$\tilde{\psi}_n = \frac{1}{\sqrt{L}} \int_0^L \psi(x) e^{-ik_n x} dx$$

We too have Parsval

$$1 = \int_0^L |\psi(x)|^2 dx = \sum_{n=-\infty}^{\infty} |\tilde{\psi}_n(k)|^2$$

and

$$|\tilde{\psi}_n(k)|^2 = \text{prob of finding momentum } p_n = \hbar k_n$$

We can summarize the structures discussed above: the wave functions make up a ∞ dimensional complex vector space (called Hilbert space) which obey the following properties

1. If A, B vectors, so is $A + B$
2. If A is a vector, c complex number, cA is also a vector.
3. $c(A + B) = cA + cB$
4. $(a + b)A = aA + bA$
5. There is a zero vector, 0_{vec}, s.t.

$$0_{vec} + A = A \qquad 0A = 0_{vec}$$

To talk about length, we define inner product

1. $(A, B + C) = (A, B) + (A, C)$
2. $(A, cB) = c(A, B)$
3. $(A, B) = (B, A)^*$
4. $(A, A) \geq 0$ $(A, A) = 0 \iff A = 0$
5. $(\psi_A, \psi_B) = \int_{-\infty}^{\infty} \psi_A^*(x)\psi_B(x)dx$

We used orthonormal vectors as Fourier basis vector. In the example above

$$\psi(x) = \sum_{n=-\infty}^{\infty} \frac{e^{ip_n x/\hbar}}{\sqrt{L}} \tilde{\psi}_n \tag{1.5}$$

for

$$\int_0^L \frac{e^{-ip_m x/\hbar}}{\sqrt{L}} \frac{e^{ip_n x/\hbar}}{\sqrt{L}} dx = \delta_{mn}$$

Fourier gives us two ways to compute length

$$\|\psi\|^2 = \int_0^L |\psi(x)|^2 dx = \sum_{n=-\infty}^{\infty} |\tilde{\psi}_n|^2$$

Lecture 2 (9/9/13)

Dirac notation says $|\psi\rangle$ to represent ψ as a vector. $|\psi\rangle$ is a vector without specifying basis (later we will show it can be in either positive or momentum space.) Applying idea from linear algebra, we write (1.5)

$$|\psi\rangle = \sum_{n=-\infty}^{\infty} \tilde{\psi}_n |p_n\rangle$$

$$|p_n\rangle \leftrightarrow \frac{e^{ip_n x/\hbar}}{\sqrt{L}} \qquad p_n = \frac{2\pi}{L}\hbar n \tag{1.6}$$

1.2 Discrete Measurement

First let's consider "yes-no" experiments for the discrete cases. For example does the particles have momentum p_{n_0}?

$$\begin{aligned} |\tilde{\psi}_{n_0}|^2 &= \text{prob of answer to be yes} \\ 1 - |\tilde{\psi}_{n_0}|^2 &= \text{prob of answer to be no} \end{aligned}$$

We will associate with this measurement a projection operator P_{n_0}.

A projection operator obeys:

1. $P^2 = P$
2. $P^\dagger = P$

A linear operator obeys:

1. for each vector A in the inner space, OA is also a vector
2. $O(cA) = cOA$
3. $O(A+B) = OA + OB$

An adjoint or hermitian conjugate of O is $O^\dagger$ obeys:

$$(B, O^\dagger A) = (OB, A)$$

A projection operator divide our vector space into two subspaces:
1. the image of P

$$\{PA \text{ where } A \text{ is a vector}\}$$

2. the orthogonal component of the image of P.
That is for any $|\psi\rangle$

$$|\psi\rangle = P\,|\psi\rangle + (1-P)\,|\psi\rangle$$

and

$$((1-P)\,|\psi\rangle\,, P\,|\psi\rangle) = (P(1-P)\,|\psi\rangle\,, |\psi\rangle) = \big((P-P^2)\,|\psi\rangle\,, |\psi\rangle\big) = 0$$

That P_{n_0} is the projection onto $|p_{n_0}\rangle$ means

$$P_{n_0}\,|\psi\rangle = P_{n_0}\sum_{n=-\infty}^{\infty}\tilde{\psi}_n\,|p_n\rangle = \tilde{\psi}_{n_0}\,|p_{n_0}\rangle$$

Now the beauty of Dirac appears, that is

$$P_{n_0}\,|\psi\rangle = \tilde{\psi}_{n_0}\,|p_{n_0}\rangle = \langle p_{n_0}|\psi\rangle\,|p_{n_0}\rangle = \underbrace{|p_{n_0}\rangle\,\langle p_{n_0}|}_{\equiv P_{n_0}}\,|\psi\rangle$$

We say

$$\begin{aligned}\langle A|B\rangle &= \text{inner product}\\ |A\rangle\,\langle B| &= \text{outer product}\end{aligned}$$

Associated with our “yes-no” experiment is the projection operator

$$P_{n_0} = |p_{n_0}\rangle\,\langle p_{n_0}|$$

$$\text{prob getting yes} = \langle\psi|P_{n_0}|\psi\rangle = \left\langle\psi\middle|P_{n_0}^2\middle|\psi\right\rangle = \langle P_{n_0}\psi|P_{n_0}\psi\rangle = |\tilde{\psi}_{n_0}|^2$$

The state after the result yes is obtained is not $P_{n_0}\left|\psi\right\rangle$, should be

$$\frac{P_{n_0}\left|\psi\right\rangle}{\sqrt{\left\langle\psi\middle|P_{n_0}^2\middle|\psi\right\rangle}} = \frac{\tilde{\psi}_{n_0}}{\sqrt{\tilde{\psi}^*_{n_0}\tilde{\psi}_{n_0}}}\left|p_{n_0}\right\rangle = \left|p_{n_0}\right\rangle$$

Note that the denominator $\left\langle\psi\middle|P_{n_0}^2\middle|\psi\right\rangle$ is not 0, because $\tilde{\psi}_{n_0} \neq 0$ otherwise yes is never obtained. Note that $\tilde{\psi}_{n_0}/\sqrt{\tilde{\psi}^*_{n_0}\tilde{\psi}_{n_0}}$ represents a phase, which is not important, because the observer cannot two measurements at the same time, hence no interference between measurements.

Similarly

$$\text{prob getting no} = \langle\psi|I - P_{n_0}|\psi\rangle = 1 - \langle\psi|P_{n_0}|\psi\rangle$$

If no is found, the resulting state is

$$\frac{(I - P_{n_0})\left|\psi\right\rangle}{\sqrt{\langle\psi|(I - P_{n_0})|\psi\rangle}}$$

Is $(I - P_{n_0})$ necessary a projection?

$$(I - P_{n_0})^\dagger = I^\dagger - P_{n_0}^\dagger = I - P_{n_0}$$

$$(I - P_{n_0})^2 = I - 2P_{n_0} + P_{n_0}^2 = 1 - P_{n_0}$$

Now we ask further "Does the momentum lie in a set of momenta $\{p_{\sigma_i}\}_{1\leq i\leq k}$?" The associated projection is

$$P_{\{\sigma_i\}} = \sum_{1\leq i\leq k} P_{\sigma_i}$$

Indeed it is a projection

$$P_{\{\sigma_i\}}^\dagger = \sum P_{\sigma_i}^\dagger = \sum P_{\sigma_i}$$

$$P_{\{\sigma_i\}}^2 = \sum_i P_{\sigma_i}\sum_j P_{\sigma_j} = \sum_i P_{\sigma_i}$$

for states are orthogonal

$$P_{\sigma_i} P_{\sigma_j} = P_{\sigma_i} \delta_{ij}$$

The expectation value is the average results on many measurements

$$\langle p \rangle = \sum_{n=-\infty}^{\infty} p_n |\tilde{\psi}_n|^2 \tag{1.7}$$

which is equivalent to the statistical definition

$$\langle p \rangle = \lim_{N \to \infty} \frac{\sum_{n=-\infty}^{\infty} p_n N_i}{N}$$

N_i number of times p_n is found and N is the total number of measurements.

In turns of projection operator we can write (1.10)

$$\langle p \rangle = \sum_{n=-\infty}^{\infty} p_n \langle \psi | P_n | \psi \rangle = \left\langle \psi \middle| \sum_{n=-\infty}^{\infty} p_n P_n \middle| \psi \right\rangle$$

We define momentum operator $p_{op} = \sum_{n=-\infty}^{\infty} p_n P_n$, which is hermitian. This is the best way of thinking of measurement in QM. If one wants to measure p^{27}, the expectation

$$\left\langle p^{27} \right\rangle = \left\langle \psi \middle| (p_{op})^{27} \middle| \psi \right\rangle = \left\langle \psi \middle| \sum_{n=-\infty}^{\infty} p_n^{27} P_n \middle| \psi \right\rangle$$

Hence we decompose the operator in its spectrum, for any analytic function (i.e. has convergent Taylor expansion) F of p

$$\langle F(p) \rangle = \left\langle \psi \middle| \sum_{n=-\infty}^{\infty} F(p_n) P_n \middle| \psi \right\rangle$$

The state $|p_{n_0}\rangle$ with a definite value of the momentum obey a simple relation

$$p_{op} |p_{n_0}\rangle = \sum_{n=-\infty}^{\infty} p_n P_n |p_{n_0}\rangle = p_{n_0} |p_{n_0}\rangle$$

Hence $|p_{n_0}\rangle$ is an eigenvector of p_{op} and p_{n_0} is the eigenvalue.

In general if an observable O has only a discrete set of allowed values λ_n, each corresponds to a state $|\lambda_n\rangle$ with that value. QM operator associated with O measurement

$$O_{op} = \sum_n \lambda_n P_n = \sum_n \lambda_n |\lambda_n\rangle \langle\lambda_n|$$

$$O_{op} |\lambda_n\rangle = \lambda_n |\lambda_n\rangle$$

Is this true for all observables? It is clearly true if the space of states is finite dimensional. Not true in general.

1.3 Continuum Measurement

Suppose we let $L \to \infty$ in (1.6). We immediately face two problems. $|p_n\rangle$ is not normalizable. The difference $\Delta p = p_{n+1} - p_n = 2\pi\hbar/L$ is so small that we loss the sense of having definite momentum.

Naturally we should talk about a range of momentum.

$$P_{[p_a,p_b]} = \lim_{\Delta p \to 0} \{ \sum_{p_a \le p_n \le p_b} P_{p_n} \} \tag{1.8}$$

Consider continuous variables x

$$\begin{aligned} (P_{[p_a,p_b]} |\psi\rangle)(x) &= \sum_{p_a \le p_n \le p_b} (|p_n\rangle (x) \langle p_n|\psi\rangle) \\ &= \sum_{p_a \le p_n \le p_b} \frac{e^{ip_n x/\hbar}}{\sqrt{L}} \int \frac{e^{-ip_n y/\hbar}}{\sqrt{L}} \psi(y) dy \end{aligned}$$

When $\Delta p \to 0$, we can convert the summation to integration. Recall Riemann integral

$$\sum f(p_n)\Delta p \to \int dp f(p)$$

Here

$$\sum_{p_a \le p_n \le p_b} \frac{e^{ip_n x/\hbar}}{L} \to \int_{p_a}^{p_b} \frac{dp}{2\pi\hbar} e^{ipx/\hbar}$$

Hence

$$P_{[p_a,p_b]} |\psi\rangle = \int_{p_a}^{p_b} \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \int \frac{dy}{\sqrt{2\pi\hbar}} \psi(y) e^{-ipy/\hbar}$$

meaning $\tilde{\psi}(p) = \int \frac{dy}{\sqrt{2\pi\hbar}}\psi(y)e^{-ipy/\hbar}$ Fourier transform ψ into momentum space, then treat it as the momentum amplitude of the plane waves $e^{ipx/\hbar}$ with momentum lie in p_a and p_b.

Conventionally, we define

$$E(p) = P_{[-\infty,p]}$$

$$E(p)\,|\psi\rangle\,(x) = \int_{-\infty}^{p} \frac{dp'}{\sqrt{2\pi\hbar}} e^{ip'x/\hbar} \int_{-\infty}^{\infty} \frac{dx'}{\sqrt{2\pi\hbar}} \psi(x') e^{-ipx'/\hbar} \tag{1.9}$$

so

$$P_{[p_a,p_b]} = E(p_b) - E(p_a) \tag{1.10}$$

$E(\lambda)$ is called a resolution of the identity. It obeys

1. E is a projection operator $(E(\lambda))^2 = E(\lambda)$, $E(\lambda)^\dagger = E(\lambda)$

2. $E(\lambda_1)E(\lambda_2) = E(\min(\lambda_1,\lambda_2))$ This is saying product of two projection is one projection of whatever the smaller the one to be.

3. $E(+\infty) = I$, because

$$E(+\infty)\,|\psi\rangle = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \int \frac{dy}{\sqrt{2\pi\hbar}} \psi(y) e^{-ipy/\hbar} = |\psi\rangle$$

Fourier then inverse Fourier. And this suggests why it is named.

Lecture 3 (9/11/13)

We know (1.8) is a projection before taking the limit. Is it still a projection? Form (1.10)

$$\begin{aligned} P^2_{[p_a,p_b]} &= E(p_b)^2 - E(p_b)E(p_a) - E(p_a)E(p_b) + E(p_a)^2 \\ &= E(p_b) - 2E(p_a) + E(p_a) = P_{[p_a,p_b]} \end{aligned}$$

Given a state $|\psi\rangle$

$$\langle\psi|E(\lambda_1) - E(\lambda_2)|\psi\rangle = \text{prob of finding } \lambda_1 \le \lambda \le \lambda_2$$

If the resolution is yes, then the state becomes

$$\frac{(E(\lambda_1) - E(\lambda_2))\,|\psi\rangle}{\sqrt{\langle\psi|E(\lambda_1) - E(\lambda_2)|\psi\rangle}}$$

Similarly as before we can construct an operator O_{op} obeying

$$\begin{aligned}\langle O\rangle &= \langle\psi|O_{op}|\psi\rangle = \lim_{\Delta\to 0}\sum \lambda_n \langle\psi|E(\lambda_1) - E(\lambda_2)|\psi\rangle \\ O_{op} &= \lim_{\Delta\to 0}\sum \lambda_n (E(\lambda_1) - E(\lambda_2)) = \int \lambda dE\end{aligned}$$

which is a stieltjes integral.

What is dE?

For momentum measurement, (1.9) shows

$$E(p) = \int |p'\rangle \langle p'| \, dp' = \int dE$$

so momentum measure

$$dE = |p\rangle \langle p| \, dp$$

$|p\rangle$ is not normalized but has definite p value and still dE is a well defined mathematical object. Later we will do decay. We will encounter such object again

$$| \langle p|H|n\rangle |^2$$

n energy states.

$$\int_{p_2}^{p_1} | \langle p|H|n\rangle |^2 dp = \left\langle n \middle| H \int_{p_2}^{p_1} dp \middle| p \right\rangle \langle p|H|n\rangle = \langle n|H[E(p_2) - E(p_1)]H|n\rangle$$

For position measurement,

$$(E(x)\,|\psi\rangle)(x') = \theta(x - x')\psi(x') \tag{1.11}$$

This is clearly projection operator.

What does

$$dE = |x\rangle \langle x| \, dx \tag{1.12}$$

mean?

From (1.11)

$$\frac{dE(x)}{dx} |\psi\rangle (x') = \frac{d}{dx}\theta(x - x')\psi(x') \tag{1.13}$$

By (1.12)

$$\frac{dE(x)}{dx} |\psi\rangle (x') = |x\rangle (x') \langle x|\psi\rangle$$

$$\frac{d}{dx}\theta(x-x') = \delta(x-x')$$

Dirac says $\langle x|\psi\rangle = \psi(x)$, $\langle x|$ acts on state $|\psi\rangle$. Note that $\langle x|$ is not normalizable but it has definite position. So (1.13) becomes

$$|x\rangle (x')\psi(x) = \delta(x-x')\psi(x') = \delta(x-x')\psi(x)$$

This shows we should identify

$$|x\rangle (x') = \delta(x-x')$$

or using the same idea for $\langle x|\psi\rangle = \psi(x)$, we say

$$|x\rangle (x') = \langle x'|x\rangle = \delta(x-x')$$

Similarly

$$\langle p'|p\rangle = \int_{-\infty}^{\infty} \frac{e^{-ip'x/\hbar}}{\sqrt{2\pi\hbar}} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} dx = \delta(p-p')$$

We have seen momentum can be discrete or continuous. If the spectrum is discrete, what does $E(\lambda)$ look like?

$$E(\lambda) = \sum_{\lambda_n<\lambda} |\lambda_n\rangle \langle\lambda_n| = \sum_n \theta(\lambda-\lambda_n) |\lambda_n\rangle \langle\lambda_n|$$

In general spectrum can be both discrete and continuous, and from spectrum theory we know discrete values are always below then approaches to a limit point after the limit point, spectrum is continuous.

For example energy eigenvalues for Hydrogen atom are discrete below 0 and continuous above 0,

$$E = -\frac{Z^2e^4m}{2n^2\hbar^2}$$

one way to memorize this formula is to memorize fine constant

$$\alpha = \frac{e^2}{\hbar c}$$

which is dimensionless. Since

$$E = -\frac{Z^2 e^4 mc^2}{2n^2\hbar^2 c^2} = -\frac{Z^2}{2n^2}\alpha^2 mc^2$$

Indeed α is dimensionless.

Again by spectral theory, once we find E resolution of the identity (could be both discrete and continuous) for a self adjoint operator O, then

$$O_{op} = \int \lambda dE$$

1.4 Uncertainty Principle

Later we will "derive" Schrodinger equation from classical mechanics. We will see most QM is just reformulation classical mechanics. The real teeth come in when we do Fourier trick, which shows x and p are related. This connection has many unique consequences.

For an easy example, say we have

$$\psi(x) = \frac{1}{\sqrt{\sqrt{\pi}d}} e^{-\frac{(x-x_0)^2}{2d^2}}$$

$$\begin{aligned}
\tilde{\psi}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \frac{1}{\pi^{\frac{1}{4}} d^{\frac{1}{2}}} e^{-\frac{(x-x_0)^2}{2d^2}} dx \\
&= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \frac{1}{\pi^{\frac{1}{4}} d^{\frac{1}{2}}} e^{-\frac{(x-x_0+ipd^2/\hbar)^2}{2d^2}} dx e^{-ipx_0/\hbar} e^{-p^2 d^2/2\hbar^2} \\
&= \frac{1}{\sqrt{\pi\hbar}} e^{-ipx_0/\hbar} e^{-\frac{p^2}{2(\frac{\hbar}{d})^2}}
\end{aligned}$$

Before we derive uncertainty principal in general, we try it on Gaussian wave above

$$\langle\psi|x_{op}|\psi\rangle = x_0$$

$$\langle\psi|p_{op}|\psi\rangle = 0$$

Fluctuation

$$\langle\psi|x_{op} - x_0|\psi\rangle = 0$$

so we look at

$$\Delta x^2 = \left\langle\psi\middle|(x_{op} - x_0)^2\middle|\psi\right\rangle = \frac{d^2}{2}$$

one can show

$$\Delta p^2 = (\frac{\hbar}{d})^2\frac{1}{2}$$

Hence

$$\Delta x \Delta p = \frac{\hbar}{2}$$

so Gaussian function saturates the uncertainty principle.

Lecture 4 (9/16/13)

We now derive uncertainty in general.

Recall

$$\begin{aligned}
x_{op}\psi(x) &= x\psi(x) \\
p_{op}\psi(x) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp e^{ipx/\hbar} p\tilde{\psi}(p) \\
&= \frac{1}{\sqrt{2\pi\hbar}}\frac{\hbar}{i}\frac{d}{dx}\int_{-\infty}^{\infty} dp e^{ipx/\hbar}\tilde{\psi}(p) = \frac{\hbar}{i}\frac{d}{dx}\psi(x)
\end{aligned}$$

thus

$$[x_{op}, p_{op}]\psi(x) = \frac{\hbar}{i}[x\frac{d}{dx} - \frac{d}{dx}x]\psi = i\hbar\psi$$

Let $X_{op} = x_{op} - \bar{x}$, $P_{op} = p_{op} - \bar{p}$, then

$$[X_{op}, P_{op}] = [x_{op}, p_{op}] = i\hbar$$

Consider $\alpha \in \mathbb{R}$, and $|\psi\rangle$ is normalized to 1,

$$\|(X_{op} + i\alpha P_{op})\,|\psi\rangle\|^2 \geq 0$$

Since $X_{op},\ P_{op}$ are hermitian,

$$\|(X_{op}+i\alpha P_{op})\,|\psi\rangle\|^2 = (|\psi\rangle\,, (X_{op}-i\alpha P_{op})(X_{op}+i\alpha P_{op})\,|\psi\rangle) \geq 0 \tag{1.14}$$

$$(X_{op}-i\alpha P_{op})(X_{op}+i\alpha P_{op}) = X_{op}^2+\alpha P_{op}^2+i\alpha[X_{op},P_{op}] = X_{op}^2+\alpha P_{op}^2-\alpha\hbar$$

Then define $(\Delta x)^2 = \langle\psi|X_{op}^2|\psi\rangle$, $(\Delta p)^2 = \langle\psi|P_{op}^2|\psi\rangle$

$$\langle\psi|X_{op}^2+\alpha P_{op}^2-\alpha\hbar|\psi\rangle = (\Delta x)^2+\alpha^2(\Delta p)^2-\alpha\hbar \geq 0$$

saying that the determinant of above is < 0, i.e. α has no real root so the graph is always above x axis.

$$\hbar^2-4(\Delta x)^2(\Delta p)^2 \leq 0$$

i.e.

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

Finally we show that kind of wave function gives the equality.

The equality is obtained in (1.14), so

$$X_{op}+i\alpha P_{op}\,|\psi\rangle = 0$$

Assume $\bar{x}=0$ and $\bar{p}=0$,

$$(x+i\alpha\frac{\hbar}{i}\frac{d}{dx})\psi = 0 \implies \psi = e^{-\alpha\hbar\frac{x^2}{2}}$$

If we prepare many identical particles in boxes, we then measure momentum and find they have value

$$p_n = \frac{2\pi}{L}\hbar n$$

for some n with uncertainty $\frac{2\pi}{L}\hbar$. Then we know the particles are now like waves with wavelength $\lambda = h/p$, the wave function

$$\langle x|p_n\rangle = \frac{e^{ip_nx/\hbar}}{\sqrt{L}}$$

If we then measure position, we will have uncertainty within a wavelength, $x_1 \leq$

$x \leq x_2$, so the wave function is

$$[\theta(x - x_1) - \theta(x - x_2)] \frac{e^{ip_n x/\hbar}}{\sqrt{L}}$$

1.5 Experiments Validate Uncertainty Principle

Discuss three experiments trying to invalidate uncertainty principle, and of course they get defeat, and in turns they support QM.

Experiment 1: Single slit diffraction

Beam of e^- far away, then enter the slit. Initial no uncertainty vertical y direction , then diffracted by the slit causes

$$\Delta p_y = p\Delta\theta$$

where $\Delta\theta$ is the 1st highest intensity after the central one. So $\Delta\theta = \lambda/D = h/pD$, where D is the width of the slit, which is the uncertainty in vertical position after the beam just passes the slit, so

$$\Delta p_y \Delta y = h$$

Question: what if we measure slit's momentum before and after the collision, then we can know exact the momentum of beam, then it may discredit uncertainty principle. But our slit was classical, if we try to measure slit's momentum we have to treat it quantum mechanically, then we don't have precisely the position of the slit.

Experiment 2: Heisenberg Microscopy

This turns out to have the same mathematics as single slit diffraction above but the mechanism is different.

A particle coming in along horizontal line with some momentum. An apparatus has a hole D and distant L straight above the path of the particle. Lights are coming out of the hole. Light may collide with the particle and get reflected back to the hole. From these lights we can infer the position and momentum of the particle.

The diffraction angle is

$$\Delta\theta = \frac{\lambda}{D}$$

the uncertainty of position of the particle when light collides it

$$\Delta x = L\Delta\theta = \frac{\lambda}{D}L$$

The uncertainty of the momentum of the particle is the same as the uncertainty of the x component momentum of the photons right after collision

$$\Delta p = \frac{h}{\lambda}\Delta\theta_\gamma = \frac{h}{\lambda}\frac{D}{L}$$

So

$$\Delta x \Delta p = h$$

Here $\Delta p \neq 0$ because we have to treat photon quantum mechanically. It has recoil, just like beam of e^- passing diffraction slit.

Experiment 3:

Eisenstein proposed to Bohr as counterexample of quantum mechanics.

The experiment consists a box. A clock is inside the box. There is a door of the box control of the clock, and a particle insider the box is ready to come out as soon as the door is open. One can make the clock very accurate $\Delta t \ll 1$ and at time t the door is open. One can weight the whole system before t and after t, then by

$$\Delta E = \frac{W_{before} - W_{after}}{g}c^2$$

We can make Δt and ΔE separately accurate. So

$$\Delta E \Delta t \geq \frac{\hbar}{2} \tag{1.15}$$

doesn't hold.

First show (1.15) from uncertainty principle.

$$\Delta x = v\Delta t + v\Delta t$$

$$\Delta p = \frac{\Delta E}{\frac{dE}{dp}} = \frac{\Delta E}{v}$$

$$\Delta x \Delta p = \frac{\Delta E}{v}(\Delta v t + v \Delta t) \geq \frac{\hbar}{2}$$

Let $t \to 0$,

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

Bohr explanation: gravitational red shift.

To get weights, we need to know vertical momentum. Measure W by measuring p at two time separated by T

$$\Delta W = \frac{\Delta p}{T}$$

$$\Delta E = \frac{c^2}{g} \frac{\Delta p}{T}$$

Light moves up down. Frequency changes.

$$h\nu + mg\Delta y = h\nu_0 \tag{1.16}$$

the mass equivalent for light is

$$m \sim \frac{h\nu}{c^2}$$

So (1.16) says

$$T_0 + T_0 \frac{g\Delta y}{c^2} = T$$

or

$$\frac{\Delta t}{T} = \frac{g\Delta y}{c^2}$$

so

$$\Delta E \Delta t = \frac{c^2}{g} \frac{\Delta p}{T} \frac{g\Delta y}{c^2} T = \Delta p \Delta y$$

1.6 Space Translation

First consider space translation

active shift $\psi(\vec{r})$ to $\psi(\vec{r} - \vec{D})$, $\vec{D}$ is a constant vector.

Claim

$$e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar} \tag{1.17}$$

carries out such a translation.

Since

$$\psi(\vec{r}) = \int d^3p \frac{e^{i\vec{p}\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}}\tilde{\psi}(\vec{p})$$

then

$$e^{-i\vec{p}\cdot\vec{D}/\hbar}\psi(\vec{r}) = \int d^3p \frac{e^{i\vec{p}\cdot(\vec{r}-\vec{D})/\hbar}}{(2\pi\hbar)^{3/2}}\tilde{\psi}(\vec{p}) = \psi(\vec{r}-\vec{D}) \tag{1.18}$$

Lecture 5 (9/18/13)

We want to see some insight (1.17).

$$e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar} = \sum_{n=0}^{\infty}\frac{1}{n!}(-i\vec{p}\cdot\vec{D})^n$$

What about

$$e^{-i\vec{p}_{op}\cdot\vec{D}_A/\hbar}e^{-i\vec{p}_{op}\cdot\vec{D}_B/\hbar} = e^{-i\vec{p}_{op}\cdot(\vec{D}_A+\vec{D}_B)/\hbar}?$$

This is indeed correct because $[p_i, p_j] = 0$ if $i \neq j$ and $\vec{D}$ is a constant, so commute with $\vec{p}$.

More we claim $e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}$ preserves the norm of a state, i.e.

$$\left\| e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}\left|\psi\right\rangle \right\| = \left\| \left|\psi\right\rangle \right\| \tag{1.19}$$

that is $e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}$ is unitary.

Mathematically U is unitary iff

$$(UA, UB) = (A, B)$$

this implies

$$(A, U^\dagger UB) = (A, B)$$

so

$$U^\dagger U = I \text{ or } U^\dagger = U^{-1}$$

Proof of (1.19)

$$[e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}]^\dagger = e^{i\vec{D}\cdot\vec{p}_{op}/\hbar} = e^{i\vec{p}_{op}\cdot\vec{D}/\hbar} = [e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}]^{-1}$$

Now we give an alternative way than (1.18) to show $e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}$ is a translation, i.e. after applying $e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}$

$$\left(e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}\left|\psi\right\rangle, \vec{r}_{op}e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar}\left|\psi\right\rangle\right) = (\left|\psi\right\rangle, \vec{r}_{op}\left|\psi\right\rangle) + \vec{D}$$

It is enough to show

$$e^{i\vec{p}_{op}\cdot\vec{D}/\hbar}\vec{r}_{op}e^{-i\vec{p}_{op}\cdot\vec{D}/\hbar} = \vec{r}_{op} + \vec{D}$$

Put

$$\vec{R}_{op}(\alpha) = e^{i\alpha\vec{p}_{op}\cdot\vec{D}/\hbar}\vec{r}_{op}e^{-i\alpha\vec{p}_{op}\cdot\vec{D}/\hbar}$$

Solve ODE with initial $\vec{R}_{op}(0) = \vec{r}_{op}$

$$\frac{d}{d\alpha}[\vec{R}_{op}(\alpha)]_i = e^{i\alpha\vec{p}_{op}\cdot\vec{D}/\hbar}\frac{i}{\hbar}\left(\vec{p}_{op}\cdot\vec{D}(\vec{r}_{op})_i - (\vec{r}_{op})_i\vec{p}_{op}\cdot\vec{D}\right)e^{-i\alpha\vec{p}_{op}\cdot\vec{D}/\hbar}$$

$$\vec{p}_{op}\cdot\vec{D}(\vec{r}_{op})_i - (\vec{r}_{op})_i\vec{p}_{op}\cdot\vec{D} = \sum_{j=1}^{3}[(p_j)D_j,\ (\vec{r}_{op})_i] = \sum_{j=1}^{3}(-i\hbar)\delta_{ij}D_j$$

$$\frac{d}{d\alpha}[\vec{R}_{op}(\alpha)]_i = D_i$$

so

$$\vec{R}_{op}(\alpha) = \vec{r}_{op} + \alpha\vec{D}$$

Set $\alpha = 1$, the claim is proven.

1.7 Time Evolution

We describe time evolution by allowing our states to change with time, i.e. given $|\psi(0)\rangle$, find $|\psi(t)\rangle$.

Assume $U(t_2, t_1)$ unitary operator translating state from t_1 to t_2 s.t.

$$|\psi(t_2)\rangle = U(t_2, t_1) |\psi(t_1)\rangle$$

U also satisfies

$$U(t_3, t_1) = U(t_3, t_2)U(t_2, t_1)$$

i.e. state evolution as what we expect if no measurement interrupted.

Assuming potential doesn't dependent on time, we expect time translation invariant i.e.

$$U(t_2 + T, t_1 + T) = U(t_2, t_1)$$

then set $T = -t_1$

$$U(t_2, t_1) = U(t_2 - t_1, 0) = U(t_2 - t_1)$$

that is U is operator of 1 variable.

What should U look like?

$$U(t)U^\dagger(t) = I$$

Differentiate wrt t

$$\frac{dU}{dt}U^\dagger + U\frac{dU^\dagger}{dt} = 0$$

or

$$\left(\frac{dU}{dt}U^\dagger\right)^\dagger = -\frac{dU}{dt}U^\dagger$$

i.e. $\frac{dU}{dt}U^\dagger$ is anti hermitian.

$$\frac{d}{dt}U(t) = \frac{d}{dt}[U(t - t')U(t')] = \left(\frac{d}{dt}U(t - t')\right)U(t')$$

Now put $t = t'$

$$\frac{d}{dt}U(t) = \frac{d}{dt}U(0)U(t) \tag{1.20}$$

or

$$\frac{d}{dt}U(0) = \left(\frac{dU(t)}{dt}\right)_{t=0} = \frac{dU(t)}{dt}U^\dagger(t)$$

is hermitian, so we define

$$\frac{d}{dt}U(0) = -i\frac{H}{\hbar}$$

or

$$H = i\hbar\frac{d}{dt}U(0)$$

H has unit of energy, for $\hbar \sim Et$, and U is unit less.

From (1.20)

$$\frac{d}{dt}U(t) = -\frac{i}{\hbar}HU(t)$$

$$|\psi(t)\rangle = U(t)\,|\psi(0)\rangle \qquad \frac{d}{dt}\,|\psi(t)\rangle = -\frac{i}{\hbar}H\,|\psi(t)\rangle$$

we derived Schrodinger equation.

What is H?

Suppose we look at

$$\begin{aligned}
\frac{d}{dt}\,\langle\psi(t)|x_{op}|\psi(t)\rangle &= \left\langle \psi(t) \middle| \frac{i}{\hbar}Hx_{op} - \frac{i}{\hbar}x_{op}H \middle| \psi(t) \right\rangle \\
&= \left\langle \psi(t) \middle| -\frac{i}{\hbar}[x_{op}, H] \middle| \psi(t) \right\rangle
\end{aligned}$$

From Hamiltonian mechanics

$$-\frac{i}{\hbar}[x_{op}, H] = \left(\frac{\partial H}{\partial p}\right)_{p=p_{op}} \tag{1.21}$$

And by Hamiltonian equations

$$\left(\frac{\partial H}{\partial p}\right)_{p=p_{op}} = \left(\frac{dx}{dt}\right)_{x=x_{op}}$$

if we take H here to be the Hamiltonian in Hamiltonian mechanics.

Similarly

$$\frac{d}{dt}\,\langle\psi(t)|p_{op}|\psi(t)\rangle = \left\langle \psi(t) \middle| -\frac{i}{\hbar}[p_{op}, H] \middle| \psi(t) \right\rangle = \left\langle \psi \middle| -\frac{\partial H}{\partial x} \middle| \psi \right\rangle$$

We can verify (1.21) using

$$H = \frac{p^2}{2m} + V(x)$$

compute

$$\begin{aligned}
[x_{op}, p_{op}^2] &= x_{op}p_{op}^2 - p_{op}^2 x_{op} \\
&= [x_{op}, p_{op}]p_{op} + p_{op}x_{op}p_{op} + p_{op}[x_{op}, p_{op}] - p_{op}x_{op}p_{op} \\
&= 2i\hbar p_{op}
\end{aligned}$$

In general any operator is a polynomial of x and p so the following are useful

$$[x_{op}, p_{op}^n] = i\hbar n p_{op}^{n-1} = i\hbar \left(\frac{\partial p^n}{\partial p}\right)_{p=p_{op}}$$

$$[x_{op}^n, p_{op}] = i\hbar n x_{op}^{n-1} = i\hbar \left(\frac{\partial x^n}{\partial x}\right)_{x=x_{op}}$$

1.8 Hamiltonian Classical Mechanics

Recall for N degrees of freedom, we describe the system by q_i and $\dot{q}_i$, $1 \le i \le N$,

$$L(q_i, \dot{q}_i) = T - V(q)$$

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$$

Define conjugate momentum

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

If we are able to invert, we get

$$\dot{q}_i = \dot{q}_i(q, p)$$

Define

$$H(q,p) = \sum_{i=1}^{N} p_i \dot{q}_i - L(q,\dot{q})$$

Then compute

$$\left(\frac{\partial H(q,p)}{\partial p_i}\right)_{\substack{\text{fix } q_j \; 1 \le j \le N \\ \text{fix } p_j \; j \neq i}} = \dot{q}_i + \sum_{j=1}^{N} p_j \frac{\partial \dot{q}_j}{\partial p_i} - \sum_{j=1}^{N} \frac{\partial L}{\partial \dot{q}_j} \frac{\partial \dot{q}_j}{\partial p_i} = \dot{q}_i$$

Similarly

$$\left(\frac{\partial H(q,p)}{\partial q_i}\right)_{\substack{\text{fix } p_j \; 1 \le j \le N \\ \text{fix } q_j \; j \neq i}} = -\dot{p}_i$$

Lecture 6 (9/23/13)

Consider

$$q_i \to q_i + \delta q_i \qquad p_i \to p_i + \delta p_i \tag{1.22}$$

Make a $G(q,p)$ function such that

$$\delta q_i = \epsilon \frac{\partial G}{\partial p_i} \quad \delta p_i = -\epsilon \frac{\partial G}{\partial q_i} \tag{1.23}$$

this is doable, because they are partial derivatives, no worry about correlations.

Define Poisson bracket

$$\{A(q,p), B(q,p)\} = \sum_{i=1}^{N} \left[\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right]$$

then clearly by Hamiltonian equations

$$\dot{q}_i = \{q_i, H\} \quad \dot{p}_i = \{p_i, H\}$$

In fact it's true for any operator with no explicit time dependence

$$\frac{d}{dt} O_{op}(q,p) = \sum_{i=1}^{N} \frac{\partial O}{\partial q_i} \dot{q}_i + \frac{\partial O}{\partial p_i} \dot{p}_i = \{O, H\}$$

Moreover (1.22), (1.23) say

$$q_i \to q_i + \epsilon\{q_i, G\} \quad p_i \to p_i + \epsilon\{p_i, G\}$$

Many standard transformation can be generated this way. For example

Translation in space by $\vec{D}$

$$G(q,p) = \vec{p} \cdot \vec{D}$$

Rotation about $\vec{w}$ is

$$G(q,p) = (\vec{r} \times \vec{p}) \cdot \vec{w} = \vec{L} \cdot \vec{w}$$

If H is invariant under a transformation generated by G,

$$0 = \sum_{i=1}^{N} \frac{\partial H}{\partial q_i} \delta q_i + \frac{\partial H}{\partial p_i} \delta p_i = \{H, G\} = -\frac{dG}{dt}$$

Hence G is conversed. E.g. H is invariant under $\vec{D}$, then $\vec{D} \cdot \vec{p}$ is constant.

We are now constructing quantum mechanics from classical Hamiltonian theory by equating

$$\begin{gathered} q_i \to q_i^{op} \qquad p_i \to p_i^{op} \\ \{q_i, p_i\} \to -\frac{i}{\hbar}[q_i^{op}, p_i^{op}] \\ H(q,p) \to H(q^{op}, p^{op}) \end{gathered}$$

Then for example, the time derivative of the average value of operator O

The above process is called canonical quantization. It holds provided

1. we can neglect issues of operators ordering
2. neglect things like

$$\langle \psi(t) | (q_i^{op})^n | \psi(t) \rangle = \langle \psi(t) | (q_i^{op}) | \psi(t) \rangle^n$$

i.e. the wave is not spread too widely.

The quantum mechanics we study here is non-relativistic. So we treat t and $\vec{x}$

very different. If one wants to do relativistic way, one should start from Lagrangian mechanics and get Feynman path integral. But the drawback is that path integral is not easy for everyday computations.

Example 1

a particle in one dimension

$$H = \frac{p^2}{2m} + V(x)$$

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m} \qquad \dot{p} = -\frac{\partial H}{\partial x} = -\frac{\partial V}{\partial x}$$

Example 2

A charge particle moving in 3D in a magnetic field $\vec{B}$, the Humiliation is very important when we solve Hydrogen.

$$H = \frac{[\vec{p} - \frac{Q}{c}\vec{A}(\vec{r})]^2}{2m} \tag{1.24}$$

In classical EM $\vec{A}$ is a manic to help solving problems. In QM $\vec{A}$ is essential, e.g. ψ has effects where $\vec{B} = 0$ but $\vec{A} \neq 0$.

Since $\vec{B} = \nabla \times \vec{A}$, $\vec{A}$ is not unique, so H is not unique, so Schrodinger equation is not unique. This idea led to Gauge invariant, which is promising to be the grand unification of all forces.

Let's check (1.24) is correct.

$$\dot{r}_i = \frac{\partial H}{\partial p_i} = \frac{p_i - \frac{Q}{c}A_i}{m} \implies \vec{p} = m\dot{\vec{r}} + \frac{Q}{c}\vec{A}$$

$$\dot{p}_i = -\frac{\partial H}{\partial r_i} = -\frac{1}{m}\sum_{j=1}^{3}(p_j - \frac{Q}{c}A_j)(-\frac{Q}{c}\frac{\partial A_j}{\partial r_i})$$

thus

$$\begin{aligned}
m\ddot{r}_i &= \dot{p}_i - \frac{Q}{c}\dot{A}_i \\
&= \frac{Q}{c}\sum_{j=1}^{3}\left(\dot{r}_j\frac{\partial A_j}{\partial r_i} - \frac{\partial A_i}{\partial r_j}\dot{r}_j\right) = \frac{Q}{c}\sum_{j\neq i}\left(\dot{r}_j\frac{\partial A_j}{\partial r_i} - \frac{\partial A_i}{\partial r_j}\dot{r}_j\right) \\
&= \frac{Q}{c}(\dot{\vec{r}}\times(\nabla\times\vec{A}))_i = \frac{Q}{c}(\dot{\vec{r}}\times\vec{B})_i
\end{aligned}$$

2 Fundamentals II

2.1 Simple Harmonic Oscillator

Schrodinger equation

$$i\hbar\frac{d}{dt}\left|\psi(t)\right\rangle = H\left|\psi(t)\right\rangle \tag{2.1}$$

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

solving by diagonalizing H

$$H\left|\psi_n\right\rangle = E_n\left|\psi_n\right\rangle$$

then any solution

$$\left|\psi(t)\right\rangle = \sum_{n=0}^{\infty} c_n(t)\left|\psi_n\right\rangle$$

By (2.1)

$$i\hbar\sum_{n=0}^{\infty} c_n'(t)\left|\psi_n\right\rangle = \sum_{n=0}^{\infty} c_n(t)E_n\left|\psi_n\right\rangle$$

Since $\left|\psi_n\right\rangle$ are orthogonal

$$i\hbar c_n'(t) = c_n(t)E_n \implies c_n(t) = c_n(0)e^{-iE_nt/\hbar}$$

Thus we want to solve time independent Schrodinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}mw^2x^2\right)\psi_n(x) = E_n\psi_n(x)$$

For very large x, we can ignore E_n and guess from the asymptotic behavior

$$\frac{d^2}{dx^2}\psi(x) \approx \frac{m^2w^2}{\hbar^2}x^2\psi(x)$$

$$\psi(x) \approx e^{-\frac{mw}{2\hbar}x^2} \text{ drop+}$$

this is the leading 2nd order term. Second derivative gives 1st and 0th order polynomial in front, but for large x, they are not comparable with $x^2e^{-x^2}$.

We then try

$$\psi_n(x) = \sum_{n=0} b_n x^n e^{-\frac{mw}{2\hbar}x^2}$$

This gives an iterative relation $b_n = f(b_{n-1}, b_{n-2})$. If the series don't terminate, it becomes $\sum b_n x^n \approx e^{\frac{mw}{\hbar}x^2}$, so

$$\psi \approx e^{\frac{mw}{2\hbar}x^2}$$

not good. This implies the series to terminate, thus gives Hermite polynomials.

We are going to do the ladder operators: raising a^+ and its hermitian conjugate a lower operator.

We want

$$[H, a^+] = \Delta E a^+ \tag{2.2}$$

This equation implies that a^+ raises the energy of any eigenstate of H by amount ΔE. If $|\psi\rangle$ is an energy eigenstate

$$H|\psi_n\rangle = E_n|\psi_n\rangle$$

$$Ha^+|\psi_n\rangle = \big\{[H, a^+] + a^+H\big\}|\psi_n\rangle = (\Delta E + E_n)a^+|\psi_n\rangle$$

What is a^+?

$$\begin{aligned}\frac{d}{dt}\langle\psi(t)|a^+|\psi(t)\rangle &= \frac{i}{\hbar}\langle\psi|[H, a^+]|\psi\rangle \\ &= \frac{i}{\hbar}\Delta E\langle\psi|a^+|\psi\rangle\end{aligned}$$

so

$$\langle\psi|a^+|\psi\rangle = ce^{i\Delta Et/\hbar}$$

Recall in classical mechanics, SHO

$$x(t) = A\cos wt \qquad p(t) = m\dot{x} = -Amw\sin wt$$

then

$$x - i\frac{1}{mw}p = Ae^{iwt}$$

So we guess

$$a^+ = \sqrt{\frac{mw}{2\hbar}}(x - \frac{i}{mw}p) \tag{2.3}$$

the extra factor is to make it dimensionless, see below

Check (2.3) is correct so it should agree (2.2)

$$\begin{aligned}\left[\frac{p^2}{2m} + \frac{1}{2}mw^2x^2, \sqrt{\frac{mw}{2\hbar}}x - \frac{i}{\sqrt{2mw\hbar}}p\right] &= -\frac{i\hbar}{2m}2p\sqrt{\frac{mw}{2\hbar}} + (-i)\frac{1}{2}mw^2x^2\frac{2x}{\sqrt{2mw\hbar}}i\hbar \\ &= \hbar w\{\sqrt{\frac{mw}{2\hbar}}x - \frac{i}{\sqrt{2mw\hbar}}p\}\end{aligned}$$

with $\Delta E = \hbar w$.

Lecture 7 (9/25/13)

Compute

$$\begin{aligned}[a, a^+] &= \left[\sqrt{\frac{mw}{2\hbar}}x + \frac{i}{\sqrt{2mw\hbar}}p, \sqrt{\frac{mw}{2\hbar}}x - \frac{i}{\sqrt{2mw\hbar}}p\right] \\ &= \frac{(-i)(i\hbar) + (i)(-i\hbar)}{2\hbar} = 1\end{aligned} \tag{2.4}$$

Claim

$$H = \hbar w(a^+a + \frac{1}{2}) \tag{2.5}$$

Indeed

$$\begin{aligned}\hbar w(a^+a) &= \hbar w(\sqrt{\frac{mw}{2\hbar}}x - \frac{i}{\sqrt{2mw\hbar}}p)(\sqrt{\frac{mw}{2\hbar}}x + \frac{i}{\sqrt{2mw\hbar}}p) \\ &= \frac{1}{2}mw^2x^2 + \frac{p^2}{2m} + \hbar w\frac{1}{2\hbar}i(xp - px) = H - \frac{\hbar w}{2}\end{aligned}$$

So if we consider

$$\langle\psi|H|\psi\rangle = \hbar w \left\|a\left|\psi\right\rangle\right\|^2 + \hbar w\frac{1}{2}$$

Hence energy

$$E \geq \hbar w\frac{1}{2} \tag{2.6}$$

Taking complex conjugate of (2.2) gives

$$aH - Ha = \Delta E a$$

or

$$[H, a] = -\Delta E a \tag{2.7}$$

This says if $|\psi_E\rangle$ is an eigenstate with energy E, then

$$Ha^n\left|\psi_E\right\rangle = (E - n\Delta E)a^n\left|\psi_E\right\rangle$$

Because of (2.6), for given $|\psi_E\rangle$ there is a largest value of n_0 for which

$$a^{n_0}\left|\psi_E\right\rangle$$

does not vanish.

Define

$$|0\rangle = a^{n_0}\left|\psi_E\right\rangle N$$

N normalization, and

$$a\left|0\right\rangle = 0$$

so

$$(\sqrt{\frac{mw}{2\hbar}}x + \frac{i}{\sqrt{2mw\hbar}}p)\psi_0 = (\sqrt{\frac{mw}{2\hbar}}x + \sqrt{\frac{\hbar}{2mw}}\frac{d}{dx})\psi_0 = 0$$

so

$$\psi_0(x) = ce^{-\frac{mw}{2\hbar}x^2} \quad c = \left(\frac{mw}{\hbar\pi}\right)^{\frac{1}{4}}$$

hence $|0\rangle$ is unique independent of initial $|\psi_E\rangle$.

Define

$$|n\rangle = (a^+)^n |0\rangle N_n$$

We want to find N_n.

Claim

$$\left\| (a^+)^n |0\rangle \right\|^2 = \left\langle 0 \middle| (a)^n (a^+)^n \middle| 0 \right\rangle = n!$$

Proof by induction

True when $n = 0$ for $0! = 1$

Assume true for $n - 1$

$$\begin{aligned}
\left\langle 0 \middle| (a)^n (a^+)^n \middle| 0 \right\rangle &= \left\langle 0 \middle| a^{n-1} a (a^+)^n \middle| 0 \right\rangle \\
&= \left\langle 0 \middle| a^{n-1} \left\{ [a, (a^+)^n] + (a^+)^n a \right\} \middle| 0 \right\rangle \\
&= \left\langle 0 \middle| a^{n-1} [a, (a^+)^n] \middle| 0 \right\rangle
\end{aligned}$$

Use (2.4)

$$\begin{aligned}
[a, (a^+)^n] &= [a, a^+](a^+)^{n-1} + a^+[a, (a^+)^{n-1}] \\
&= (a^+)^{n-1} + a^+[a, a^+](a^+)^{n-2} + (a^+)^2[a, (a^+)^{n-2}] \\
&= \dots \\
&= n(a^+)^{n-1}
\end{aligned}$$

so

$$\left\langle 0 \middle| (a)^n (a^+)^n \middle| 0 \right\rangle = n \left\langle 0 \middle| a^{n-1} (a^+)^{n-1} \middle| 0 \right\rangle = n(n-1)! = n!$$

Therefore

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^+)^n |0\rangle \tag{2.8}$$

defines normalized states.

Now compute

$$\begin{aligned}
\langle n\big|a^+a\big|n\rangle &= \frac{1}{n!}\left\langle 0\big|(a)^n a^+a(a^+)^n\big|0\right\rangle \\
&= \frac{1}{n!}\left\langle 0\big|(a)^n(aa^+-[a,a^+])(a^+)^n\big|0\right\rangle \\
&= \frac{1}{n!}\left\langle 0\big|(a)^{n+1}(a^+)^{n+1}\big|0\right\rangle - \langle n|n\rangle \\
&= (n+1)\langle n+1|n+1\rangle - 1 \\
&= n
\end{aligned}$$

Compare this with (2.5), we find

$$E_n = \langle n|H|n\rangle = \hbar w(n+\frac{1}{2})$$

Note surprising that $E_0 \neq 0$. Because if it were 0, then particle would be sitting at the minimal potential, so $x = 0$ not allowed by uncertainty principle.

Does (2.8) give all energy states?

Suppose we have

$$H|\psi_E\rangle = E|\psi_E\rangle$$

Does $|\psi_E\rangle = |n\rangle$ for some n?

We know from before there exists some m

$$a^m|\psi_E\rangle = N|0\rangle \tag{2.9}$$

Since $a^+a = aa^+ - 1$,

$$\begin{aligned}
a^+a^m &= (aa^+-1)a^{m-1} \\
&= a(aa^+-1)a^{m-2} - a^{m-1} \\
&= a^2(aa^+-1)a^{m-3} - 2a^{m-1} \\
&\dots \\
&= a^{m-1}a^+a - (m-1)a^{m-1} \\
&= a^{m-1}\left(\frac{H}{\hbar w} - \frac{1}{2}\right) - (m-1)a^{m-1}
\end{aligned}$$

Apply a^+ to (2.9),

$$LHS = a^{m-1}\left|\psi_E\right\rangle\left(\frac{E}{\hbar w} - \frac{1}{2} - m + 1\right)$$

$$RHS = a^+ N\left|0\right\rangle$$

If we keep applying a^+ m times,

$$(a^+)^m N\left|0\right\rangle = \left|\psi_E\right\rangle$$

hence

$$\left|\psi_E\right\rangle = \left|m\right\rangle$$

What does $\left|n\right\rangle$ look like?

$$\begin{aligned}
\langle x|n\rangle &= \frac{1}{\sqrt{n!}}\left\langle x\middle|(a^+)^n\middle|0\right\rangle \\
&= \frac{1}{\sqrt{n!}}\left(\sqrt{\frac{mw}{2\hbar}}x - \frac{\hbar}{\sqrt{2mw\hbar}}\frac{d}{dx}\right)^n e^{-\frac{mw}{2\hbar}x^2}\left(\frac{mw}{\hbar\pi}\right)^{\frac{1}{4}}
\end{aligned}$$

Let $z = \sqrt{\frac{mw}{\hbar}}x$

$$\langle x|n\rangle = \frac{1}{\sqrt{n!}}\frac{1}{2^n}(z - \frac{d}{dz})^n e^{-\frac{1}{2}z^2}\left(\frac{mw}{\hbar\pi}\right)^{\frac{1}{4}}$$

Since

$$e^{z^2/2}\left(-\frac{\partial}{\partial z}\right)e^{-z^2/2}\psi(z) = (z - \frac{\partial}{\partial z})\psi(z)$$

$$e^{z^2/2}\left(-\frac{\partial}{\partial z}\right)^n e^{-z^2/2} = (z - \frac{\partial}{\partial z})^n$$

Thus

$$\begin{aligned}
\langle x|n\rangle &= \frac{1}{\sqrt{n!}}\frac{1}{2^n}\left(\frac{mw}{\hbar\pi}\right)^{\frac{1}{4}} e^{z^2/2}\left(-\frac{\partial}{\partial z}\right)^n e^{-z^2} \\
&= \frac{1}{\sqrt{n!}}\frac{1}{2^n}\left(\frac{mw}{\hbar\pi}\right)^{\frac{1}{4}} e^{-z^2/2}\underbrace{e^{z^2}\left(-\frac{\partial}{\partial z}\right)^n e^{-z^2}}_{\equiv h_n(z)}
\end{aligned}$$

where $h_n(z)$ Hermite polynomials.

$$\begin{aligned}
h_0(z) &= 1 \\
h_1(z) &= 2z \\
h_2(z) &= 4z^2 - 2
\end{aligned}$$

One interesting property

$$h_n(-z) = (-1)^n h_n(z)$$

Hence h_n is odd (even) function if n is odd (even).

Another property about Hermite.

$$\sum_{n=0}^{\infty} s^n \frac{1}{n!} h_n(z) = e^{-s^2+2sz} \tag{2.10}$$

e^{-s^2+2sz} is called generating function for Hermite polynomials.

Proof of (2.10)

$$LHS = \sum_{n=0}^{\infty} s^n \frac{1}{n!} e^{z^2}\left(-\frac{\partial}{\partial z}\right)^n e^{-z^2} = e^{z^2} e^{-(z-s)^2}$$

2.2 Coherent States

For $E \gg \hbar w$ ($n \gg 1$),

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

looks roughly continuous as we expect from classical mechanics, however ψ_n ($n \gg 1$) doesn't look like classically at all. ψ_n has many many oscillations.

The classical behavior for the SHO is easily seen by examining coherent state $|A\rangle$, which are eigenvectors of lowing operator

$$a\,|A\rangle = A\,|A\rangle$$

Since a is not hermitian, A is complex, $A = |A|e^{i\phi}$.

If we look at

$$\bar{x} = \langle A|x|A\rangle = \left\langle A\middle|\sqrt{\frac{\hbar}{2mw}}(a+a^+)\middle|A\right\rangle = \sqrt{\frac{\hbar}{2mw}}(A+A^*) = \sqrt{\frac{2\hbar}{mw}}|A|\cos\phi = R\cos\phi$$

$$\bar{p} = \langle A|p|A\rangle = \left\langle A\middle|\sqrt{2mw\hbar}\frac{1}{2i}(a-a^+)\middle|A\right\rangle = \sqrt{2mw\hbar}|A|\sin\phi = mwR\sin\phi$$

put $R = \sqrt{\frac{2\hbar}{mw}}|A|$.

Lecture 8 (9/30/13)

Since $|A\rangle$ is not stationary state, it is interesting to see how it evolves.

By (2.7)

$$\begin{aligned} ae^{-iHt/\hbar}\,|A\rangle &= e^{-iwt}e^{-iHt/\hbar}a\,|A\rangle \\ &= Ae^{-iwt}e^{-iHt/\hbar}\,|A\rangle \end{aligned}$$

Hence $e^{-iHt/\hbar}\,|A\rangle$ is eigenvector with eigenvalue Ae^{-iwt}.

Denote

$$\left|Ae^{-iwt}\right\rangle = e^{-iHt/\hbar}\,|A\rangle$$

Then like last time and now $\phi \to \phi - wt$

$$\bar{x}(t) = \left\langle Ae^{-iwt}\middle|x\middle|Ae^{-iwt}\right\rangle = R\cos(\phi - wt) \tag{2.11}$$

$$\bar{p}(t) = \left\langle Ae^{-iwt}\middle|p\middle|Ae^{-iwt}\right\rangle = mwR\sin(\phi - wt) = m\dot{\bar{x}} \tag{2.12}$$

As $|A\rangle$ evolves its expectation appears to be classical.

What does $|A\rangle$ look like?

$$\left(\sqrt{\frac{mw}{2\hbar}}x + \frac{\hbar}{\sqrt{2mw\hbar}}\frac{d}{dx}\right)\psi_A(x) = A\psi_A(x)$$

That is

$$\frac{d}{dx}\psi_A(x) = -\frac{mw}{\hbar}(x - A\sqrt{\frac{2\hbar}{mw}})\psi_A(x)$$

so

$$\psi_A(x) = Ne^{-\frac{1}{2}\frac{mw}{\hbar}(x-A\sqrt{\frac{2\hbar}{mw}})^2}$$

Combining with (2.11), (2.12), we see that ψ_A evolves as a Gaussian wave stay the same shape and oscillates back and forth.

Finally we can express $|A\rangle$ in energy eigenstates

$$|A\rangle = \sum_{n=0}^{\infty} c_n |n\rangle$$

$$a|A\rangle = A|A\rangle = \sum_{n=0}^{\infty} c_n a|n\rangle = \sum_{n=0}^{\infty} c_n\sqrt{n}\,|n-1\rangle$$

Since $|n\rangle$ are orthogonal,

$$c_n A = c_{n+1}\sqrt{n+1}$$

so

$$c_n = \frac{A^n}{\sqrt{n!}}c_0$$

so

$$|A\rangle = \sum_{n=0}^{\infty}\frac{A^n}{\sqrt{n!}}c_0|n\rangle$$

Find c_0

$$1 = \langle A|A\rangle = |c_0|^2\sum_{n=0}^{\infty}\frac{|A|^{2n}}{n!} = |c_0|^2 e^{|A|^2} \implies c_0 = e^{-|A|^2/2}$$

Hence

$$|A\rangle = \sum_{n=0}^{\infty}\frac{A^n}{n!}(a^+)^n|0\rangle\, e^{-|A|^2/2}$$

2.3 WKB

The next topic is semiclassical limit of Schrodinger wave mechanics and WKB approximation. Its assumptions are $\hbar$ very small, so is $\lambda = h/p$ very small compared to the scale over which $V(x)$ varies. More precisely

$$\frac{\partial V}{\partial x} \cdot \lambda \ll E - V(x)$$

Intuitively that is because $H(p,x)\psi = E\psi$ in which $p = \frac{\hbar}{i}\frac{\partial}{\partial x}$, since $\hbar$ is very small, to have contribution of $\partial/\partial x$, we need rapidly oscillating ψ, i.e. small λ. The analogous thing happens in geometric optic where light is treated as classical ray as long as the wave length is small compared to the shape of the apparatus.

Now suppose

$$\psi_E(x) = e^{\pm \frac{i}{\hbar}\int^x \sqrt{2m(E-V(x'))}dx'} \tag{2.13}$$

solves the 1 dimensional time independent Schrodinger equation, we obtain

$$-\frac{d^2}{dx^2}\psi_E = \frac{2m(E-V(x))}{\hbar^2}\psi_E + O(\frac{1}{\hbar})$$

with the leading order term in $1/\hbar^2$, showing (2.13) is the leading approximate solution.

We can do better than (2.13), try

$$\psi_E(x) = e^{\frac{i}{\hbar}S_E(x)}$$

where $S_E(x) = S^{(0)}(x) + \hbar S^{(1)}(x) + \hbar^2 S^{(2)}(x)$, then plug into time independent Schrodinger equation, the $1/\hbar^2$ order gives

$$-\frac{\hbar^2}{2m}(\frac{i}{\hbar}\frac{\partial S^{(0)}}{\partial x})^2\psi_E + V(x)\psi_E = E\psi_E$$

so

$$\frac{\partial S^{(0)}}{\partial x} = \pm\sqrt{2m(E-V(x))} \implies S^{(0)}(x) = \int_{x_0}^{x} \sqrt{2m(E-V(x'))}dx'$$

The $1/\hbar$ order

$$-\frac{\hbar^2}{2m}\left[\frac{\partial}{\partial x}\frac{i}{\hbar}\frac{\partial S^{(0)}}{\partial x}+2\frac{\partial S^{(0)}}{\partial x}\frac{\partial S^{(1)}}{\partial x}\frac{i^2}{\hbar}\right]\psi_E=0$$

so

$$\frac{\partial S^{(1)}}{\partial x}=\frac{i}{2}\frac{\partial^2 S^{(0)}}{\partial x^2}\frac{1}{\frac{\partial S^{(0)}}{\partial x}}=\frac{i}{2}\frac{\partial}{\partial x}\ln\frac{\partial S^{(0)}}{\partial x}$$

Therefore

$$\begin{aligned}\psi_E(x) &= e^{\pm\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V(x'))}dx'}e^{i\frac{i}{2}\ln\frac{\partial S^{(0)}}{\partial x}}\\ &= \frac{1}{(2m(E-V(x)))^{1/4}}e^{\pm\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V(x'))}dx'}\end{aligned}\tag{2.14}$$

Compare this to (2.13), we get an additional factor which, as we will see, makes probability current conserved. Suppose $E>V$ and V is increasing then as the wave enter high potential region

$$p=\sqrt{2m(E-V(x'))}$$

deceases. $\lambda\uparrow$ and amplitude $\downarrow$.

Recall probability density $\rho(x)=\psi^*(x)\psi(x)$ and probability current $\vec{j}(x)=\frac{\hbar}{2mi}[\psi^*\nabla\psi-\psi\nabla\psi^*]$, where $\psi=\psi_E e^{-iEt/\hbar}$, so for (2.14) to the leading $1/\hbar$ order

$$\vec{j}(x)\sim\frac{d}{dx}(\psi^*\frac{d\psi}{dx}-\frac{d\psi^*}{dx}\psi)\sim\frac{d}{dx}(\frac{1}{\sqrt{2m(E-V(x))}}2\sqrt{2m(E-V(x))})=0$$

Here we have assume $E>V$, for $E<V$ at turning points we will get imaginary p.

Lecture 9 (10/2/13)

Plane wave WKB solutions are not so interesting. We can form wave package to reproduce classical behaviors. Suppose $C(E)$ is a real slowly varying function but sharply peaked at $E=E_0$, then we evaluate the time evolution wave function

$$\psi(x,t)=\int dE C(E)\frac{1}{(2m(E-V(x)))^{1/4}}e^{\frac{i}{\hbar}\int_{x_0}^{x}\sqrt{2m(E-V(x'))}dx'}e^{-iEt/\hbar}$$

(taking only + for right moving solution)

By stationary phase approximation, $\psi(x,t)$ is largest for $x = x(t)$ such that

$$\frac{d}{dE}[\int_{x_0}^{x} p_E(x')dx' - Et] = 0$$

or

$$t = \int_{x_0}^{x} \frac{dx'}{p/2m} = \int_{x_0}^{x} \frac{dx'}{v'}$$

this agrees classical behavior with the choice $x(t_0) = x_0$.

Remark: there is a N dimensional version of WKB,

$$H(p_1, .., p_N, q_1, ..., q_N)\psi_E(q_1, ..., q_N) = E\psi_E(q_1, ..., q_N) \tag{2.15}$$

$$\psi(q_1, ..., q_N) = e^{\frac{i}{\hbar}S(q_1,...,q_N)} \tag{2.16}$$

but no one knows how to deal with turning points for N variable WKB.

Substitute (2.16) in (2.15) since $p_i = \frac{\hbar}{i}\frac{\partial}{\partial q_i}$,

$$H(\frac{\partial S}{\partial q_1}, ..., \frac{\partial S}{\partial q_N}, q_1, ..., q_N)e^{\frac{i}{\hbar}S} = Ee^{\frac{i}{\hbar}S}$$

or

$$H(\frac{\partial S}{\partial q_1}, ..., \frac{\partial S}{\partial q_N}, q_1, ..., q_N) = E \tag{2.17}$$

This is called the Hamilton-Jacobin equation and S is the Hamilton characteristic function. Byproduct we showed

$$p_i = \frac{\partial S}{\partial q_i} \tag{2.18}$$

One can solve (2.17) for $S(q_1, ..., q_N, \alpha_1, ..., \alpha_N)$ where S depends on $N + 1$ integration constants which can be reduced to N if we ignore an additive constant to E, and say E is uniquely determined by $\alpha_1, ..., \alpha_N$ too.

Construct the wave packets

$$\psi(q_1, ..., q_N) = \prod_{i=1}^{N} \int d\alpha_i C(\alpha_1, ..., \alpha_N)e^{\frac{i}{\hbar}S(q_1,...,q_N,\alpha_1,...,\alpha_N)}e^{-\frac{i}{\hbar}E(\alpha_1,...,\alpha_N)t}$$

again C is sharply peaked about $\bar{\alpha}_1, ..., \bar{\alpha}_N$. Apply stationary phase approximation, obtain

$$\frac{\partial S(q_1,...,q_N,\bar{\alpha}_1,...,\bar{\alpha}_N)}{\partial \alpha_i} - \frac{\partial E(\bar{\alpha}_1,...,\bar{\alpha}_N)}{\partial \alpha_i} t = 0 \tag{2.19}$$

for $i = 1,...,N$ which should determine $q_1(t),...,q_N(t)$ which should in fact obey Hamilton equations. Indeed differentiate (2.19) with respect to t

$$\sum_{j=1}^{N} \frac{\partial^2 S}{\partial q_j \partial \alpha_i} \frac{\partial q_j}{\partial t} - \frac{\partial E}{\partial \alpha_i} = 0$$

Differentiate (2.17) with respect to α_i

$$\sum_{j=1}^{N} \frac{\partial H}{\partial p_j} \frac{\partial^2 S}{\partial q_j \partial \alpha_i} = \frac{\partial E}{\partial \alpha_i}$$

Combining two above

$$\sum_{j=1}^{N} \frac{\partial^2 S}{\partial q_j \partial \alpha_i} \left(\frac{\partial q_j}{\partial t} - \frac{\partial H}{\partial p_j} \right) = 0$$

If the matrix $\frac{\partial^2 S}{\partial q_j \partial \alpha_i}$ is invertible, then

$$\frac{\partial q_j}{\partial t} - \frac{\partial H}{\partial p_j} = 0$$

or

$$\dot{q}_j = \frac{\partial H}{\partial p_j}$$

this gives one of the two Hamiltonian equations. Differentiate (2.17) with respect to q_i,

$$\sum_j \frac{\partial H}{\partial p_j} \frac{\partial^2 S}{\partial q_j \partial q_i} + \frac{\partial H}{\partial q_i} = 0$$

and by (2.18),

$$\dot{p}_j = \sum_{k=1}^{N} \frac{\partial^2 S}{\partial q_j \partial q_k} \frac{\partial q_k}{\partial t} = \sum_{k=1}^{N} \frac{\partial^2 S}{\partial q_j \partial q_k} \frac{\partial H}{\partial p_k} = -\frac{\partial H}{\partial q_i}$$

2.4 Connecting Formulas

We will only do 1D WKB. Suppose $V(x)$ is increasing and $E = V(0)$, hence in $x < 0$, region I, $V(x) < E$; while in $x > 0$, region II, $V(x) > E$. The reason we get singularity of the WKB solution is purely the breakdown of our approximation; there is nothing peculiar to the physical nature of the wave near the turning point, nor any non analyticity to the Schrodinger equation.

Region I:

$$\psi(x) = \frac{A}{\sqrt{p_E(x)}} e^{\frac{i}{\hbar}\int_x^0 p_E(x')dx'} + \frac{B}{\sqrt{p_E(x)}} e^{-\frac{i}{\hbar}\int_x^0 p_E(x')dx'}$$

Region II:

$$\psi(x) = \frac{A'}{\sqrt{|p_E(x)|}} e^{\frac{1}{\hbar}\int_0^x |p_E(x')|dx'} + \frac{B}{\sqrt{|p_E(x)|}} e^{-\frac{1}{\hbar}\int_0^x |p_E(x')|dx'}$$

We want to find a relation between A, B and A', B'. Two ways to do this

Way 1: Airy Functions

The smaller the $\hbar$ is in comparison to the scale of the problem, the better the leading $1/\hbar^2$ term is, so (2.13) suffice no need to get to (2.14) so no trouble get to $p \to 0$. This means λ is very small and $V'(x)$ is not too small, so we assume WKB solutions extends into the region where

$$V \approx E + V'(0)x \tag{2.20}$$

is valid. Then we solve

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E}{dx^2} + V'(0)x\psi_E(x) = 0$$

gives Airy equations with solution that are Bessel function of order 1/3

$$\psi = aJ_{1/3} + bJ_{-1/3}$$

then use asymptotic behavior. The situation is ambiguous if both A, B or both A', B' are presented.

Way 2: Analytic Continuation

Lecture 10 (10/7/13)

In region near 0 where (2.20) is valid,

$$|p(x)| = \sqrt{2mV'(0)}|x|^{1/2}$$

so in region II

$$\psi(x) \sim \frac{1}{|x|^{1/4}} e^{\pm\frac{1}{\hbar}\sqrt{2mV'(0)}\frac{2}{3}|x|^{3/2}}$$

Let $z^{3/2} = \sqrt{2mV'(0)}\frac{2}{3\hbar}x^{3/2}$, so in region II

$$\psi(z) \sim \frac{A'}{|z|^{1/4}} e^{|z|^{3/2}} + \frac{B'}{|z|^{1/4}} e^{-|z|^{3/2}}$$

Similarly in region I

$$\psi(z) \sim \frac{A}{z^{1/4}} e^{iz^{3/2}} + \frac{B}{z^{1/4}} e^{-iz^{3/2}}$$

Here again the situation is ambiguous if both A, B or both A', B' are presented. Before it was due to ambiguity in asymptotic behavior; now the ambiguity is due to multivalued in complex contour (known as the Stokes' phenomenon). Let us assume B' is given and A' is 0.

Let $\phi = \arg z$, consider counterclockwise move z from $\phi : 0 \to \pi$, then

$$z^{3/2} = |z|^{3/2} e^{i\frac{3}{2}\phi} : |z|^{3/2} \to -i|z|^{3/2} \tag{2.21}$$

and

$$z^{1/4} = |z|^{1/4} e^{i\frac{1}{4}\phi} : |z|^{1/4} \to |z|^{1/4} e^{i\frac{\pi}{4}} \tag{2.22}$$

Cleverly we move z from $z > 0$, region II to $z < 0$, region I without passing $z = 0$ so (2.22) doesn't blow up. There seems to be a problem in (2.21).

$$z^{3/2} = |z|^{3/2}(\cos\frac{3}{2}\phi + i\sin\frac{3}{2}\phi)$$

When $2\pi/3 > \phi > \pi/2$, $\cos\phi < 0$, so $e^{-z^{3/2}}$ grows exponentially for $|z|$ large. But that is fine after $\phi > 2\pi/3$. The actual problem is multivalued in (2.21), so we need a branch cut say $z < 0$ axis. Then moving counterclockwise from $\phi : 0 \to \pi$ is not the same as moving clockwise from $\phi : 0 \to -\pi$. Indeed counterclockwise gives

$$\frac{e^{-z^{3/2}}}{z^{1/4}} \to \frac{e^{i|z|^{3/2}}}{|z|^{1/4}e^{i\pi/4}}$$

clockwise gives

$$\frac{e^{-z^{3/2}}}{z^{1/4}} \to \frac{e^{-i|z|^{3/2}}}{|z|^{1/4}e^{-i\pi/4}}$$

Adding the two and use $e^{-i\pi/4} = e^{i\pi/4}/i$, $e^{i\pi/4} = -e^{-i\pi/4}/i$, we get

$$\frac{e^{-z^{3/2}}}{z^{1/4}} \to \frac{2\sin\left(|z|^{3/2} + \frac{\pi}{4}\right)}{|z|^{1/4}}$$

Or

$$\frac{e^{-\frac{1}{\hbar}\int_0^x |p(x')|dx'}}{\sqrt{|p(x)|}} \to \frac{2\sin\left(\frac{1}{\hbar}\int_x^0 p(x')dx' + \frac{\pi}{4}\right)}{\sqrt{p(x)}}$$

Similar we can show the second connection formula which is orthogonal to the 1st,

$$\frac{\sin\left(\frac{1}{\hbar}\int_x^0 p(x')dx' + \frac{\pi}{4}\right)}{\sqrt{p(x)}} \to \frac{e^{\frac{1}{\hbar}\int_0^x |p(x')|dx'}}{\sqrt{|p(x)|}}$$

Example. Suppose $V(x)$ has two turning points $x_1 < x_2$, find bound state energy.

First assuming exponential decay in $x > x_2$

$$\psi = \frac{1}{|p(x)|^{1/2}} e^{\frac{1}{\hbar}\int_{x_2}^x |p(x')|dx'} \to \frac{2\sin\left(\frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}\right)}{\sqrt{p(x)}}$$

Also assume exponential increase in $x < x_1$

$$\psi = \frac{1}{|p(x)|^{1/2}} e^{-\frac{1}{\hbar}\int_x^{x_1} |p(x')|dx'} \to \frac{2\sin\left(\frac{1}{\hbar}\int_{x_1}^x p(x')dx' + \frac{\pi}{4}\right)}{\sqrt{p(x)}}$$

Hence in $x_1 < x < x_2$ region

$$\sin\left(\frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}\right) = \pm\sin\left(\frac{1}{\hbar}\int_{x_1}^{x} p(x')dx' + \frac{\pi}{4}\right)$$

The $\pm$ sign has two reasons: 1) both left and right are real functions, so if they are off by a phase, that phase must be ± 1; 2) $\pm$ will give odd/even solutions.

Then

$$RHS = \sin\left(\xi - \left(\frac{1}{\hbar}\int_x^{x_2} p(x')dx' + \frac{\pi}{4}\right)\right)$$

where $\xi = \frac{1}{\hbar}\int_{x_1}^{x_2} p(x')dx' + \frac{\pi}{2}$. So

$$\xi = n\pi$$

or

$$\oint p(x')dx' = 2\pi\hbar(n + \frac{1}{2})$$

$\oint$ means integrate the full cycle, e.g. $x_1 \to x_2 \to x_1$. This is called Bohr quantization. We will revisit WKB when we study α decay.

2.5 Angular Momentum and Rotation

We all know rotations belong to group $O(3)$. In general a group $\mathcal{G}$, has the following

1. $g, g' \in \mathcal{G}$, so is $g \cdot g' \in \mathcal{G}$
2. $g(g'g'') = (gg')g''$
3. Exists $e \in \mathcal{G}$ such that $ge = eg = g$
4. for $g \in \mathcal{G}$, $\exists\ g^{-1} \in \mathcal{G}$ such that $gg^{-1} = g^{-1}g = e$.

For quantum mechanics, we expect to each element of $g \in \mathcal{G}$ there should be a linear unitary transformation $G(g)$ that carries out the transformation on our states

$$|\psi\rangle \to G(g)\,|\psi\rangle$$

For rotation $\mathcal{G} = O(3)$, but the same setup can be used to describe other symmetry transformation as well.

Lecture 11 (10/9/13)

$O(3) = 3 \times 3$ orthogonal matrices, i.e.

$$O^T O = I = \begin{pmatrix} 1 & 0 & 0 \\ & 1 & 0 \\ & & 1 \end{pmatrix} \tag{2.23}$$

then $(\det O)^2 = \det O \det O^T = 1 \implies \det O = \pm 1$. (2.23) restricts 6 equations for nine elements of $O(3)$. Think this as 9 elements on the hyper surface, it has 2 continuous components. If require $\det O = 1$, we get $SO(3)$, so purely rotation no reflection.

Rotation of vector $\vec{r}$,

$$r_i \to SO_{ij}(g) r_j$$

Another way to characterize rotation is to parametrize it by a direction $\hat{n}$ and an angle $0 \leq \theta \leq \pi$,

$$\theta \hat{n}$$

if $\theta = 0$ identity.

We can identify $\theta \hat{n}$ to be a vector from the origin pointing in $\hat{n}$ direction with magnitude θ, then we can associate

$$SO(3) \leftrightarrow \text{solid sphere of radius } \pi/\text{antipodes pt}$$

The reason to module antipodes is because

$$\pi \hat{n} = -\pi \hat{n}$$

If one walks on the surface of the solid sphere of radius π ball from one point to its antipodes and perform serial of rotations, one should see the end results of the serial of rotations rotate the object by 2π. But we claim this is not I from the view of higher dimensional geometry. If the person walks on the surface of the solid sphere of radius π ball from one point to the starting point and perform serial of rotations, he should see the end results of the serial of rotations rotate the object by 4π, which is I.

Take a square shaped object and attach four strings to the corners. If the square is rotated through 2π, the bands will become entangled and it can be shown that there is no way by stretching or looping to disentangled the strings. However if we rotate the square through 4π, the bands can be disentangled without moving the square. From a more geometric view the 2π path is not homotopic a point while the 4π path is.

More should be true $R(\hat{e}_i, \theta)$

$$R(\hat{e}_i, \theta_1)R(\hat{e}_i, \theta_2) = R(\hat{e}_i, \theta_1 + \theta_2) \tag{2.24}$$

then

$$R(\hat{e}_i, \theta)R(\hat{e}_i, \theta)^T = I$$

take derivative

$$\frac{dR(\hat{e}_i, \theta)}{d\theta}R(\hat{e}_i, \theta)^T + R(\hat{e}_i, \theta)\frac{dR(\hat{e}_i, \theta)^T}{d\theta} = 0$$

put $\theta = 0$

$$\frac{dR(\hat{e}_i, \theta)}{d\theta} + \frac{dR(\hat{e}_i, \theta)^T}{d\theta} = 0$$

Hence we let

$$\left.\frac{dR(\hat{e}_i, \theta)}{d\theta}\right|_{\theta=0} = -\frac{i}{\hbar}J_i$$

We will show J_i is the hermitian generator of rotation in the ith direction.

Shift $\theta \to \theta + \theta_0$

$$\left.\frac{dR(\hat{e}_i, \theta + \theta_0)}{d\theta}\right|_{\theta=0} = \left.\frac{dR(\hat{e}_i, \theta)}{d\theta}\right|_{\theta=0} R(\hat{e}_i, \theta_0)$$

Or

$$\left.\frac{dR(\hat{e}_i, \theta)}{d\theta}\right|_{\theta=\theta_0} = -\frac{i}{\hbar}J_i R(\hat{e}_i, \theta_0)$$

so

$$R(\hat{e}_i, \theta) = e^{-iJ_i\theta/\hbar}$$

This turns out to be the easiest way to represent rotation, much easier than Euler angles.

Claim

$$R(\hat{n}, \theta) = e^{-i\vec{J}\cdot\hat{n}\theta/\hbar} \tag{2.25}$$

Because of (2.24), it is enough to show

$$R(\hat{n}, \delta\theta) = I - i\vec{J} \cdot \hat{n}\theta/\hbar + O(\delta\theta^2)$$

How does a vector $\vec{v} = (v_1, v_2, v_3)$ transform under a rotation about $\hat{n}$ through $\delta\theta$?

$$\begin{aligned}
\vec{v} &\rightarrow \vec{v} + \delta\theta\hat{n} \times \vec{v} + O(\delta\theta^2) &(2.26)\\
&= \vec{v} + \delta\theta n_1\hat{e}_1 \times \vec{v} + \delta\theta n_2\hat{e}_2 \times \vec{v} + \delta\theta n_3\hat{e}_3 \times \vec{v} + O(\delta\theta^2)\\
&= (1 + \delta\theta n_1\hat{e}_1\times)(1 + \delta\theta n_2\hat{e}_2\times)(1 + \delta\theta n_3\hat{e}_3\times)\vec{v} + O(\delta\theta^2)
\end{aligned}$$

So

$$\begin{aligned}
R(\hat{n}, \delta\theta) &= R(\hat{e}_1, n_1\delta\theta)R(\hat{e}_2, n_2\delta\theta)R(\hat{e}_3, n_3\delta\theta) + O(\delta\theta^2)\\
&= (1 - iJ_1n_1\delta\theta/\hbar)(1 - iJ_2n_2\delta\theta/\hbar)(1 - iJ_3n_3\delta\theta/\hbar)
\end{aligned}$$

The above multiplication is in Hilbert space.

Finally

$$R(\hat{n}, \delta\theta) = I - i\frac{\delta\theta}{\hbar}(J_1n_1 + J_2n_2 + J_3n_3) = I - i\frac{\delta\theta}{\hbar}\vec{J} \cdot \hat{n}$$

What makes rotation special is its commutation relation. Clearly

$$R(\hat{n}, \theta)R(\hat{n}', \delta\theta')R(\hat{n}, \theta)^{-1} \approx I$$

So we extrapolate that

$$R(\hat{n}, \theta)(1 - i\frac{\delta\theta'}{\hbar}\hat{n}' \cdot \vec{J})R(\hat{n}, \theta)^{-1} = I - i\frac{\delta\theta'}{\hbar}\sum_{ij} J_iM_{ij}(\hat{n}, \theta)n'_j \qquad (2.27)$$

This has to be the case because LHS is linear in $i\frac{\delta\theta'}{\hbar}$. So

$$R(\hat{n}, \theta)J_jR(\hat{n}, \theta)^{-1} = \sum_i J_iM_{ij}(\hat{n}, \theta)$$

Now let $\theta \to \delta\theta$, the LHS of (2.27) becomes

$$(1 - i\frac{\delta\theta}{\hbar}\hat{n}\cdot\vec{J})(1 - i\frac{\delta\theta'}{\hbar}\hat{n}'\cdot\vec{J})(1 + i\frac{\delta\theta}{\hbar}\hat{n}\cdot\vec{J}) \tag{2.28}$$

From idea of (2.26), suppose $\delta\theta \not\sim \delta\theta'$, otherwise they cancel, not good

$$\begin{aligned}
(1+\delta\theta\hat{n}\times)(1+\delta\theta'\hat{n}'\times)(1-\delta\theta\hat{n}\times)\vec{v} &= \vec{v} + \delta\theta'\left\{\hat{n}'\times\vec{v} + \delta\theta[\hat{n}\times(\hat{n}'\times\vec{v})] - \delta\theta[\hat{n}'\times(\hat{n}\times\vec{v})]\right\} \\
&= \vec{v} + \delta\theta'\left\{\hat{n}'\times\vec{v} + \delta\theta[\hat{n}'(\hat{n}\cdot\vec{v}) - \hat{n}(\hat{n}'\cdot\vec{v})]\right\} \\
&= \vec{v} + \delta\theta'\left\{\hat{n}'\times\vec{v} + \delta\theta[(\hat{n}\times\hat{n}')\times\vec{v}]\right\} \\
&= R(\hat{n}' + \delta\theta(\hat{n}\times\hat{n}'), \delta\theta')\vec{v}
\end{aligned}$$

Hence (2.28) is equal to

$$I - i\frac{\delta\theta'}{\hbar}[\hat{n}' + \delta\theta(\hat{n}\times\hat{n}')]\cdot\vec{J} = I - i\frac{\delta\theta'}{\hbar}\vec{J}\cdot\hat{n}' - \frac{1}{\hbar^2}\delta\theta\delta\theta'[\vec{J}\cdot\hat{n}, \vec{J}\cdot\hat{n}']$$

where

$$[\vec{J}\cdot\hat{n}, \vec{J}\cdot\hat{n}'] = i\hbar(\hat{n}\times\hat{n}')\cdot\vec{J}$$

If $\hat{n} = \hat{e}_i$, $\hat{n}' = \hat{e}_j$, above says

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k \tag{2.29}$$

Lecture 12 (10/14/13)

We will soon make connection between generator of rotation with the classical quantity of angular momentum. From (2.29) it is possible to figure the matrix form of $\vec{J}$.

First try $\infty\times\infty$ matrix (later do spin, matrix will be finite)

Define J^2 to be

$$J^2 = J_1^2 + J_2^2 + J_3^2 \tag{2.30}$$

check

$$[J_i, J^2] = 0$$

Conventionally we choose to work with eigenstates of J^2 and J_z, $|j,m\rangle$ s.t.

$$\langle j', m'|j, m\rangle = \delta_{j'j}\delta_{m'm}$$

and

$$\begin{aligned} J^2 \left|j,m\right\rangle &= \hbar^2 j(j+1) \left|j,m\right\rangle \\ J_z \left|j,m\right\rangle &= \hbar m \left|j,m\right\rangle \end{aligned}$$

Consider $J_x \pm iJ_y$, check

$$[J^2, J_x \pm iJ_y] = 0$$

By (2.29)

$$[J_z, J_x \pm iJ_y] = i\hbar J_y \pm i(-i\hbar J_x) = \pm\hbar(J_x \pm iJ_y)$$

Hence $J_x \pm iJ_y$ are raising/lowing operators

$$(J_x \pm iJ_y) \left|j,m\right\rangle = N^{\pm}_{j,m} \left|j,m\pm 1\right\rangle \tag{2.31}$$

Find normalization $N^{\pm}_{j,m}$, apply $\langle j, m \pm 1|$

$$\begin{aligned} N^{\pm}_{j,m} &= \langle j, m\pm 1|J_x \pm iJ_y|j,m\rangle \\ &= \frac{1}{N^{\pm *}_{j,m}} \langle j,m|(J_x \mp iJ_y)(J_x \pm iJ_y)|j,m\rangle \end{aligned}$$

$$\begin{aligned} \left|N^{\pm}_{j,m}\right|^2 &= \left\langle j,m\middle|J_x^2 + J_y^2 \pm i[J_x, J_y]\middle|j,m\right\rangle \\ &= \left\langle j,m\middle|J^2 - J_z^2 \mp \hbar J_z\middle|j,m\right\rangle \\ &= \hbar^2 j(j+1) - \hbar^2 m^2 \mp \hbar^2 m \end{aligned}$$

Choose $N^{\pm}_{j,m}$ be real positive (Condon-Shortley phase conventions)

$$N^{\pm}_{j,m} = \hbar\sqrt{(j\mp m)(j\pm m+1)}$$

Indeed inside the square root is always non negative because of (2.30)

$$\hbar^2 j(j+1) \geq \hbar m^2 \implies |m| \leq j \tag{2.32}$$

By definition of quantum numbers $|j,m\rangle$, the states $m=\pm j$ exists, then by (2.32), $2j$ must be an integer, or $j=$ half integer.

Total number of states: $2j+1$

$$J_z = \hbar \begin{pmatrix} j & & & \\ & j-1 & & \\ & & \ddots & \\ & & & -j \end{pmatrix} \tag{2.33}$$

One can show

$$J_x + iJ_y = \begin{pmatrix} & \sqrt{(j-(j-1))(j+(j-1)+1)} & & \\ & & \sqrt{(j-(j-2))(j+(j-2)+1)} & \\ & & & \ddots \\ & & & \end{pmatrix} \tag{2.34}$$

Now back to (2.25), cannot change j

$$e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}|j,m\rangle = \sum_{m=-j}^{j} \mathcal{D}^{(j)}_{m',m}(\hat{n},\theta)|j,m'\rangle \tag{2.35}$$

where $\mathcal{D}^{(j)}_{m',m}(\hat{n},\theta)$ is $(2j+1)\times(2j+1)$ matrix, the subindices m',m in $\mathcal{D}$ are arranged so that it agrees matrix multiplication

$$\begin{aligned} e^{-i\vec{J}\cdot\hat{n}'\theta'/\hbar}e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}|j,m\rangle &= \sum_{m'=-j}^{j} e^{-i\vec{J}\cdot\hat{n}'\theta'/\hbar}\mathcal{D}^{(j)}_{m',m}(\hat{n},\theta)|j,m'\rangle \\ &= \sum_{m'',m'} \mathcal{D}^{(j)}_{m'',m'}(\hat{n}',\theta')\mathcal{D}^{(j)}_{m',m}(\hat{n},\theta)|j,m''\rangle \end{aligned}$$

2.6 Pauli Matrices

The case $j=1$, $2j+1=3$ describes the normal rotation of vectors.

Consider $j=\frac{1}{2}$, there are two basis states

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle, \ \left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

$$J_z = \hbar \begin{pmatrix} \frac{1}{2} & \\ & -\frac{1}{2} \end{pmatrix}$$

J_z acts on vector $\begin{pmatrix} a_{\frac{1}{2}} \\ a_{-\frac{1}{2}} \end{pmatrix}$ which are coefficients of

$$\psi = a_{\frac{1}{2}} \left| \frac{1}{2}, \frac{1}{2} \right\rangle + a_{-\frac{1}{2}} \left| \frac{1}{2}, -\frac{1}{2} \right\rangle$$

Similarly

$$J_x + iJ_y = \hbar \begin{pmatrix} 0 & \sqrt{(\frac{1}{2} - (-\frac{1}{2}))(\frac{1}{2} + (-\frac{1}{2}) + 1)} \\ 0 & 0 \end{pmatrix} = \hbar \begin{pmatrix} & 1 \\ 0 & \end{pmatrix}$$

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

Hence

$$J_x = \frac{\hbar}{2} \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} \quad J_y = \frac{\hbar}{2} \begin{pmatrix} & -i \\ i & \end{pmatrix} \quad J_z = \frac{\hbar}{2} \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

So define Pauli matrices

$$\sigma_x = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} \quad \sigma_y = \begin{pmatrix} & -i \\ i & \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

Then

$$J_i = \frac{\hbar}{2} \sigma_i$$

and

$$\sigma_i \sigma_j = i\epsilon_{ijk}\sigma_k + \delta_{ij}$$

so

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k$$

From above one can check (even without using the Pauli representations)

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$$

$$(\vec{\sigma} \cdot \hat{n})^2 = \begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix}^2 = I \tag{2.36}$$

Or more general

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = \vec{A} \cdot \vec{B} I + i\vec{\sigma} \cdot (\vec{A} \times \vec{B})$$

The quantity

$$aI - i\vec{b} \cdot \vec{\sigma} \tag{2.37}$$

$a \in \mathbb{R}$, $\vec{b} \in \mathbb{R}^3$ is closed under multiplication and addition and it makes up the only 4 generators non-commutative algebra known as the quaternions. For example

$$(aI - i\vec{b} \cdot \vec{\sigma})(a'I - i\vec{b}' \cdot \vec{\sigma}) = (aa' - \vec{b} \cdot \vec{b})I - i(a\vec{b}' + a'\vec{b} - \vec{b} \times \vec{b}')\vec{\sigma}$$

Now we can compute, by (2.36)

$$\begin{aligned} e^{-i\vec{J}\cdot\hat{n}\theta/\hbar} &= e^{-i\vec{\sigma}\cdot\hat{n}\frac{\theta}{2}} \\ &= \sum_{l=0}^{\infty} \frac{1}{l!}(-i\frac{\theta}{2})^l (\vec{\sigma} \cdot \hat{n})^l \\ &= \sum_{l=0}^{\infty} \frac{1}{(2l)!}(-i\frac{\theta}{2})^{2l} + (\vec{\sigma} \cdot \hat{n}) \sum_{l=0}^{\infty} \frac{1}{(2l+1)!}(-i\frac{\theta}{2})^{2l+1} \\ &= \cos\frac{\theta}{2} - i(\vec{\sigma} \cdot \hat{n})\sin\frac{\theta}{2} \qquad (2.38) \\ &= \begin{pmatrix} \cos\frac{\theta}{2} - in_z \sin\frac{\theta}{2} & -i\sin\frac{\theta}{2}(n_x - in_y) \\ -i\sin\frac{\theta}{2}(n_x + in_y) & \cos\frac{\theta}{2} + in_z\sin\frac{\theta}{2} \end{pmatrix} \qquad (2.39) \end{aligned}$$

So in the sense of (2.35)

$$\mathcal{D}^{(\frac{1}{2})}_{m'm}(\hat{n}, \theta) = \delta_{m'm}\cos\frac{\theta}{2} - i(\vec{\sigma} \cdot \hat{n})_{m'm}\sin\frac{\theta}{2}$$

Two shocking things

The above is not $SO(3)$; it's $SU(2)$. We have to reverse our attitude, and switch what fundamental of rotations is.

Put $\theta = 2\pi$, gives

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

Note: one can use this method to figure out higher $\mathcal{D}^{(j)}$. Here $SU(2)$ gives all $O(3)$, it is not the case for higher j.

Why is (2.39) a general $SU(2)$? Mathematically U is unitary then there is a Hermitian H

$$U = e^{-iH}$$

and

$$\det U = e^{-i\mathrm{Tr}H}$$

Here

$$\mathrm{Tr}H = \mathrm{Tr}(\vec{\sigma} \cdot \hat{n}\frac{\theta}{2}) = 0$$

so indeed $SU(2)$.

We can rewrite (2.38)

$$e^{-i\vec{J}\cdot\hat{n}\theta/\hbar} = a - i\vec{\sigma} \cdot \vec{b}$$

where $a = \cos\frac{\theta}{2}$, $\vec{b} = \hat{n}\sin\frac{\theta}{2}$, so $a^2 + \vec{b}^2 = 1$. Hence we can represent $SU(2)$ as points on the 4 dimensional unit sphere.

Since $SU(2)$ is double cover of $SO(3)$

$$SU(2) \to SO(3) \text{ not faithful}$$

$$SO(3) \to SU(2) \text{ not well defined}$$

High SU have other usages. For example $SU(3)$ represents flavors and $SU(5)$ used in grand unification theory.

2.7 Spherical Harmonics

Lecture 13 (10/21/13)

Consider rotation acting on wave function $\psi(\vec{r})$,

$$R(\hat{n}, \delta\theta)\psi(\vec{r})$$

Here we use $L_{x,y,z}$,l instead of $J_{x,y,z}$,j etc.

$$(1 - i\frac{\delta\theta}{\hbar}\hat{n} \cdot \vec{L})\psi(\vec{r}) = \psi(\vec{r} - \delta\theta\hat{n} \times \vec{r}) \tag{2.40}$$

In comparison to (2.26), the $-$ sign on the right signifies that it is a passive rotation, then

$$\begin{aligned}
(\hat{n} \cdot \vec{L})\psi(\vec{r}) &= \frac{i\hbar}{\delta\theta}[\psi(\vec{r} - \delta\theta\hat{n} \times \vec{r}) - \psi(\vec{r})] \\
&= -i\hbar(\hat{n} \times \vec{r}) \cdot \nabla\psi(\vec{r}) \\
&= \hat{n} \cdot [\vec{r} \times (\frac{\hbar}{i}\nabla)]\psi(\vec{r})
\end{aligned}$$

Hence

$$\vec{L} = \vec{r}_{op} \times \vec{p}_{op}$$

What does $\vec{L}$ look like? In spherical coordinate $\vec{r} \to r, \theta, \phi$. Since r is unchanged, we can focus on $\psi(\theta, \phi)$.

First rotate $\delta\phi$ around z, so θ should no change. Use (2.40)

$$(1 - iL_z\frac{\delta\phi}{\hbar})\psi(\theta, \phi) = \psi(\theta, \phi - \delta\phi)$$

so

$$L_z\psi = \frac{i\hbar}{\delta\phi}[\psi(\theta, \phi - \delta\phi) - \psi(\theta, \phi)] = -i\hbar\frac{\partial\psi}{\partial\phi}$$

thus

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

Rotate about x by $\delta\alpha$

$$(1 - iL_x\frac{\delta\alpha}{\hbar})\psi(\theta, \phi) = \psi(\theta - \delta\theta, \phi - \delta\phi)$$

Relate $\delta\theta$, $\delta\phi$ to $\delta\alpha$, take an arbitrary vector $\vec{r}$, under the rotation, its z component becomes

$$z' = r\cos(\theta + \delta\theta) = r\cos\theta - r\sin\delta\theta$$

On the another hand we can compute the z component change through the rotation

$$z' = r\cos\theta\cos\delta\alpha + r\sin\theta\sin\phi\sin\delta\alpha = r\cos\theta + r\sin\theta\sin\phi\delta\alpha$$

So

$$\delta\theta = -\sin\phi\delta\alpha$$

The x component of $\vec{r}$ is unchanged

$$x' = r\sin(\theta+\delta\theta)\cos(\phi+\delta\phi) = r\sin\theta\cos\phi = x$$

So

$$\cos\theta\delta\theta\cos\phi + \sin\theta(-\sin\phi\delta\phi) = 0$$

Thus

$$\delta\phi = \frac{\cos\phi\cos\theta}{\sin\phi\sin\theta}\delta\theta = -\frac{\cos\phi\cos\theta}{\sin\theta}\delta\alpha$$

Therefore

$$L_x\psi = \frac{i\hbar}{\delta\alpha}[\psi(\theta+\sin\phi\delta\alpha, \phi + \frac{\cos\phi\cos\theta}{\sin\theta}\delta\alpha) - \psi(\theta,\phi)]$$

thus

$$L_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\theta}{\sin\theta}\cos\phi\frac{\partial}{\partial\phi}\right)$$

Similarly

$$L_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\cos\theta}{\sin\theta}\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$L^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \tag{2.41}$$

$$L_x \pm iL_y = i\hbar\left(\mp ie^{\pm i\phi}\frac{\partial}{\partial\theta} + \frac{\cos\theta}{\sin\theta}e^{\pm i\phi}\frac{\partial}{\partial\phi}\right) \tag{2.42}$$

Now define spherical harmonics

$$Y_{lm}(\theta,\phi) = \langle\theta,\phi|l,m\rangle$$

From

$$L_z Y_{lm} = \hbar m Y_{lm}$$

$$Y_{lm}(\theta,\phi) = e^{im\phi} Y_{lm}(\theta,\phi=0)$$

Find $Y_{l,-l}$

$$(L_x - iL_y)Y_{l,-l} = 0$$

By (2.42)

$$\left(ie^{-\phi}\frac{\partial}{\partial\theta} + \frac{\cos\theta}{\sin\theta}e^{-\phi}(-il)\right)Y_{l,-l} = 0$$

$$\frac{\partial}{\partial\theta}Y_{l,-l}(\theta,\phi)\bigg|_{\phi=0} = l\frac{\cos\theta}{\sin\theta}Y(\theta,0)$$

$$Y_{l,-l}(\theta,\phi) = N\sin^l\theta e^{-il\phi}$$

$$\begin{aligned}
1 &= N^2\int_0^{2\pi} d\phi \int_0^{\pi}\sin\theta d\theta \sin^{2l}\theta \\
&= N^2 2\pi \int_{-1}^{1} dz(1-z^2)^l \text{ (let } \cos\theta = z) \\
&= N^2 2\pi \int_{-1}^{1} dzz(2lz)(1-z^2)^2 \text{ (integration by parts)} \\
&\ldots \text{ (integration by parts)} \\
&= N^2 2\pi \int_{-1}^{1} z^{2l}dz 2^l l! \frac{1}{1\cdot 3\cdot \ldots \cdot (2l-1)} \\
&= N^2 2\pi \frac{2}{2l+1} 2^l l! \frac{1}{1\cdot 3\cdot \ldots \cdot (2l-1)}
\end{aligned}$$

$$N = \sqrt{\frac{2l+1}{4\pi}\frac{1}{2^l l!}1\cdot 3\cdot\ldots\cdot(2l-1)} = \frac{1}{\sqrt{4\pi}}\frac{\sqrt{(2l+1)!}}{2^l l!}$$

Then

$$\begin{aligned}
Y_{lm}(\theta,\phi) &= \frac{1}{\hbar\sqrt{(l-m+1)(l+m-1+1)}}(L_x + iL_y)Y_{l,m-1}(\theta,\phi) \\
&= \frac{i\hbar}{\hbar\sqrt{(l-m+1)(l+m)}}\left(-ie^{i\phi}\frac{\partial}{\partial\theta} + \frac{\cos\theta}{\sin\theta}e^{i\phi}\frac{\partial}{\partial\phi}\right)Y_{l,m-1}(\theta,\phi)
\end{aligned}$$

$$
\begin{aligned}
Y_{lm}(\theta,0) &= \frac{i}{\sqrt{(l-m+1)(l+m)}}\left(-i\frac{\partial}{\partial\theta}+\frac{\cos\theta}{\sin\theta}i(m-1)\right)Y_{l,m-1}(\theta,0)\\
&= \frac{1}{\sqrt{(l-m+1)(l+m)}}\underbrace{\underbrace{\underbrace{\frac{\partial}{\partial\theta}-\frac{\cos\theta}{\sin\theta}(m-1)}_{\sin^{m-1}\theta\left(\frac{\partial}{\partial\theta}\right)\sin^{-(m-1)}\theta}}_{\sin^{m}\theta\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\right)\sin^{-(m-1)}\theta}}\qquad Y_{l,m-1}(\theta,0)\\
&= \frac{1}{\sqrt{(l-m+1)(l+m)}}\frac{1}{\sqrt{(l-m+2)(l+m-1)}}\\
&\qquad\left(\sin^m\theta\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\right)^2\sin^{-(m-2)}\right)Y_{l,m-2}(\theta,0)\\
&\dots\\
&= \frac{1}{\sqrt{(l-m+1)(l+m)}}\dots\frac{1}{\sqrt{2l(2)}}\left(\sin^m\theta\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\right)^{m+l}\sin^l\right)\frac{1}{\sqrt{4\pi}}\frac{\sqrt{(2l+1)!}}{2^l l!}\sin^l\theta\\
&= \sqrt{\frac{(2l+1)(l-m)!}{(l+m)!4\pi}\frac{1}{2^l l!}}\sin^m\theta\left(-\frac{d}{d(\cos\theta)}\right)^{m+l}\sin^{2l}\theta
\end{aligned}
$$

2.8 Alpha Decay

Lecture 14 (10/23/13)

$U^{92}_{238}\to Th_{234}+\alpha$, rejecting α with energy 4.1MeV. The life time $\tau=4\times10^9$yr. We'll use WKB to calculate τ. The strong force empirically is in the range (see Griffiths problem 8.4)

$$r = 1.07A^{1/3}\text{fm} = 1.07(234)^{1/3} = 6\text{fm}$$

$$T=\frac{r}{c}=\frac{6\times10^{-13}cm}{3\times10^{-10}cm/s}\times2=4\times10^{-23}s=\frac{1}{f} \tag{2.43}$$

f is the frequency α hits the wall. Long range force is

$$2\frac{Z_{\text{th}}e^2}{r}$$

so we can find the turning point r_{rp}

$$2\frac{Z_{\text{th}}e^2}{r_{rp}} = 4.1\text{MeV} \implies r_{rp} = \frac{2\times 90}{4.1\text{MeV}}\frac{e^2}{\hbar c}\hbar c = \frac{2\times 90}{4.1}\frac{1}{137}200\text{fm} = 60\text{fm}$$

Hence the barrier is from $r = 6$fm to 60fm.

$$\text{Decay rate} = f \times \Gamma^2$$

Γ =probability of tunneling.

$$\Gamma = e^{-\frac{1}{\hbar}\int_{6\text{fm}}^{60\text{fm}}\sqrt{2m_\alpha(V(r)-E)}dr}$$

$$\text{life time}=\frac{1}{\text{decay rate}}$$

Use triangle to approximate the integral

$$\frac{1}{\hbar}\int_{6\text{fm}}^{60\text{fm}}\sqrt{2m_\alpha(V(r)-E)}dr \quad = \quad \frac{1}{\hbar}\sqrt{2\times 4000\frac{\text{MeV}}{c^2}(\frac{2\cdot 90e^2}{6\text{fm}} - 4\text{MeV})}(60-6)\text{fm}\frac{1}{2} = 81$$

$$\text{life time } \tau=\frac{10^{-23}\text{sec}}{e^{-2\cdot 81}}\frac{1\text{yr}}{\pi\times 10^7\text{sec}} \sim 10^{30}\text{yr}$$

$e \approx 10^{-1.43}$. Not so good.

We now try to do a better job

$$H = -\frac{\hbar^2}{2m_\alpha}\nabla^2 + V(r)$$

$$\nabla^2 = \frac{1}{r^2}\frac{d}{dr}(r^2\frac{d}{dr}) + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{d}{d\theta}\sin\theta\frac{d}{d\theta} + \frac{1}{r^2}\frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}$$

By (2.41)

$$H = -\frac{\hbar^2}{2m_\alpha}\frac{1}{r^2}\frac{d}{dr}(r^2\frac{d}{dr}) + \frac{L^2}{2m_\alpha r^2} + V(r)$$

We write

$$\psi(\vec{r}) = \psi(r,\theta,\phi) = \frac{1}{r}u(r)Y_{lm}(\theta,\phi) \tag{2.44}$$

One reason to put u/r is that in case we evaluate

$$\int \psi_1 \psi_2 d^3\vec{r} \sim \int \frac{1}{r}\frac{1}{r} u_1 u_2 r^2 dr = \int u_1 u_2 dr$$

Such (2.44) makes sense if

$$u(0) = 0$$

The Schrodinger equation becomes

$$\left[-\frac{\hbar^2}{2m_\alpha} \frac{1}{r^2} \frac{d}{dr} (r^2 \frac{d}{dr}) + \frac{\hbar^2 l(l+1)}{2m_\alpha r^2} \right] \frac{u(r)}{r} = E \frac{u(r)}{r}$$

Simplify

$$\begin{aligned} \frac{1}{r^2}\frac{d}{dr} r^2 \frac{d}{dr} \frac{u(r)}{r} &= \frac{1}{r^2} \frac{d}{dr} r^2 \left(-\frac{1}{r^2} u + \frac{1}{r} u' \right) \\ &= \frac{1}{r^2} \left(-u' + u' + r u'' \right) = \frac{1}{r} u'' \end{aligned} \tag{2.45}$$

Choose $l = 0$, use WKB approximation.

The barrier is in $r_1 < r < r_2$. There are two possible independent solutions $u(r)$, the same u defined above. One has exponential decay in $r_1 < r < r_2$ and the other is exponential growth in $r_1 < r < r_2$

$$u_1 = \begin{cases} \frac{1}{\sqrt{v_E(r)}} \cos\left(\frac{1}{\hbar} \int_{r_2}^{r} p_E(r') dr' + \frac{\pi}{4} \right) & r_2 < r \\ \downarrow \text{(by connecting formula)} & \\ \frac{1}{\sqrt{|v_E(r)|}} e^{\frac{1}{\hbar} \int_r^{r_2} |p_E(r')| dr'} = \frac{1}{\sqrt{|v_E(r)|}} \frac{1}{T_E} e^{-\frac{1}{\hbar} \int_{r_1}^{r} |p_E(r')| dr'} & r_1 < r < r_2 \\ \downarrow & \\ \frac{2}{\sqrt{v_E(r)}} \frac{1}{T_E} \sin\left(\frac{1}{\hbar} \int_r^{r_1} p_E(r') dr' + \frac{\pi}{4} \right) & 0 < r < r_1 \end{cases}$$

$$\text{transition amplitude } T_E = e^{-\frac{1}{\hbar} \int_{r_1}^{r_2} |p_E(r')| dr'}$$

We put $1/\sqrt{v}$ in the front, before we had $1/\sqrt{p}$, which is off by constant m_α. The reason will be evident later.

Put a extra factor to $u_2(r)$ in $0 < r < r_1$ so that u_2 will match the same factor as u_1 in $r_2 < r$, which will help to simplify later calculation

$$u_2 = \begin{cases} \frac{1}{\sqrt{v_E(r)}} \sin\left(\frac{1}{\hbar}\int_{r_2}^{r} p_E(r')dr' + \frac{\pi}{4}\right) & r_2 < r \\ \uparrow & \\ \frac{1}{\sqrt{|v_E(r)|}} \frac{T_E}{2} e^{\frac{1}{\hbar}\int_{r_1}^{r} |p_E(r')|dr'} = \frac{1}{\sqrt{|v_E(r)|}} \frac{1}{2} e^{-\frac{1}{\hbar}\int_{r}^{r_2} |p_E(r')|dr'} & r_1 < r < r_2 \\ \uparrow & \\ \frac{1}{\sqrt{v_E(r)}} \frac{T_E}{2} \cos\left(\frac{1}{\hbar}\int_{r}^{r_1} p_E(r')dr' + \frac{\pi}{4}\right) & 0 < r < r_1 \end{cases}$$

We require $u(r)$ vanish at origin, define

$$\eta = \frac{1}{\hbar}\int_0^{r_1} p(r')dr' + \frac{\pi}{4} \tag{2.46}$$

then

$$u_1(0) = \frac{2}{\sqrt{v(0)}}\frac{1}{T_E}\sin\eta \qquad u_2(0) = \frac{1}{\sqrt{v(0)}}\frac{T_E}{2}\cos\eta$$

So the solution is

$$u_E(r) = N_E\left(\frac{T_E}{2}\cos\eta u_1(r) - \frac{2}{T_E}\sin\eta u_2(r)\right)$$

which not only vanishes at $r = 0$ and it decreases as fast as r as $r \to 0$.

Lecture 15 (10/28/13)

Clearly stationary solutions are orthogonal

$$\int_0^\infty u_{E'}(r)u_E(r)dr = \delta(E - E') \tag{2.47}$$

Put

$$w_E = \sqrt{\left(\frac{T_E}{2}\cos\eta\right)^2 + \left(\frac{2}{T_E}\sin\eta\right)^2} \qquad \tan\phi = \left(\frac{2}{T_E}\right)^2\tan\eta$$

then our goal is to find N_E,

$$u_E = N_E(w\cos\phi u_1 - w\sin\phi u_2)$$

So in region $0 < r < r_1$

$$\begin{aligned} u_E &= N_E \frac{1}{\sqrt{v_E}} \left(\cos\eta \sin\left(\frac{1}{\hbar} \int_r^{r_1} p_E(r')dr' + \frac{\pi}{4} \right) - \sin\eta\cos\left(\frac{1}{\hbar} \int_r^{r_1} p_E(r')dr' + \frac{\pi}{4} \right) \right) \\ &= N_E \frac{1}{\sqrt{v_E}} \sin\left(\frac{1}{\hbar} \int_r^{r_1} p_E(r')dr' + \frac{\pi}{4} - \eta \right) \\ &= -N_E \frac{1}{\sqrt{v_E}} \sin\left(\frac{1}{\hbar} \int_0^{r} p_E(r')dr' \right) \end{aligned} \tag{2.48}$$

In region $r > r_2$

$$u_E = N_E w \frac{1}{\sqrt{v_E}} \cos\left(\frac{1}{\hbar} \int_{r_2}^{r} p_E(r')dr' + \frac{\pi}{4} + \phi \right)$$

From (2.47), since the wave amplitude is much larger in $r > r_2$ region and $r_2 \ll 1$, we restrict the integral from r_2 to ∞

$$\begin{aligned} \delta(E-E') &= \int_{r_2}^{\infty} dr \frac{N_E w_E N_{E'} w_{E'}}{\sqrt{v_E v_{E'}}} \cos\left(\frac{1}{\hbar} \int_{r_2}^{r} p_E(r')dr' + \frac{\pi}{4} + \phi \right) \cos\left(\frac{1}{\hbar} \int_{r_2}^{r} p_{E'}(r')dr' + \frac{\pi}{4} + \phi \right) \\ &\approx \int_{r_2}^{\infty} dr \frac{N_E w_E N_{E'} w_{E'}}{\sqrt{v_E v_{E'}}} \cos\left(\frac{p_E}{\hbar} r + \theta \right) \cos\left(\frac{p_{E'}}{\hbar} r + \theta \right) \end{aligned}$$

by assumption $p_{E,E'}(r)$ are slowly varying and absorb other constants into θ.

Continue

$$\begin{aligned} \delta(E-E') &\approx \int_{0}^{\infty} dr \cos\left(\frac{p_E}{\hbar} r + \theta \right) \cos\left(\frac{p_{E'}}{\hbar} r + \theta \right) \frac{N_E w_E N_{E'} w_{E'}}{\sqrt{v_E v_{E'}}} \\ &= \int_{0}^{\infty} dr \frac{N_E w_E N_{E'} w_{E'}}{\sqrt{v_E v_{E'}}} \frac{e^{i(\frac{p_E}{\hbar} r + \theta)} + e^{-i(\frac{p_E}{\hbar} r + \theta)}}{2} \frac{e^{i(\frac{p_{E'}}{\hbar} r + \theta)} + e^{-i(\frac{p_{E'}}{\hbar} r + \theta)}}{2} \\ &= \frac{N_E^2 w_E^2}{4 v_E} \left(\underbrace{\int_{-\infty}^{\infty} e^{i(p_E - p_{E'})r/\hbar} dr}_{2\pi\hbar \underbrace{\delta(p_E - p_{E'})}_{\frac{\delta(E-E')}{\frac{\partial p}{\partial E} = v_E}}} + \int_0^{\infty} e^{i(p_E + p_{E'})r/\hbar + i2\theta} dr + \int_{-\infty}^{0} e^{i(p_E + p_{E'})r/\hbar - i2\theta} \right) \end{aligned}$$

We can treat $N_E = N_{E'}$, $v_E = v_{E'}$, ... because of the $\delta(p_E - p_{E'})$ term. The other two terms are 0 due to steepest descent.

Continue

$$\delta(E-E') \approx \frac{N_E^2 w_E^2}{4v_E} 2\pi\hbar v_E \delta(E-E')$$

Hence

$$N_E = \frac{1}{w_E}\sqrt{\frac{2}{\pi\hbar}}$$

Let us take an initial wave function α particle inside of nuclear

$$u_0(r) = \begin{cases} 0 & r > r_1 \\ N\frac{1}{\sqrt{v}}\sin\left(\frac{1}{\hbar}\int_0^r p(r')dr'\right) & r < r_1 \end{cases} \tag{2.49}$$

which is not an eigenstate.

$$\sin\left(\frac{1}{\hbar}\int_0^r p(r')dr'\right) = \sin\left(\eta - \left(\int_r^{r_1} p(r')dr' + \frac{\pi}{4}\right)\right)$$

η is defined in (2.46). By Bohr quantization condition, we choose E_0 s.t.

$$\eta_{E_0} = n\pi \tag{2.50}$$

Time evolution wave function

$$u_0(r) = \int_{-\infty}^{\infty} dE C_E u_E, \quad C_E = \int_0^{\infty} u_0 u_E dr$$

and

$$u(r,t) = \int_{-\infty}^{\infty} dE C_E u_E e^{-iEt/\hbar} \tag{2.51}$$

First find N in (2.49)

$$1 = \int_0^{r_1} |u_0|^2 dr = N^2 \int_0^{r_1} \underbrace{\sin^2\left(\frac{1}{\hbar}\int_0^r p(r')dr'\right)}_{\approx\frac{1}{2}} \frac{1}{v(r)}dr = N^2\frac{1}{2}\underbrace{\int_0^{r_1}\frac{1}{v(r)}dr}_{=\frac{T}{2}}$$

Because $\hbar$ is very small, $\sin^2(\frac{1}{\hbar}...)$ is rapidly oscillating, so closed to 1/2. So

$$N = \frac{2}{\sqrt{T}}$$

T is defined in (2.43). Use (2.48) and compute

$$C_E = \int_0^{r_1} dr \frac{2}{\sqrt{T}} \frac{1}{\sqrt{v_{E_0}}} \sin\left(\frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right) \frac{1}{w_E}\sqrt{\frac{2}{\pi\hbar}} \frac{1}{\sqrt{v_E}} \sin\left(\frac{1}{\hbar}\int_0^r p_E(r')dr'\right)$$

Expect C_E to be sharply peaked, so is p_E, but not necessarily for w_E.

$$\begin{aligned} C_E &= \int_0^{r_1} \underbrace{\sin^2\left(\frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right)}_{=\frac{1}{2}} \frac{dr}{v_{E_0}} \frac{2}{\sqrt{T}} \frac{1}{w_E}\sqrt{\frac{2}{\pi\hbar}} = \frac{1}{2}\frac{T}{2}\frac{2}{\sqrt{T}}\frac{1}{w_E}\sqrt{\frac{2}{\pi\hbar}} \\ &= \frac{\sqrt{2}\sqrt{T}}{2\sqrt{\pi\hbar}} \frac{1}{\sqrt{\left(\frac{T_E}{2}\cos\eta_E\right)^2 + \left(\frac{2}{T_E}\sin\eta_E\right)^2}} \end{aligned}$$

Rewrite w_E by expending

$$\cos\eta_E = \cos\eta_{E_0} - \sin\eta_{E_0} \left.\frac{\partial \eta_E}{\partial E}\right|_{E=E_0} (E-E_0) + O((E-E_0)^2)$$

$$\sin\eta_E = \sin\eta_{E_0} + \cos\eta_{E_0} \left.\frac{\partial \eta_E}{\partial E}\right|_{E=E_0} (E-E_0) + O((E-E_0)^2)$$

$\sin\eta_{E_0} = 0$, $\cos\eta_{E_0} = \pm 1$ by (2.50), $\left.\frac{\partial\eta_E}{\partial E}\right|_{E=E_0} = \frac{1}{\hbar}\int_0^{r_1}\frac{\partial p_E}{\partial E}dr = \frac{1}{\hbar}\frac{T}{2}$, so

$$\begin{aligned} C_E &= \sqrt{\frac{T}{2\pi\hbar}} \frac{1}{\sqrt{\left(\frac{T_E}{2}\right)^2 + \left(\frac{2}{T_E}\frac{1}{\hbar}\frac{T}{2}(E-E_0)\right)^2}} \\ &= \frac{1}{\sqrt{2\pi}} \frac{\sqrt{\Gamma}}{\sqrt{\left(\frac{\Gamma}{2}\right)^2 + (E-E_0)^2}} \end{aligned} \tag{2.52}$$

putting $\Gamma = \frac{T_E^2\hbar}{T} \approx \frac{T_{E_0}^2\hbar}{T}$. (2.52) shows resonant. One way to check (2.52) is to check Parseval

$$\int_{-\infty}^{\infty} C_E^2 dE = \|u_0\|^2 = 1$$

Indeed

$$\int_{-\infty}^{\infty} \frac{1}{2\pi} \frac{\Gamma}{\left(\frac{\Gamma}{2}\right)^2 + (E-E_0)^2} dE = \frac{1}{2\pi} \int_{-\infty}^{\infty} dE \frac{\Gamma}{(E-E_0-i\frac{\Gamma}{2})(E-E_0+i\frac{\Gamma}{2})}$$

One can choose to close the contour either upper half or lower half

$$\int_{-\infty}^{\infty} C_E^2 dE = \frac{1}{2\pi} 2\pi i \frac{\Gamma}{2i\frac{\Gamma}{2}} = 1$$

Lecture 16 (11/11/13)

Now we are ready to compute decay rate.
The probability amplitude of finding α within r_1

$$A(t) = \int_0^{\infty} u_0(r) u(r,t) dr$$

$u(r,t)$ is given in (2.51).

$$\begin{aligned} A(t) &= \int_0^{r_1} dr \frac{2}{\sqrt{T}} \frac{1}{\sqrt{v_{E_0}}} \sin\left(\frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right) \int_{-\infty}^{\infty} dE \frac{1}{\sqrt{2\pi}} \frac{\sqrt{\Gamma}}{\sqrt{\left(\frac{\Gamma}{2}\right)^2 + (E-E_0)^2}} \\ &\quad \frac{1}{w_E}\sqrt{\frac{2}{\pi\hbar}} \frac{1}{\sqrt{v_E}} \sin\left(\frac{1}{\hbar}\int_0^r p_E(r')dr'\right) e^{-iEt/\hbar} \end{aligned}$$

where

$$\frac{1}{w_E} = \frac{C_E}{\sqrt{\frac{T}{2\pi\hbar}}} = \frac{\sqrt{\Gamma\frac{\hbar}{T}}}{\sqrt{\left(\frac{\Gamma}{2}\right)^2 + (E-E_0)^2}}$$

So

$$\begin{aligned}
A(t) &\approx \int_0^{r_1} dr \frac{2}{\sqrt{T}} \frac{1}{v_{E_0}} \underbrace{\sin^2\left(\frac{1}{\hbar}\int_0^r p_{E_0}(r')dr'\right)}_{=\frac{1}{2}} \int_{-\infty}^{\infty} dE \frac{1}{\pi\sqrt{T}} \frac{\Gamma}{\left(\frac{\Gamma}{2}\right)^2 + (E-E_0)^2} e^{-iEt/\hbar} \\
&= \frac{2}{T}\frac{1}{2}\frac{T}{2}\frac{1}{\pi}\int_{-\infty}^{\infty} dE \frac{\Gamma}{\left(\frac{\Gamma}{2}\right)^2 + (E-E_0)^2} e^{-iEt/\hbar} \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} dE \frac{\Gamma e^{-iEt/\hbar}}{(E-E_0-i\frac{\Gamma}{2})(E-E_0+i\frac{\Gamma}{2})} \\
&= \frac{1}{2\pi}(-2\pi i)\frac{\Gamma e^{-i(E_0-i\frac{\Gamma}{2})t/\hbar}}{-2i\frac{\Gamma}{2}} = e^{-iE_0t/\hbar}e^{-\frac{\Gamma}{2\hbar}t}
\end{aligned}$$

Because of the $e^{-iEt/\hbar}$, must close the contour lower half plane.

Then the probability of finding α within r_1 is diminishing

$$P(t) = |A(t)|^2 = e^{-\frac{\Gamma}{\hbar}t}$$

Hence the decay rate is $\Gamma/\hbar$, and the life time

$$\frac{\hbar}{\Gamma} = \frac{T}{T_E^2}$$

The analysis is little imperfect; there are small correction we didn't consider. Later we'll revisit them.

3 Time Independent Perturbation

3.1 Hydrogen like Atoms

$$H = \frac{p^2}{2m} - \frac{Ze^2}{r}$$

There are ∞ number of bound states

$$E_n = -\frac{me^4Z^2}{2\hbar^2n^2} = -\frac{Z^2e^2}{2a_0n^2} \quad n \in \mathbb{Z}^+$$

Bohr radius

$$a_0 = \frac{\hbar}{mc}\frac{\hbar c}{e^2} = \text{compton wavelength} \times \tfrac{1}{\alpha} = 4.3 \times 10^{-11}\text{cm} \cdot 137 = 0.5E - 8\text{cm}$$

showing that as charge gets weaker or EM coupling weaker $\alpha \downarrow \Longrightarrow a_0 \uparrow$.

Let

$$\psi_E(r) = R_{n,l}(r) Y_{l,m}(\theta, \phi)$$

From (2.45), we know $R_{n,l}$ is given by

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2m} - \frac{Ze^2}{r} \right) r R_{n,l}(r) = E_n r R_{n,l}(r)$$

Use power series to solve above ode, and use asymptotic behavior to terminate the series, so the polynomial has to be L_p^k, associated Laguerre polynomial.

$$R_{n,l}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{2rZ}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2rZ}{na_0}\right) e^{-\frac{rZ}{na_0}} \tag{3.1}$$

The exponent is like SHO, but doesn't decay nearly as fast as SHO; SHO exponent $\sim -x^2$.

The reason that E_n doesn't depend on l is because there is another conserved quantity, Lenz vector.

$$\vec{K} = \frac{1}{m}(\vec{p} \times \vec{L}) - \frac{e^2}{r}\vec{r}$$

$$\frac{d\vec{K}}{dt} = 0 \qquad [H, \vec{K}] = 0$$

This is analogous to classical gravitational motion.

Hydrogen serves a good model for motivating what we are going to study, and provides a good experimental test for the theories.

Now add $\vec{B}$

$$\vec{B} = \nabla \times \vec{A} \qquad \nabla \cdot \vec{B} = 0 \qquad \nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$$

So

$$\nabla \times \left(\vec{E} + \frac{1}{c}\dot{\vec{A}} \right) = 0 \Longrightarrow \vec{E} = -\frac{1}{c}\dot{\vec{A}} - \nabla\phi$$

Gauge transformation

$$\vec{A}' = \vec{A} + \nabla\Lambda$$

then

$$\vec{E} = -\frac{1}{c}\dot{\vec{A}}' + \frac{1}{c}\nabla\dot{\Lambda} - \nabla\phi = -\frac{1}{c}\dot{\vec{A}}' - \nabla\phi'$$

so correspondingly

$$\phi' = \phi - \frac{1}{c}\dot{\Lambda}$$

The Hamilton in the present of $\vec{B}$

$$H = \frac{[\vec{p} + \frac{e}{c}\vec{A}]^2}{2m} - e\phi \tag{3.2}$$

Does the solution depend on gauge?

$$\left(\frac{(-i\hbar\nabla + \frac{e}{c}\vec{A}')^2}{2m} - e\phi'\right)\psi' = i\hbar\frac{\partial}{\partial t}\psi' \tag{3.3}$$

then

$$\psi'(\vec{r}, t) = e^{-i\frac{e}{\hbar c}\Lambda(\vec{r},t)}\psi(\vec{r}, t)$$

Indeed

$$\begin{aligned}
(-i\hbar\nabla + \frac{e}{c}\vec{A}')\psi' &= e^{-i\frac{e}{\hbar c}\Lambda(\vec{r},t)}[-i\hbar\nabla + \frac{e}{c}A]\psi + \psi[-i\hbar(-i\frac{e}{\hbar c}\nabla\Lambda) + \frac{e}{c}\nabla\Lambda]e^{-i\frac{e}{\hbar c}\Lambda(\vec{r},t)} \\
&= e^{-i\frac{e}{\hbar c}\Lambda(\vec{r},t)}(-i\hbar\nabla + \frac{e}{c}A)\psi
\end{aligned}$$

$$\begin{aligned}
(-i\hbar\nabla + \frac{e}{c}\vec{A}')^2\psi' &= (-\frac{e}{c}\nabla\Lambda + \frac{e}{c}\nabla\Lambda)e^{-i\frac{e}{\hbar c}\Lambda(\vec{r},t)}(-i\hbar\nabla + \frac{e}{c}A)\psi + e^{-i\frac{e}{\hbar c}\Lambda(\vec{r},t)}(-i\hbar\nabla + \frac{e}{c}A)^2\psi \\
&= e^{-i\frac{e}{\hbar c}\Lambda(\vec{r},t)}(-i\hbar\nabla + \frac{e}{c}A)^2\psi
\end{aligned}$$

$$i\hbar\frac{\partial}{\partial t}\psi' = e^{-i\frac{e}{\hbar c}\Lambda(\vec{r},t)}(-\frac{e}{c}\dot{\Lambda}\psi + i\hbar\frac{\partial}{\partial t}\psi)$$

Since ψ solves

$$\left(\frac{(-i\hbar\nabla + \frac{e}{c}A)^2}{2m} - e\phi\right)\psi = i\hbar\frac{\partial}{\partial t}\psi$$

we have

$$e^{i\frac{e}{\hbar c}\Lambda(\vec{r},t)}\left(\frac{(-i\hbar\nabla+\frac{e}{c}A')^2}{2m}-e\phi\right)\psi' = e^{i\frac{e}{\hbar c}\Lambda(\vec{r},t)}\left(i\hbar\frac{\partial}{\partial t}\psi'+\frac{e}{c}\dot{\Lambda}\psi'\right)$$

which in turn gives (3.3).

The local gauge transformation in (3.3) serves a prototype for standard model and QCD, where $\Lambda(\vec{r},t)$ becomes 2 or 3 unitary matrix.

Lecture 17 (11/13/13)

We can solve for (3.2). Say $\vec{B}=B\hat{z}$, $\vec{A}(\vec{r})=\frac{1}{2}(\vec{B}\times\vec{r})$

$$\begin{aligned} H &= \frac{(\vec{p}+\frac{e}{c}A)^2}{2m}-\frac{e^2}{|\vec{r}|} \\ &= \frac{\vec{p}^2}{2m}-\frac{e^2}{|\vec{r}|}+e\frac{\vec{p}\cdot A}{mc}+\underbrace{\frac{1}{2m}\vec{A}^2}_{\text{ignore}} \\ &= \frac{\vec{p}^2}{2m}-\frac{e^2}{|\vec{r}|}+\underbrace{e\frac{\vec{p}\cdot(\vec{B}\times\vec{r})}{2mc}}_{\underbrace{e\frac{\vec{L}}{2mc}}_{-\vec{\mu}}\cdot\vec{B}} \end{aligned} \tag{3.4}$$

Magnitude $\frac{\vec{p}^2}{2m}$ and $\frac{e^2}{|\vec{r}|}$ about same $\sim 13\text{eV}$. Magnitude

$$e\frac{\vec{L}\cdot\vec{B}}{2mc}\sim\frac{\hbar^2}{2mc}eB = 4.3E-11\text{cm}\cdot\text{e Gauss}B = 13E-9\text{eV}B$$

We will neglect A^2 term unless:

$B\sim 10^5$Gauss; or if the motion is unbounded $r\to\infty$; or if $O(A)$ term happens to vanish.

What is all we can do with hydrogen without perturbation:

Zeemen effect

$$E_{n,m_l} = -\frac{me^4}{2\hbar^2n^2}+\frac{eB\hbar m_l}{2mc}\quad m_l=-1,0,1$$

for $l=0$. If $l\neq 0$, there will be spin-orbital correct, typical at the order comparable to Zeeman, later we will show the simple calculation need to be modified.

Adding electron spin

$$\vec{\mu}_{\text{spin}} = \frac{ge}{2mc}\vec{S} \quad g = 2(1 + \frac{\alpha}{2\pi} + ...)$$

$$H = \frac{\vec{p}^2}{2m} - \frac{e^2}{|\vec{r}|} - \vec{\mu}_L \cdot \vec{B} - \vec{\mu}_{\text{spin}} \cdot \vec{B} = \frac{\vec{p}^2}{2m} - \frac{e^2}{|\vec{r}|} + e\frac{\vec{L} \cdot \vec{B}}{2mc} + e\frac{g\vec{S} \cdot \vec{B}}{2mc} \tag{3.5}$$

$\vec{S} = \frac{\hbar}{2}\vec{\sigma}$

$$\vec{S} \cdot \vec{B} = S_z B_z = B_z \frac{\hbar}{2} \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$$

Hence since $g = 2$, the amount of spin-B energy shift is the same as the orbital-B energy shift.

3.2 Non Degenerate Perturbation

Rayleigh – Schrodinger

$$H = H_0 + \lambda V$$

and $E_n^{(0)}$, $|\phi_n\rangle$ are known

$$H_0 |\phi_n\rangle = E_n^{(0)} |\phi_n\rangle$$

To solve

$$H |\psi_n\rangle = E_n |\psi_n\rangle \tag{3.6}$$

Although the solution given by perturbation $|\psi_n\rangle$ is not normalized, (3.6) is still valid. Write E_n, $|\psi_n\rangle$ in term of $E_n^{(0)}$, $|\phi_n\rangle$ as a power series in λ.

$$E_n(\lambda) = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + ...$$

$$|\psi_n\rangle = \sum_{n'} S_{n'n} |\phi_{n'}\rangle$$

hence $S_{n'n} = \langle\phi_{n'}|\psi_n\rangle$, require $\langle\psi_{n'}|\psi_n\rangle \propto \delta_{n'n}$.

$S_{n'n}$ is the unitary matrix changing from the $|\phi_n\rangle$ basis to the $|\psi_{n'}\rangle$ basis

$$S_{n'n}(\lambda) = \delta_{n'n} + \lambda S_{n'n}^{(1)} + \lambda^2 S_{n'n}^{(2)} + ... \tag{3.7}$$

If H_0 is degenerated, it is not so clearly as $\lambda = 0 \to$ non zero $\to 0$, the $|\psi_k\rangle = |\phi_k\rangle$ will be back to $|\phi_k\rangle$ (or more generally $e^{i\gamma}|\phi_k\rangle$ but by convention choose $e^{i\gamma} = 1$. Note we will require $\langle\phi_n|\psi_n\rangle = 1$), so the first term on the right of (3.7) may not be $\delta_{n'n}$. Luckily we do not have to worry about them now.

Apply $\langle\phi_{n'}|$ to (3.6), and insert identity

$$\langle\phi_{n'}| \left\{ (H_0 + \lambda V) \sum_{n''} |\phi_{n''}\rangle \langle\phi_{n''}| |\psi_n\rangle = |\psi_n\rangle E_n \right\}$$

get

$$\sum_{n''} \left(E_{n'}^{(0)} S_{n''n} \delta_{n'n''} + \lambda V_{n'n''} S_{n''n} \right) = S_{n'n} E_n \tag{3.8}$$

$V_{n'n''} = \langle\phi_{n'}|V|\phi_{n''}\rangle$

That is

$$\begin{aligned} &\sum_{n''} (E_{n'}^{(0)} \delta_{n'n''} + \lambda V_{n'n''})(\delta_{n''n} + \lambda S_{n''n}^{(1)} + \lambda^2 S_{n''n}^{(2)} + \ldots) \\ &\qquad = (\delta_{n'n} + \lambda S_{n'n}^{(1)} + \lambda^2 S_{n'n}^{(2)} + \ldots)(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots) \end{aligned} \tag{3.9}$$

In compact form

$$\sum_{n''} H_{n'n''} S_{n''n} = S_{n'n} E_n$$

or

$$HS = SE$$

E is diagonal,

$$(S^{-1} H S)_{n'n} = E_n \delta_{n'n}$$

1st Order, $O(\lambda)$, (3.9)

$$V_{n'n} + E_{n'}^{(0)} S_{n'n}^{(1)} = S_{n'n}^{(1)} E_n^{(0)} + \delta_{n'n} E_n^{(1)} \tag{3.10}$$

If $n = n'$

$$E_n^{(1)} = V_{nn}$$

If $n \neq n'$

$$S^{(1)}_{n'n} = \frac{V_{n'n}}{E^{(0)}_n - E^{(0)}_{n'}} \tag{3.11}$$

To get the 1st correction wave, we need $S^{(1)}_{nn}$ as well.

Assume $S^{(1)}_{nn}$ is real. Since S is unitary, $S^\dagger S = I$

$$\sum_{n''}(\delta_{nn''} + \lambda S^{(1)*}_{nn''} + \lambda^2 S^{(2)*}_{nn''} + ...)(\delta_{n'n} + \lambda S^{(1)}_{n'n} + \lambda^2 S^{(2)}_{n'n} + ...) = \delta_{n'n} \tag{3.12}$$

In 1st order

$$S^{(1)*}_{nn'} + S^{(1)}_{n'n} = 0 \tag{3.13}$$

But $S^{(1)}_{nn}$ is real, so $S^{(1)}_{nn} = 0$. One can also check (3.11) agrees (3.13)

$$\frac{V^*_{nn'}}{E^{(0)}_{n'} - E^{(0)}_n} + \frac{V_{n'n}}{E^{(0)}_n - E^{(0)}_{n'}} = 0$$

2nd Order, $O(\lambda^2)$, (3.9)

$$E^{(0)}_{n'} S^{(2)}_{n'n} + \sum_{n''} V_{n'n''} S^{(1)}_{n''n} = S^{(1)}_{n'n} E^{(1)}_n + \delta_{n'n} E^{(2)}_n + S^{(2)}_{n'n} E^{(0)}_n \tag{3.14}$$

If $n = n'$

$$E^{(2)}_n = \sum_{n''} V_{n'n''} S^{(1)}_{n''n} = \sum_{n''\neq n} \frac{V_{nn''}V_{n''n}}{E^{(0)}_n - E^{(0)}_{n''}} = \sum_{n'\neq n} \frac{|V_{nn'}|^2}{E^{(0)}_n - E^{(0)}_{n'}} \tag{3.15}$$

So the 2nd order ground state shift is always negative.

If $n \neq n'$

$$\begin{aligned} S^{(2)}_{n'n} &= \frac{1}{E^{(0)}_n - E^{(0)}_{n'}} (\sum_{n''} V_{n'n''} S^{(1)}_{n''n} - S^{(1)}_{n'n} E^{(1)}_n) \\ &= \frac{1}{E^{(0)}_n - E^{(0)}_{n'}} \left(\sum_{n''\neq n} \frac{V_{n'n''}V_{n''n}}{E^{(0)}_n - E^{(0)}_{n''}} - \frac{V_{nn}V_{n'n}}{E^{(0)}_n - E^{(0)}_{n'}} \right) \end{aligned} \tag{3.16}$$

To find $S_{nn}^{(2)}$, assume it is real and from (3.12), in 2nd order

$$2\text{Re}\left(S_{nn}^{(2)}\right) + \sum_{n''} S_{n''n}^{(1)*} S_{n''n}^{(1)} = 0$$

then

$$S_{nn}^{(2)} = -\frac{1}{2} \sum_{n' \neq n} \frac{|V_{n'n}|^2}{\left(E_n^{(0)} - E_{n'}^{(0)}\right)^2} \tag{3.17}$$

Lecture 18 (11/18/13)

In summary, non degenerated perturbation with assumption $\langle \phi_n | \psi_n \rangle$ real, we find

$$E_n = E_n^{(0)} + \lambda \langle \phi_n | V | \phi_n \rangle + \lambda^2 \sum_{n' \neq n} \frac{|V_{n'n}|^2}{E_n^{(0)} - E_{n'}^{(0)}}$$

$$\begin{aligned} |\psi_n\rangle \;=\; & |\phi_n\rangle + \lambda \sum_{n' \neq n} \frac{V_{n'n}}{E_n^{(0)} - E_{n'}^{(0)}} |\phi_{n'}\rangle + \lambda^2 \left\{ \sum_{n' \neq n} \frac{|\phi_{n'}\rangle}{E_n^{(0)} - E_{n'}^{(0)}} \left(\sum_{n'' \neq n} \frac{V_{n'n''} V_{n''n}}{E_n^{(0)} - E_{n''}^{(0)}} - \frac{V_{nn} V_{n'n}}{E_n^{(0)} - E_{n'}^{(0)}} \right) \right. \\ & \left. - \frac{|\phi_n\rangle}{2} \sum_{n' \neq n} \frac{|V_{n'n}|^2}{\left(E_n^{(0)} - E_{n'}^{(0)}\right)^2} \right\} \end{aligned} \tag{3.18}$$

not yet normalized

Wigner – Brillouin

This method is less symmetrical but more systematical.

$$(H_0 + V) |\psi_n\rangle = E_n |\psi_n\rangle$$

$$\langle \phi_{n'} | H_0 + V | \psi_n \rangle = E_n \langle \phi_{n'} | \psi_n \rangle$$

$$LHS = E_{n'}^{(0)} \langle \phi_{n'} | \psi_n \rangle + \langle \phi_{n'} | V | \psi_n \rangle$$

so

$$\langle \phi_{n'} | \psi_n \rangle = \frac{1}{E_n - E_{n'}^{(0)}} \langle \phi_{n'} | V | \psi_n \rangle$$

If $n = n'$, put $|\psi_n\rangle = |\phi_n\rangle$ to above, i.e.

$$E_n - E_n^{(0)} = \langle\phi_{n'}|V|\psi_n\rangle$$

or

$$E_n = E_n^{(0)} + \langle\phi_{n'}|V|\psi_n\rangle \tag{3.19}$$

Therefore

$$\begin{aligned}|\psi_n\rangle &= \sum_{n'} |\phi_{n'}\rangle \langle\phi_{n'}|\psi_n\rangle \\ &= |\phi_n\rangle + \sum_{n'\neq n} \frac{|\phi_{n'}\rangle}{E_n - E_{n'}^{(0)}} \langle\phi_{n'}|V|\psi_n\rangle \end{aligned} \tag{3.20}$$

which is not yet normalized.

Check the leading order in (3.20) is leading order in (3.18), put $E_n = E_n^{(0)}$ and $|\psi_n\rangle = |\phi_n\rangle$ into right side of (3.20).

Next order substitute (3.20) into the right side of (3.20)

$$|\psi_n\rangle = |\phi_n\rangle + \sum_{n'\neq n} \frac{|\phi_{n'}\rangle}{E_n - E_{n'}^{(0)}} \langle\phi_{n'}|V|\phi_n\rangle + \sum_{n'\neq n}\sum_{n''\neq n} \frac{|\phi_{n'}\rangle \langle\phi_{n'}|V|\phi_n\rangle \langle\phi_{n''}|V|\psi_n\rangle}{(E_n - E_{n'}^{(0)})(E_n - E_{n''}^{(0)})} \tag{3.21}$$

then put $E_n = E_n^{(0)}$ and $|\psi_n\rangle = |\phi_n\rangle$ into right side above, we recover three terms of (3.18). The fourth term in (3.18) is given by putting

$$E_n = E_n^{(0)} + \langle\phi_n|V|\phi_n\rangle$$

which is 1st order approximation to (3.19), into the second term in (3.21), that is

$$\sum_{n'\neq n} \frac{|\phi_{n'}\rangle \langle\phi_{n'}|V|\phi_n\rangle}{E_n^{(0)} + \langle\phi_n|V|\phi_n\rangle - E_{n'}^{(0)}} = \sum_{n'\neq n} \frac{|\phi_{n'}\rangle \langle\phi_{n'}|V|\phi_n\rangle}{E_n - E_{n'}^{(0)}} + \sum_{n'\neq n} - \frac{|\phi_{n'}\rangle \langle\phi_{n'}|V|\phi_n\rangle \langle\phi_n|V|\phi_n\rangle}{\left(E_n^{(0)} - E_{n'}^{(0)}\right)^2}$$

The fourth term in (3.18) can be derived from normalization of Brillouin-Wigner solution.

3.3 Helium like Atom

$$H = \sum_{i=1}^{2} \left(\frac{p_i^2}{2m} - \frac{Ze^2}{r_i} \right) + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$$

The first term on the right $\sim Z^2$ and the second term $\sim Z$ because

$$\langle r \rangle \sim \frac{\hbar^2}{mZ}$$

So for $Z = 2$, the validity of perturbation is not obvious. What we can do is to apply perturbation to Z large then take $Z \to 2$ see if the result consistently and cheat by experiment.

Consider the ground state of Helium and find the first order energy shift for $e^- e^-$ repulsion, don't consider e^- spin, no Pauli statistics. Suppose $n = 1$, $l = 0$ for both e^-, refer (3.1)

$$\psi_{1s,1s}(\vec{r}_1, \vec{r}_2) = \left(\frac{1}{\pi} \left(\frac{Z}{a_0} \right)^{3/2} \right)^2 e^{-\frac{Z}{a_0} r_1} e^{-\frac{Z}{a_0} r_2}$$

Choose $\vec{r}_1$ to be the z direction to define $\vec{r}_2$

$$\begin{aligned}
E^{(1)}_{ground} &= \langle 1s, 1s | V | 1s, 1s \rangle \\
&= \int d^3 r_1 \int d^3 r_2 \frac{1}{\pi^2} \left(\frac{Z}{a_0} \right)^6 e^{-\frac{2Z}{a_0} r_1} e^{-\frac{2Z}{a_0} r_2} \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \\
&= \int d^3 r_1 \int_0^\infty r_2^2 dr_2 \int_0^{2\pi} d\phi \int_{-1}^{1} d(\cos\theta) e^{-2\frac{r_1 + r_2}{a_0} Z} \frac{e^2}{(r_1^2 + r_2^2 - 2 r_1 r_2 \cos\theta)^{1/2}} \frac{1}{\pi^2} \left(\frac{Z}{a_0} \right)^6 \\
&= \frac{e^2}{\pi^2} \left(\frac{Z}{a_0} \right)^6 4\pi 2\pi \int_0^\infty r_1^2 d^2 r_1 \int_0^\infty r_2^2 dr_2 e^{-2\frac{r_1 + r_2}{a_0} Z} \frac{1}{r_1 r_2} \\
&\qquad \times \underbrace{[\underbrace{(r_1^2 + r_2^2 + 2 r_1 r_2)^{1/2}}_{(r_1 + r_2)} - \underbrace{(r_1^2 + r_2^2 - 2 r_1 r_2)^{1/2}}_{|r_1 - r_2|}]}_{2 \min(r_1, r_2)}
\end{aligned}$$

Integrate over the bigger first, when $r_1 > r_2$ switch $r_1 \leftrightarrow r_2$

$$\begin{aligned} E^{(1)}_{ground} &= 2 \times 8e^2 \left(\frac{Z}{a_0}\right)^6 \int_0^\infty r_1^2 d^2 r_1 \int_{r_1}^\infty r_2^2 dr_2 e^{-2\frac{r_1+r_2}{a_0}Z} \frac{2}{r_2} \\ &= \frac{5}{8}\frac{Zme^4}{\hbar^2} \end{aligned}$$

$$E_{ionization} = -\left(-\frac{Z^2 e^4 m}{2\hbar^2} + \frac{5}{8}\frac{Zme^4}{\hbar^2}\right)$$

Use variational method

$$H\left|\psi_n\right\rangle = E_n \left|\psi_n\right\rangle$$

$$\left|\psi\right\rangle = \sum_n c_n \left|\psi_n\right\rangle \tag{3.22}$$

$$\langle\psi|H|\psi\rangle = \sum_n |c_n|^2 E_n \geq \sum_n |c_n|^2 E_0 = E_0$$

The step requires the wave function (3.22) to be properly normalized.

Pick a trial function with screening

$$\psi^\alpha_{1s,1s}(\vec{r}_1, \vec{r}_2) = \left(\frac{1}{\pi}\left(\frac{\alpha Z}{a_0}\right)^{3/2}\right)^2 e^{-\frac{\alpha Z}{a_0}r_1} e^{-\frac{\alpha Z}{a_0}r_2}$$

$$\begin{aligned} E &= \left\langle \psi^\alpha \middle| \sum_{i=1}^2 \left(\frac{p_i^2}{2m} - \frac{Ze^2}{r_i}\right) + \frac{e^2}{|\vec{r}_1 - \vec{r}_2|} \middle| \psi^\alpha \right\rangle \\ &= \frac{\alpha^2 Z^2 e^4 m}{\hbar^2} - 2\frac{\alpha Z^2 e^4 m}{\hbar^2} + \frac{5}{8}\frac{Zme^4}{\hbar^2} \end{aligned}$$

Then impose

$$\frac{\partial E}{\partial \alpha} = 0$$

to find the minimal E. The results are listed below in the unit $E_{ionization}/\left(\frac{Z^2 e^4 m}{2\hbar^2}\right)$

	exper	1st ord perturb	variation meth
He	0.9035	0.75	0.8477
Li^-	2.7798	2.625	2.7287

3.4 Degenerated Perturbation

Lecture 19 (11/20/13)

Consider

$$H_0 |\phi_n\rangle = E_n^{(0)} |\phi_n\rangle$$

where a set T_k of N_k states all have same energy $E_k^{(0)}$. For simplicity we assume only one energy level is degenerated. As mentioned before, as $\lambda = 0 \to$ non zero $\to 0$, then $|\psi_k\rangle = |\phi_k\rangle$ will not be back to $|\phi_k\rangle$ but

$$\lim_{\lambda \to 0} |\psi_n(\lambda)\rangle = \sum_{n' \in T_k} S_{n'n} |\phi_{n'}\rangle$$

1st Order degenerated Perturbation

$$|\psi_n\rangle = \sum_{n'} S_{n'n} |\phi_n\rangle$$

Following the same procedure starting from (3.2) up to (3.10). (3.10) says $V_{n'n} = V_{nn}\delta_{n'n}$ no off diagonal elements.

We know for 1st order non degenerated perturbation

$$\langle \psi_{n'} | H_0 + \lambda V | \psi_n \rangle$$

is automatically diagonal. Indeed using (3.18),

$$\begin{aligned}
\langle \psi_m | H_0 + \lambda V | \psi_n \rangle &= (\langle \phi_m | + \lambda \sum_{m' \neq m} \frac{V^*_{m'm}}{E_m^{(0)} - E_{m'}^{(0)}} \langle \phi_{m'} |)(H_0 + \lambda V) \\
&\qquad (|\phi_n\rangle + \lambda \sum_{n' \neq n} \frac{V_{n'n}}{E_n^{(0)} - E_{n'}^{(0)}} |\phi_{n'}\rangle) && (3.23) \\
&= \lambda V_{mn} + \lambda E_m^{(0)} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} + \lambda E_n^{(0)} \frac{V^*_{nm}}{E_m^{(0)} - E_n^{(0)}} + O(\lambda^2) && (3.24) \\
&= O(\lambda^2) && (3.25)
\end{aligned}$$

if $n \neq m$. And

$$\langle\psi_n|H_0 + \lambda V|\psi_n\rangle = E_n^{(0)} + \lambda V_{nn} + O(\lambda^2)$$

But now if $|\psi_m\rangle, |\psi_n\rangle \in T_k$

$$\begin{aligned}
\langle\psi_m|H_0 + \lambda V|\psi_n\rangle &= (\langle\phi_m| + \lambda \sum_{m' \notin T_k} \frac{V^*_{m'm}}{E_m^{(0)} - E_{m'}^{(0)}} \langle\phi_{m'}|)(H_0 + \lambda V) \\
&\qquad (|\phi_n\rangle + \lambda \sum_{n' \notin T_k} \frac{V_{n'n}}{E_n^{(0)} - E_{n'}^{(0)}} |\phi_{n'}\rangle) \\
&= \lambda V_{mn} + O(\lambda^2) = O(\lambda^2)
\end{aligned}$$

if $n \neq m$. And if $|\psi_m\rangle \notin T_k, |\psi_n\rangle \in T_k$

$$\begin{aligned}
\langle\psi_m|H_0 + \lambda V|\psi_n\rangle &= (\langle\phi_m| + \lambda \sum_{m' \neq m} \frac{V^*_{m'm}}{E_m^{(0)} - E_{m'}^{(0)}} \langle\phi_{m'}|)(H_0 + \lambda V) \\
&\qquad (|\phi_n\rangle + \lambda \sum_{n' \notin T_k} \frac{V_{n'n}}{E_n^{(0)} - E_{n'}^{(0)}} |\phi_{n'}\rangle) \\
&= \lambda V_{mn} + \lambda E_m^{(0)} \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}} + \lambda E_n^{(0)} \frac{V^*_{nm}}{E_m^{(0)} - E_n^{(0)}} + O(\lambda^2) = O(\lambda^2)
\end{aligned}$$

same as (3.24).

So the "energy expectation" (quotation because ψ is not normalized) has off diagonal $N_k \times N_k$ block corresponding the states in T_k

$$\langle\psi_m|H_0 + \lambda V|\psi_n\rangle = \begin{pmatrix}
E_a^{(0)} + \lambda V_{aa} & & & & & \\
& \ddots & & & & \\
& & E_k^{(0)} + \lambda V_{11} & \cdots & \lambda V_{mn} & & \\
& & \vdots & & \vdots & & \\
& & \lambda V_{nm} & \cdots & E_k^{(0)} + \lambda V_{nn} & & \\
& & & & & \ddots & \\
& & & & & & E_b^{(0)} + \lambda V_{bb}
\end{pmatrix} \tag{3.26}$$

What we need to do is to first pick orthonormal $|\phi_n\rangle \in T_k$, calculate V_{mn}'s, then diagonal the block

$$\begin{pmatrix} \lambda V_{11} & \cdots & \lambda V_{mn} \\ \vdots & & \vdots \\ \lambda V_{nm} & \cdots & \lambda V_{nn} \end{pmatrix}$$

the resulting eigenvalues are the energy corrections, which are just

$$\langle \phi_n | V | \phi_n \rangle$$

evaluated using the eigenvectors and the wave function corrections, if $n \in T_k$

$$|\psi_n\rangle = |\phi_n\rangle + \lambda \sum_{n' \notin T_k} \frac{V_{n'n}}{E_n^{(0)} - E_{n'}^{(0)}} |\phi_{n'}\rangle$$

If $n \notin T_k$

$$|\psi_n\rangle = |\phi_n\rangle + \lambda \sum_{n' \neq n} \frac{V_{n'n}}{E_n^{(0)} - E_{n'}^{(0)}} |\phi_{n'}\rangle$$

Question what happens, if we first pick a different set of orthonormal $|\phi_n\rangle \in T_k$, then calculating V_{mn} will give different numbers? Luckily the two sets of orthonormal $|\phi_n\rangle$ are unitary related, so the new V_{mn} is

$$U^\dagger V U$$

of the old V_{mn} so the eigenvalues are the same.

2nd Order degenerated Perturbation

(3.16), (3.17) have to be modified.

For (3.16) if at least one of $n, n' \notin T_k$

$$S_{n'n}^{(2)} = \frac{1}{E_n^{(0)} - E_{n'}^{(0)}} (\sum_{n''} V_{n'n''} S_{n''n}^{(1)} - S_{n'n}^{(1)} E_n^{(1)})$$

and use result from 1st order degenerated perturbation, put $S_{ij}^{(1)}$ to 0 if $i, j \in T_k$.

The problem raises when both $n, n' \in T_k$. Suppose $n_1, n_2 \in T_k$. Let us focus on (3.14), put $n = n_1$ $n' = n_2$ into (3.14). Ignoring $S_{n_1 n_2}^{(2)}$, because it is higher order, then (3.14) becomes

$$\sum_{n''\notin T_k} V_{n_2n''}S^{(1)}_{n''n_1} + \underbrace{V_{n_2n_1}}_{0}S^{(1)}_{n_1n_1} + V_{n_2n_2}S^{(1)}_{n_2n_1} + \underbrace{V_{n_2n_3}}_{0}S^{(1)}_{n_3n_1} + ... = S^{(1)}_{n_2n_1}V_{n_1n_1}$$

$V_{n_2n_1} = V_{n_2n_3} = ... = 0$ because of the diagonalization we did before. So we find

$$S^{(1)}_{n_2n_1} = \frac{1}{V_{n_1n_1} - V_{n_2n_2}} \sum_{n''\notin T_k} V_{n_2n''} \frac{V_{n''n_1}}{E^{(0)}_{n_1} - E^{(0)}_{n''}} \tag{3.27}$$

This is nominal 1st order, but it is actually 2nd order, because it has the form whose numerator is V^2 and denominator is $\sim \Delta E^2$.

Hence the corrected wave function is, if $n \notin T_k$, same as (3.18). If $n \in T_k$

$$\begin{aligned}
|\psi_n\rangle &= |\phi_n\rangle + \lambda \sum_{n'\notin T_k} \frac{V_{n'n}}{E^{(0)}_n - E^{(0)}_{n'}} |\phi_{n'}\rangle + \\
&\lambda^2 \left\{ \sum_{n'\notin T_k} \frac{|\phi_{n'}\rangle}{E^{(0)}_n - E^{(0)}_{n'}} \left(\sum_{n''\notin T_k} \frac{V_{n'n''}V_{n''n}}{E^{(0)}_n - E^{(0)}_{n''}} - \frac{V_{nn}V_{n'n}}{E^{(0)}_n - E^{(0)}_{n'}} \right) - \frac{|\phi_n\rangle}{2} \sum_{n'\notin T_k} \frac{|V_{n'n}|^2}{\left(E^{(0)}_n - E^{(0)}_{n'}\right)^2} \right\} \\
&+\lambda^2 \{ \sum_{\substack{n' \in T_k \\ n' \neq n}} \frac{|\phi_{n'}\rangle}{V_{nn} - V_{n'n'}} \sum_{n''\notin T_k} V_{n'n''} \frac{V_{n''n}}{E^{(0)}_n - E^{(0)}_{n''}} \}
\end{aligned}$$

The 2nd order energy correction is similar to (3.15), if $n \in T_k$,

$$E^{(2)}_n = \sum_{n'} V_{nn'}S^{(1)}_{n'n} = \sum_{n'\notin T_k} \frac{|V_{nn'}|^2}{E^{(0)}_n - E^{(0)}_{n'}} + \sum_{\substack{n' \in T_k \\ n' \neq n}} \frac{V_{nn'}}{V_{nn} - V_{n'n'}} \sum_{n''\notin T_k} V_{n'n''} \frac{V_{n''n}}{E^{(0)}_n - E^{(0)}_{n''}}$$

Everything looks good excepts what if $V_{n_1n_1} = V_{n_2n_2}$ so (3.27) doesn't apply, then we have to diagonalize matrix again. Similar to (3.26), below we illustrate a 2×2 block up to 2nd order.

$$\langle\psi_m|H_0 + \lambda V|\psi_n\rangle =$$

$$
\begin{pmatrix}
E_n^{(0)} + \lambda V_{nn} + \lambda^2 \sum\limits_{n' \neq n} \frac{|V_{nn'}|^2}{E_n^{(0)} - E_{n'}^{(0)}} & & & \\
& \ddots & & \\
& & \boxed{} & \\
& & & \ddots
\end{pmatrix}
$$

where the block looks like

$$
\begin{pmatrix}
E_{n_1}^{(0)} + \lambda V_{n_1 n_1} + \lambda^2 \sum\limits_{n' \notin T_k} \frac{\left|V_{n_1 n'}\right|^2}{E_{n_1}^{(0)} - E_{n'}^{(0)}} & \lambda^2 \sum\limits_{n' \notin T_k} \frac{V_{n_1 n'} V_{n' n_2}}{E_{n_2}^{(0)} - E_{n'}^{(0)}} \\
\lambda^2 \sum\limits_{n' \notin T_k} \frac{V_{n_2 n'} V_{n' n_1}}{E_{n_1}^{(0)} - E_{n'}^{(0)}} & E_{n_2}^{(0)} + \lambda V_{n_2 n_2} + \lambda^2 \sum\limits_{n' \notin T_k} \frac{\left|V_{n_2 n'}\right|^2}{E_{n_2}^{(0)} - E_{n'}^{(0)}}
\end{pmatrix}
$$

The eigenvalue of the block will be the corrected energy up to 2nd order.

3.5 Stark Effect

This is an example of 1st order degenerated perturbation theory.

Apply a uniform electric field $E\hat{z}$ to Hydrogen atom. We will see this gives 2 polarizations. Although classically we only see wrongly one polarization, e^- move toward $-z$, reducing energy and producing electric dipole

$$
\vec{D} = \alpha \vec{E}
$$

Classically the energy shift will be

$$
\epsilon = -\vec{D} \cdot \vec{E} \propto -E^2
$$

QM gives linear E dependence and quadratic dependence, depending on the strength of the $\vec{E}$ field.

Lecture 20 (11/25/13)

$$
H = \frac{\vec{p}^2}{2m} - \frac{e^2}{r} + eEr\cos\theta
$$

suppose E is small, 1st order perturbation

$$E_{nlm}^{(1)} = \langle nlm|eEr\cos\theta|nlm\rangle = 0$$

hence we have degenerate perturbation for each n. Suppose we are interested in energy shift for $n = 2$ and $n = 2$ has 4 unperturbed states $|2s\rangle$, $|2p\rangle$, but

$$\langle n'l'm'|z|nlm\rangle = 0$$

if $m \neq m'$, so that in the basis of $\{|2s0\rangle, |2p,0\rangle, |2p,1\rangle, |2p,-1\rangle\}$

$$V = \begin{pmatrix} 0 & V_{2s0,2p0} & & \\ V_{2p0,2s0} & 0 & & \\ & & 0 & \\ & & & 0 \end{pmatrix} \tag{3.28}$$

we only have to diagonalize 2×2 matrix

$$\begin{aligned}
\langle\vec{r}|2s, m = 0\rangle &= \frac{1}{2\sqrt{\pi}}\left(\frac{1}{2a}\right)^{3/2}(2 - \frac{r}{a})e^{-r/2a} \\
\langle\vec{r}|2p, m = 0\rangle &= \frac{1}{2\sqrt{\pi}}\cos\theta\left(\frac{r}{\sqrt{3}a}\right)\left(\frac{1}{2a}\right)^{3/2} e^{-r/2a}
\end{aligned}$$

$$\begin{aligned}
V_{2s0,2p0} &= \int d\Omega\int r^2 dr\frac{1}{4\pi}\left(\frac{1}{2a}\right)^{3/2}\cos^2\theta eEr(2 - \frac{r}{a})\frac{r}{a}e^{-r/a} \\
&= \frac{1}{3}\left(\frac{1}{2a}\right)^{3/2} eEa\int_0^\infty dye^{-y}(2y^4 - y^5) \text{ set } y = r/a \\
&= \frac{eEa}{24}4\cdot 3\cdot 2\cdot(2 - 5) \\
&= -3eEa
\end{aligned}$$

So the block in (3.28)

$$-3eEa\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$$

has eigenstates, eigenvalues

$$\begin{aligned} |\psi_\pm\rangle &= \frac{1}{\sqrt{2}}(|2s0\rangle \pm |2p0\rangle) \\ E_\pm^{(1)} &= \mp 3eEa \end{aligned}$$

We get linear Stark effect, no seen classically.

What do $|\psi_\pm\rangle$ look like?

$$|\psi_\pm|^2 \sim (2 - \frac{r}{a} \pm z)^2 e^{-r/a}$$

For $|\psi_+\rangle$, it changes the spherical symmetric $|2s0\rangle$ e^- cloud. If $r/a < 2$, then more probable that the e^- will be found the top of the spherical shell; if $r/a > 2$, then more probable that the e^- will be found the bottom of the spherical shell. So the e^- cloud is no longer spherical symmetric. It is elongated and the center of e^- cloud is draft downward, which creates a upward dipole moment that is parallel to the external $\vec{E}$ so the energy is lower.

$|\psi_-\rangle$ is opposite.

How to get quadratic Stark effect?

Take H_2O molecule. It has intrinsic dipole moment. The chemical bond forces of H_2O are strong so in the present of external $\vec{E}$ we assume H_2O will only rotate i.e. the shape does not change

$$H = \frac{L^2}{2I} + aeE\cos\theta$$

$I \sim Ma^2$, $a =$ Bohr radius. If E not strong, $aeE\cos\theta$ is perturbation, but unlike before,

$$V_{2s0,2p0} = 0$$

We need 2nd order degenerated perturbation, which will give quadratic Stark effect.

However if $\vec{E}$ is very strong, we will take $\frac{L^2}{2I}$ to be perturbation, and the result is linear Stark effect. The boundary between weak and strong field is

$$\frac{\hbar^2}{2Ma^2} \text{ v.s.} eaE \implies E \sim 10^5 \frac{\text{vols}}{\text{cm}}$$

3.6 Fine Structure

This is historically first correction to Balmer series, including lowest order of relativistic effect on Hydrogen spectrum.

We argue it is at the order of

$$\frac{v^2}{c^2}$$

$v \sim p/m \sim \hbar/am$, $a = \hbar^2/me^2$, $v/c \sim e^2/\hbar c = \alpha$, hence fine structure correction is at order of α^2. One can do the whole fine structure business in the content of Dirac equation. But that will bring in all the complication associate with Pauli matrices, e^-e^+ etc. We don't do that way.

$$\begin{aligned} E &= \sqrt{m^2c^4 + p^2c^2} = mc^2\left(1 + \frac{p^2}{m^2c^2}\right)^{1/2} \\ &= mc^2\left(1 + \frac{p^2}{2m^2c^2} - \frac{1}{8}\frac{p^4}{m^4c^4} + ...\right. \\ &= mc^2 + \frac{p^2}{2m} - \frac{1}{8}\frac{p^4}{m^3c^2} + ... \end{aligned}$$

$$E_{n,l}^{(1)} = \left\langle n, l \middle| -\frac{p^4}{8m^3c^2} \middle| n, l \right\rangle$$

This is 1st order degenerated perturbation for each n, but luckily it is already diagonalized.

$$E_{n,l}^{(1)} = -\frac{1}{2mc^2}\left\langle n, l \middle| \left(\frac{p^2}{2m} - \frac{e^2}{r} + \frac{e^2}{r}\right)^2 \middle| n, l \right\rangle$$

$$\begin{aligned} \left(\frac{p^2}{2m} - \frac{e^2}{r} + \frac{e^2}{r}\right)^2 &= (H_0 + \frac{e^2}{r})^2 \\ &= H_0^2 + 2H_0\frac{e^2}{r} + \frac{e^4}{r^2} \end{aligned}$$

H_0, $\frac{e^2}{r}$ commute,

$$\left\langle n\left|\frac{1}{r}\right|n\right\rangle = \frac{1}{n^2 a} \quad \left\langle n\left|\frac{1}{r^2}\right|n\right\rangle = \frac{1}{n^3 a^2 (l+\frac{1}{2})}$$

so

$$\begin{aligned} E^{(1)}_{n,l} &= -\frac{1}{2mc^2}\left[\left(\frac{me^4}{2n^2\hbar^2}\right)^2 - 4\left(\frac{me^4}{2n^2\hbar^2}\right)\left(\frac{me^4}{n^2\hbar^2}\right) + \frac{e^4}{n^3a^2(l+\frac{1}{2})}\right] \\ &= \frac{me^4}{8n^4\hbar^2}\alpha^2\left(3 - \frac{4n}{l+\frac{1}{2}}\right) \end{aligned} \tag{3.29}$$

The l dependence will be canceled later. This takes care of relativistic effect on kinetic energy.

We now study the other relativistic effect. Suppose e^- is moving with $\vec{v}$ in electric field $\vec{E}$, in the rest frame of e^-, it will see a magnetic field although no B-field in the lab frame, which is the rest of frame of the nuclear, because

$$\begin{cases} E'_{\|=} & E_{\|} \\ E'_{\perp} = & \gamma(\vec{E}_{\perp} + \frac{\vec{v}}{c}\times\vec{B}) \\ B'_{\|=} & B_{\|} \\ B'_{\perp} = & \gamma(B_{\perp} - \frac{\vec{v}}{c}\times\vec{E}) \end{cases}$$

prime for the rest frame of e^-, unprime states for the lab frame. $\|$ is the direction parallel to $\vec{v}$. $\vec{B}=\vec{0}$. The torque on magnetic moment is

$$\frac{d\vec{S}}{dt'} = \vec{\mu}\times\vec{B}' \quad \vec{\mu} = -\frac{ge}{2mc}\vec{S} \quad g = 2(1+\frac{\alpha}{2\pi}+...)$$

So

$$\frac{d\vec{S}}{dt} = \frac{1}{\gamma}\vec{\mu}\times\vec{B}' \tag{3.30}$$

so the extra Hamilton is

$$\frac{1}{\gamma}\left(-\frac{ge}{2mc}\vec{S}\right)\cdot\left(-\gamma\frac{\vec{v}}{c}\times\vec{E}\right) \sim \vec{L}\cdot\vec{S}$$

The electric field is due to central potential

$$\vec{E} = \frac{e\vec{r}}{r^3}$$

So the interaction energy

$$U = \frac{ge^2}{2m^2c^2}\frac{1}{r^3}\vec{S}\cdot(m\vec{v}\times\vec{r}) \sim \vec{S}\cdot\vec{L} \tag{3.31}$$

That is why it is called spin-orbit interaction.

3.7 Thomas Precession

It turns out that (3.31) is twice larger than it should be. We need to take Thomas precession seriously. In other words the comoving frame e^- in non collinear boosts resulting rotations, then we know even classically

$$\left.\frac{d\vec{S}}{dt}\right|_{\text{rotation coor}} = \left.\frac{d\vec{S}}{dt}\right|_{\text{rotation coor}} - \vec{w}\times\vec{S}$$

so the interaction energy is reduced by amount $\vec{w}\cdot\vec{S}$ from (3.31)

To find $\vec{w}$, suppose at the instance, e^- is changing velocity from $\vec{v}$ to $\vec{v}+\Delta\vec{v}$, and $\Delta\vec{v}$ has an angle $\Delta\theta$ with $\vec{v}$, so

$$|\vec{v}|\Delta\theta = |\Delta\vec{v}| = a\Delta t \text{ or } \Delta\theta = \frac{|\Delta\vec{v}|}{|\vec{v}|}$$

The comoving frame of e^-, which is moving at $\vec{v}$ relative to lab frame, sees

$$|\Delta\vec{v}'| = \gamma|\Delta\vec{v}|$$

so

$$\Delta\theta' = \frac{|\Delta\vec{v}'|}{|\vec{v}|} = \gamma\Delta\theta$$

This tells us the angle speed of the rotation of the comoving

$$|\vec{w}| = \frac{\Delta\theta' - \Delta\theta}{\Delta t} = \frac{(\gamma-1)a\Delta t}{v\Delta t}$$

The direction of the rotation is of course

$$\hat{v} \times \hat{a}$$

so

$$\vec{w}_{Thomas} = \vec{v} \times \vec{a}\frac{\gamma - 1}{v^2} \approx (\vec{v} \times \vec{a})\frac{1}{v^2}\left(\frac{1}{2}\frac{v^2}{c^2}\right)$$

where

$$a = \frac{e\vec{E}}{m}$$

So

$$\vec{w} \cdot \vec{S} = \frac{e}{2mc^2}\vec{S} \cdot \left(\vec{v} \times \vec{E}\right)$$

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Therefore

$$H_{SO} = -\frac{(g-1)e^2}{2m^2c^2}\frac{\vec{L} \cdot \vec{S}}{r^3} \tag{3.32}$$

$\vec{L} \cdot \vec{S}$ term is rotational invariant. We would like to define

$$\vec{J} = \vec{L} + \vec{S}$$

then $\vec{J}$ is also an angular momentum vector, because

$$[J_i, L_j] = i\hbar\epsilon_{ijk}L_k \quad [J_i, S_j] = i\hbar\epsilon_{ijk}S_k$$

imply

$$[J_i, J_j] = [J_i, L_j + S_j] = i\hbar\epsilon_{ijk}J_k$$

More

$$[J_i, \vec{L} \cdot \vec{S}] = 0$$

or

$$e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}\vec{L} \cdot \vec{S}e^{i\vec{J}\cdot\hat{n}\theta/\hbar} = \vec{L} \cdot \vec{S}$$

If we are allowed to add angular operators, we should be allowed to add states.

4 Theory of Angular Momentum

4.1 Addition of Angular Momenta

We want to combine independent QM systems. For example, states of $\vec{L}$ and states of $\vec{S}$. E.g. $l = 1$

$$Y_{11}(\theta,\phi), Y_{10}(\theta,\phi), Y_{1-1}(\theta,\phi) \quad \chi = \begin{pmatrix} \chi_{\frac{1}{2}} \\ \chi_{-\frac{1}{2}} \end{pmatrix}$$

In general we have two QM vector spaces V_1, V_2 with bases $\{v_i^{(1)}\}_{1\leq i\leq d_1}$ and $\{v_j^{(2)}\}_{1\leq j\leq d_2}$. Mathematically there are two way to combine them: Cartesian product, Tensor product.

Cartesian product

$$V_1 \oplus V_2$$

is a $d_1 + d_2$ vector space with basis $v_1^{(1)}, ..., v_{d_1}^{(1)}, v_1^{(2)}, ..., v_{d_2}^{(2)}$.

$$|\psi\rangle = \sum_{i=1}^{d_1} \psi_i v_i^{(1)} + \sum_{j=1}^{d_2} \psi_j v_j^{(2)}$$

This formula works if $v_i^{(1)}$, $v_j^{(2)}$ are orthonormal, i.e.

$$v_i^{(a)} v_j^{(b)} = \delta_{ab}\delta_{ij}$$

This formalism is very useful for classical mechanics. Say combine two particles states into one states

$$(x^{(1)}, y^{(1)}, z^{(1)}, x^{(2)}, y^{(2)}, z^{(2)})$$

However it is disaster for QM, writing

$$\psi = a\,|11\rangle + b\,|10\rangle + c\,|1-1\rangle + d\,|\uparrow\rangle + e\,|\downarrow\rangle$$

doesn't make sense.

For QM we use tensor product, which doesn't make sense for classical mechanics.

$$V_1 \otimes V_2$$

is a $d_1 \times d_2$ dimensional vector space with basis $\{v_i^{(1)} \otimes v_j^{(2)}\}_{\substack{1 \le i \le d_1 \\ 1 \le j \le d_2}}$. The we write

$$\psi = \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} c_{ij} v_i^{(1)} \otimes v_j^{(2)} \tag{4.1}$$

where $|c_{ij}|^2$ is probability of finding the eigenvalues of $\left|v_i^{(1)}\right\rangle, \left|v_j^{(2)}\right\rangle$ simultaneously. For the case of $l = 1$ combines with spin

$$\psi = \sum_{m_l=-1}^{1} \sum_{m_s=-1/2}^{1/2} c_{ij} \left|m_l\right\rangle \otimes \left|m_s\right\rangle$$

The continuous variable version of this is

$$\psi = \int d^3x \sum_{m_s=-1/2}^{1/2} c_m(x) \left|x\right\rangle \otimes \left|m_s\right\rangle$$

Notice (4.1) is not equal to

$$\left(\sum_{i=1}^{d_1} c_i^{(1)} v_i^{(1)}\right) \otimes \left(\sum_{j=1}^{d_2} c_j^{(2)} v_j^{(2)}\right)$$

This is the fundamental of entanglement.

4.2 Clebsch–Gordan coefficients

Consider two angular momentum operation

$$\vec{J}^{(1)} \ \& \ \vec{J}^{(2)}$$

For each we consider eigenstates of $\left(\vec{J}^{(a)}\right)^2$ & $\vec{J}_z^{(a)}$, $a = 1, 2$. Clearly

$$\begin{aligned} \left(\vec{J}^{(a)}\right)^2 |j_a, m_a\rangle &= \hbar^2 j_a(j_a+1) |j_a, m_a\rangle \\ \vec{J}_z^{(a)} |j_a, m_a\rangle &= \hbar m_a |j_a, m_a\rangle \end{aligned}$$

Let us designate the basis of $\vec{J}^{(1)} + \vec{J}^{(2)}$

$$|j_1, m_1; j_2, m_2\rangle \equiv |j_1, m_1\rangle \otimes |j_2, m_2\rangle$$

which is $(2j_1+1)(2j_2+1)$ dimensional. The same vector space can be characterized by another basis, eigenvectors for J^2 & J_z

$$\begin{aligned} J^2 |j, m; j_1, j_2\rangle &= \hbar^2 j(j+1) |j, m; j_1, j_2\rangle \\ J_z |j, m; j, j_2\rangle &= \hbar m |j, m; j_1, j_2\rangle \end{aligned}$$

Since $J_z = J_z^{(1)} + J_z^{(2)}$,

$$m = m_1 + m_2 \tag{4.2}$$

The conversion between $|j, m; j_1, j_2\rangle$ and $|j_1, m_1; j_2, m_2\rangle$ is

$$\begin{aligned} |j, m; j_1, j_2\rangle &= \sum_{m_1, m_2} C(jm; j_1 m_1 j_2 m_2) |j_1, m_1; j_2, m_2\rangle \\ &= \sum_{m_1+m_2=0} C(jm; j_1 m_1 j_2 m_2) |j_1, m_1; j_2, m_2\rangle \end{aligned}$$

$C(jm; j_1 m_1 j_2 m_2) = \langle j_1, m_1; j_2, m_2 | j, m; j_1, j_2\rangle$. To save chalk, we write

$$\langle j, m | j_1, m_1; j_2, m_2\rangle$$

called Clebsch–Gordan coefficients.

From (4.2),

$$\langle j, m | j_1, m_1; j_2, m_2\rangle \neq 0 \text{ unless } m = m_1 + m_2$$

Since

$$-j \leq m \leq j$$

and $j_1 + j_2$ is the largest value of j, there is only one state with $j = j_1 + j_2$ and $m = m_1 + m_2$. Hence we find the CG coefficient is 1

$$|j_1 + j_2, j_1 + j_2, j_1, j_1\rangle = 1\, |j_1 j_1\rangle \otimes |j_2 j_2\rangle \tag{4.3}$$

Using (2.31) apply $J_x - iJ_y$ to (4.3)

$$LHS = \hbar\sqrt{2(j_1 + j_2)}\, |j_1 + j_2, j_1 + j_2 - 1, j_1, j_1\rangle$$

$$RHS = \hbar\sqrt{2j_1}\, |j_1 j_1 - 1\rangle \otimes |j_2 j_2\rangle + \hbar\sqrt{2j_2}\, |j_1 j_1\rangle \otimes |j_2 j_2 - 1\rangle$$

Hence we found

$$|j_1 + j_2, j_1 + j_2 - 1, j_1, j_1\rangle = \sqrt{\frac{j_1}{j_1 + j_2}}\, |j_1 j_1 - 1\rangle \otimes |j_2 j_2\rangle + \sqrt{\frac{j_2}{j_1 + j_2}}\, |j_1 j_1\rangle \otimes |j_2 j_2 - 1\rangle \tag{4.4}$$

Then we argue since

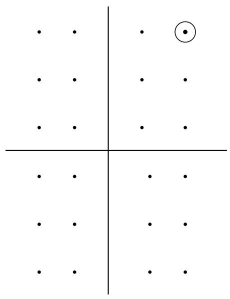
$$\sqrt{\frac{j_2}{j_1 + j_2}}\, |j_1 j_1 - 1\rangle \otimes |j_2 j_2\rangle - \sqrt{\frac{j_1}{j_1 + j_2}}\, |j_1 j_1\rangle \otimes |j_2 j_2 - 1\rangle \tag{4.5}$$

is orthogonal to $|j_1 + j_2, j_1 + j_2 - 1, j_1, j_1\rangle$, it must be

$$|j_1 + j_2 - 1, j_1 + j_2 - 1, j_1, j_1\rangle \tag{4.6}$$

because applying $J_x + iJ_y$ to (4.5) is 0.

Let x, y axes represent m_1 and m_2. The graph shows $j_1 = 2$, $j_2 = 3$. There should be dots on the axes if j_1 or j_2 is integer.



We start from $\odot$ state, then use $J_x - iJ_y$ and orthogonalization to get 2 states

$$|j_1+j_2, j_1+j_2-1, j_1, j_1\rangle\,, |j_1+j_2-1, j_1+j_2-1, j_1, j_1\rangle$$

which can be written in terms of

$$|j_1 j_1 - 1; j_2 j_2\rangle\,, |j_1 j_1; j_2 j_2 - 1\rangle$$

which are states that lie on the line right below $\odot$ with slope -1.

Note: the new orthogonal state $|j_1+j_2-1, j_1+j_2-1, j_1, j_1\rangle$ has an undetermined ± 1 phase factor. It is set by the extra symmetric impositions:

$$\langle j, m|j_1, m_1; j_2, m_2\rangle = (-1)^{j-j_1-j_2} \langle j, m|j_2, m_2; j_1, m_1\rangle \tag{4.7}$$

$$\langle j, j_1 - j_2|j_1, j_1; j_2, -j_2\rangle > 0 \tag{4.8}$$

Then use $J_x - iJ_y$ and orthogonalization to get 3 states

$$|j_1+j_2, j_1+j_2-2, j_1, j_1\rangle\,, |j_1+j_2-1, j_1+j_2-2, j_1, j_1\rangle\,, |j_1+j_2-2, j_1+j_2-2, j_1, j_1\rangle \tag{4.9}$$

which can be written in terms of states that lie on the line right below $\odot$ with slope -1 associated with $m = j_1 + j_2 - 2$.

From the last item in (4.9), it seems like we can apply the process $(j_1 + j_2)$ times to get $|0, 0, j_1, j_2\rangle$ state. Actually it is only possible if $j_1 = j_2$. Because the line with slope -1 has maximum $2\min(j_1, j_2) + 1$ elements, after that line is reached, orthogonality is not possible, because the dimension of vector space of that m is on longer increasing. Hence j stops going down. Thus

$$|j_1 - j_2| \leq j \leq j_1 + j_2$$

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From the process above, applying lowering operator always returns real coefficients and Gram-Schmidt in vector space of real coefficients returns real coefficients, so CG coefficients are real.

For consistency we check that the dimension of $J_1 + J_2$ space is the same, $(2j_1+1)(2j_2+1)$, from two base $\{|j_1 m_1\rangle \otimes |j_2 m_2\rangle\}$, $\{|j m j_1 j_2\rangle\}$. Without lost of generality assume $j_1 \leq j_2$

$$\begin{aligned}
\sum_{j=j_2-j_1}^{j_1+j_2}(2j+1) &= \sum_{j=0}^{j_1+j_2}(2j+1) - \sum_{j=j_2-j_1}^{j_2-j_1-1}(2j+1) \\
&= 2\frac{(j_1+j_2)(j_1+j_2+1)}{2} + (j_1+j_2+1) - \\
&\qquad 2\frac{(j_1-j_2)(j_1-j_2-1)}{2} - (j_1-j_2-1+1) \\
&= (j_1+j_2+1)^2 - (j_1-j_2)^2 = (2j_1+1)(2j_2+1)
\end{aligned}$$

Hence both $\{|j_1 m_1\rangle \otimes |j_2 m_2\rangle\}$, $\{|j m j_1 j_2\rangle\}$ span the $J_1 + J_2$ space. Therefore CG base transformation are unique.

Example. combine 2 e^-

$$0 \leq j \leq 1$$

$$\left|11; \frac{1}{2}; \frac{1}{2}\right\rangle = 1\,|\uparrow\rangle \otimes |\uparrow\rangle$$

apply $J_x - iJ_y$

$$\sqrt{2}\left|1, 0; \frac{1}{2}; \frac{1}{2}\right\rangle = |\downarrow\rangle \otimes |\uparrow\rangle + |\uparrow\rangle \otimes |\downarrow\rangle$$

or

$$\left|1, 0; \frac{1}{2}; \frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}|\downarrow\rangle \otimes |\uparrow\rangle + \frac{1}{\sqrt{2}}|\uparrow\rangle \otimes |\downarrow\rangle$$

orthogonal

$$\left|0, 0; \frac{1}{2}; \frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}|\downarrow\rangle \otimes |\uparrow\rangle - \frac{1}{\sqrt{2}}|\uparrow\rangle \otimes |\downarrow\rangle$$

note: why is not

$$\left|0,0;\frac{1}{2};\frac{1}{2}\right\rangle = -\frac{1}{\sqrt{2}}\left|\downarrow\right\rangle\otimes\left|\uparrow\right\rangle + \frac{1}{\sqrt{2}}\left|\uparrow\right\rangle\otimes\left|\downarrow\right\rangle?$$

because of (4.8). More (4.7) imposes $\left|1,0;\frac{1}{2};\frac{1}{2}\right\rangle$ is symmetric wrt to exchange $j_1 \leftrightarrow j_2$, and $\left|0,0;\frac{1}{2};\frac{1}{2}\right\rangle$ is antisymmetric. In other words lowering operator commutes exchanging while orthogonalization gives antisymmetric state.

Apply $J_x - iJ_y$

$$\sqrt{2}\left|1-1;\frac{1}{2};\frac{1}{2}\right\rangle = \frac{1}{\sqrt{2}}\left|\downarrow\right\rangle\otimes\left|\downarrow\right\rangle + \frac{1}{\sqrt{2}}\left|\downarrow\right\rangle\otimes\left|\downarrow\right\rangle$$

or

$$\left|1-1;\frac{1}{2};\frac{1}{2}\right\rangle = \left|\downarrow\right\rangle\otimes\left|\downarrow\right\rangle$$

4.3 Wigner 3j Symbols

This is powerful alternative to CG and it is allowed to explore the symmetry of CG.

First we show how CG transforms under rotations

$$\langle j,m|j_1,m_1;j_2,m_2\rangle = \left\langle j,m;j_1;j_2\left|e^{i\vec{J}\cdot\hat{n}\theta/\hbar}e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}\right|j_1,m_1;j_2,m_2\right\rangle$$

By (2.35) and $\vec{J}$ acts separately as J_1 and J_2,

$$e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}\left|j_1,m_1;j_2,m_2\right\rangle = \sum_{m_1',m_2'}\mathcal{D}^{(j_1)}_{m_1'm_1}(\hat{n},\theta)\mathcal{D}^{(j_2)}_{m_2'm_2}(\hat{n},\theta)\left|j_1,m_1';j_2,m_2'\right\rangle \tag{4.10}$$

and

$$\left\langle j,m;j_1;j_2\right|e^{i\vec{J}\cdot\hat{n}\theta/\hbar} = \left(\sum_{m'}\mathcal{D}^{(j)}_{m'm}(\hat{n},\theta)\left|j,m';j_1;j_2\right\rangle\right)^{\dagger}$$

so

$$\langle j,m|j_1,m_1;j_2,m_2\rangle = \sum_{m',m_1',m_2'}\mathcal{D}^{(j)*}_{m'm}(\hat{n},\theta)\mathcal{D}^{(j_1)}_{m_1'm_1}(\hat{n},\theta)\mathcal{D}^{(j_2)}_{m_2'm_2}(\hat{n},\theta)\left\langle j,m'|j_1,m_1';j_2,m_2'\right\rangle \tag{4.11}$$

Later we will show $\mathcal{D}^{(j)*}_{m'm}(\hat{n},\theta)$ is a rotation too, hence the three rotation permute indices m, m_1, m_2, hence CG coefficient is invariant tensor, just like δ_{ij}, ϵ_{ijk}.

Recall the matrices elements of J_z, $J_x \pm iJ_y$ are real, see (2.33), (2.34), so

$$J_x, J_z \text{ have real matrice elements}$$

$$J_y \text{ has purely imaginary matrice elements}$$

so

$$\left(e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}\right)^* = e^{-i[-J_xn_x+J_yn_y-J_zn_z]\theta/\hbar} \tag{4.12}$$

which is same as

$$e^{-i\pi J_y\theta/\hbar}e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}e^{i\pi J_y\theta/\hbar} \tag{4.13}$$

because the nth term Taylor expansion of (4.13) is

$$\frac{1}{n!}e^{-i\pi J_y/\hbar}[\frac{-i\theta}{\hbar}(J_xn_x+J_yn_y+J_zn_z)]e^{i\pi J_y/\hbar}e^{-i\pi J_y/\hbar}[\frac{-i\theta}{\hbar}(J_xn_x+J_yn_y+J_zn_z)]e^{i\pi J_y/\hbar}\cdot \\ \ldots\cdot e^{-i\pi J_y/\hbar}[\frac{-i\theta}{\hbar}(J_xn_x+J_yn_y+J_zn_z)]e^{i\pi J_y/\hbar} \tag{4.14}$$

There are n number of

$$e^{-i\pi J_y/\hbar}[\frac{-i\theta}{\hbar}(J_xn_x+J_yn_y+J_zn_z)]e^{i\pi J_y/\hbar} = \frac{-i\theta}{\hbar}(-J_xn_x+J_yn_y-J_zn_z)$$

Hence (4.14) is

$$\frac{1}{n!}[\frac{-i\theta}{\hbar}(-J_xn_x+J_yn_y-J_zn_z)]^n$$

which is the nth term expansion of RHS of (4.12).

To understand (4.12), we need to understand $e^{-iJ_y\pi/\hbar}$. Since

$$J_ze^{-iJ_y\pi/\hbar}|j,m\rangle = -e^{-iJ_y\pi/\hbar}J_z|j,m\rangle = -me^{-iJ_y\pi/\hbar}|j,m\rangle$$

$$e^{-iJ_y\pi/\hbar}|j,m\rangle = e^{-i\phi(j,m)}|j,-m\rangle$$

or

$$\left(e^{-iJ_y\pi/\hbar}\right)_{m'm} = \left\langle j,m'\middle|e^{-iJ_y\pi/\hbar}\middle|j,m\right\rangle = e^{i\phi}\delta_{m',-m}$$

Find $e^{i\phi(j,m)}$. We construct $|j,m\rangle$ using additive $2j$ number of spin 1/2 particles. (The construction doesn't work only when $j=0$, $|0,0\rangle$ state is known spherical symmetric.) Suppose among them there are N_+ number of spin up and N_- number of spin down, i.e.

$$|j,m\rangle = \sum c_n \left|\frac{1}{2}, m_1\right\rangle \otimes \left|\frac{1}{2}, m_2\right\rangle \otimes ... \otimes \left|\frac{1}{2}, m_{2j}\right\rangle \tag{4.15}$$

$m_i = \pm\frac{1}{2}$, and

$$m = \frac{N_+ - N_-}{2} \qquad j = \frac{N_+ + N_-}{2}$$

Since

$$e^{-iJ_y\pi/\hbar} = \cos\frac{\pi}{2} I - i\sigma_y \sin\frac{\pi}{2} = \begin{pmatrix} & -1 \\ 1 & \end{pmatrix}$$

$e^{-iJ_y\pi/\hbar}$ acting on (4.15) will flip $\uparrow$ to $\downarrow$ and flip $\downarrow$ to $\uparrow$ with a minus sign, i.e.

$$N_+ \to N_- \qquad N_- \to N_+$$

and bring an extra factor $(-1)^{N_-}$, (note before we applied $J_x - iJ_y$ operator to the tensor product, we choose to do one term at a time, while here we apply $e^{-iJ_y\pi/\hbar}$ to all terms at same time. That is because here we rotate the frame.) hence

$$e^{-iJ_y\pi/\hbar}|j,m\rangle = (-1)^{N_-}|j,-m\rangle = (-1)^{j-m}|j,-m\rangle$$

Similarly show

$$e^{iJ_y\pi/\hbar}|j,m\rangle = (-1)^{N_+}|j,-m\rangle = (-1)^{j+m}|j,-m\rangle$$

Back to (4.11). By (4.13)

$$\begin{aligned}
\mathcal{D}^{(j)*}_{m'm}(\hat{n},\theta) &= \left(e^{-iJ_y\pi/\hbar}\right)^*_{m'm} \\
&= \sum_{m'',m'''} \left\langle m'\middle|e^{-iJ_y\pi/\hbar}\middle|m''\right\rangle \mathcal{D}^{(j)*}_{m''m'''}(\hat{n},\theta) \left\langle m'''\middle|e^{iJ_y\pi/\hbar}\middle|m\right\rangle \\
&= (-1)^{j+m'}\mathcal{D}^{(j)*}_{-m',-m}(\hat{n},\theta)(-1)^{j+m}
\end{aligned}$$

Therefore

$$\begin{aligned}\langle j,m|j_1,m_1;j_2,m_2\rangle &= \sum_{m',m_1',m_2'} \mathcal{D}^{(j)*}_{m'm}(\hat{n},\theta)\mathcal{D}^{(j_1)}_{m_1'm_1}(\hat{n},\theta)\mathcal{D}^{(j_2)}_{m_2'm_2}(\hat{n},\theta)\,\langle j,m'|j_1,m_1';j_2,m_2'\rangle \\ &= (-1)^{2j+m}\sum_{m',m_1',m_2'}(-1)^{m'}\mathcal{D}^{(j)}_{-m',-m}(\hat{n},\theta)\mathcal{D}^{(j_1)}_{m_1'm_1}(\hat{n},\theta)\mathcal{D}^{(j_2)}_{m_2'm_2}(\hat{n},\theta) \\ &\qquad\qquad \langle j,m'|j_1,m_1';j_2,m_2'\rangle\end{aligned}$$

This leads to define Wigner 3j symbol

$$\begin{pmatrix} j & j_1 & j_2 \\ m & m_1 & m_2 \end{pmatrix} = \frac{(-1)^{j_1-j_2}}{\sqrt{2j+1}}(-1)^{-m}\,\langle j,-m|j_1,m_1;j_2,m_2\rangle \tag{4.16}$$

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As we will see the extra constant factor $\frac{(-1)^{j_1-j_2}}{\sqrt{2j+1}}$ will make Winger 3j symbol totally symmetrical. From above we conclude Wigner 3j obey

$$\begin{pmatrix} j & j_1 & j_2 \\ m & m_1 & m_2 \end{pmatrix} = \sum_{m',m_1',m_2'} \mathcal{D}^{(j)}_{m',m}(\hat{n},\theta)\mathcal{D}^{(j_1)}_{m_1'm_1}(\hat{n},\theta)\mathcal{D}^{(j_2)}_{m_2'm_2}(\hat{n},\theta)\begin{pmatrix} j & j_1 & j_2 \\ m' & m_1' & m_2' \end{pmatrix} \tag{4.17}$$

If we construct

$$|j,m\rangle = \sum_{m_1,m_2,m_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}|j_1,m_1\rangle\otimes|j_2,m_2\rangle\otimes|j_3,m_3\rangle \tag{4.18}$$

Clearly the coefficient is 0 if $-m_1 \neq m_2+m_3$, so $m=0$ in the above expression. Moreover it is spherical symmetric, because applying $e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}$ to (4.18) is

$$\begin{aligned}&\sum_{m_1,m_2,m_3}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}\sum_{m_1',m_2',m_3'}\mathcal{D}^{(j_1)}_{m_1',m_1}(\hat{n},\theta)\mathcal{D}^{(j_2)}_{m_2'm_1}(\hat{n},\theta)\mathcal{D}^{(j_3)}_{m_3'm_3}(\hat{n},\theta) \\ &\qquad\qquad |j_1,m_1'\rangle\otimes|j_2,m_2'\rangle\otimes|j_3,m_3'\rangle \\ =&\sum_{m_1',m_2',m_3'}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3' \end{pmatrix}^*|j_1,m_1'\rangle\otimes|j_2,m_2'\rangle\otimes|j_3,m_3'\rangle \\ =&\ (4.18)\end{aligned}$$

therefore (4.18) is $j=0$ state.

There is only one way to construct $|0,0\rangle$ using $\{|j_1,m_1\rangle\otimes|j_2,m_2\rangle\otimes|j_3,m_3\rangle\}_{-j_i\le m_i\le j_i}$ so Wigner 3j symbols are unique. Why is there only one way to construct $|0,0\rangle$ using 3 momentum, $j_{1,2,3}$.

Think this way. We need to find the states, denoted $|j_1',m_1'\rangle$, combing $\vec{j}_2+\vec{j}_3$ gives j_1. Only these states combine with $\vec{j}_1$ will give $j=0$. Hence we are adding

$$|j_1,m_1\rangle\oplus|j_1',m_1'\rangle=|0,0\rangle \tag{4.19}$$

This is only one way to do so because CG are unique. By the same token, getting $|j_1',m_1'\rangle$ for each value of m_1' is too unique.

We now discuss some symmetry properties of Wigner 3j symbols.

We will show that the columns are bound to be cyclic permutation

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}=(\epsilon_{abc})^{j_1+j_2+j_3}\begin{pmatrix} j_a & j_b & j_c \\ m_a & m_b & m_c \end{pmatrix} \tag{4.20}$$

$a,b,c=1,2,3$. Note $j_1+j_2+j_3$ will always be integers.

From (4.17) e.g. exchanging $j\leftrightarrow j_1$ and $m\leftrightarrow m_1$ will not affect (4.17), so interchange columns return Wigner 3j, hence

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}=c(a,b,c)\begin{pmatrix} j_a & j_b & j_c \\ m_a & m_b & m_c \end{pmatrix}$$

$c(a,b,c)$ is some factor. Since

$$\sum_{m_1,m_2}\left(\langle j,m|j_1,m_1;j_2,m_2\rangle\right)^2=\left\||j,m;j_1;j_2\rangle\right\|^2=1,$$

$$\sum_{m,m_1,m_2}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}^2=\frac{2j+1}{2j+1}=1$$

That is the origin of $1/\sqrt{2j+1}$ factor in (4.16). This implies

$$c(a,b,c)=\pm 1$$

Since a permutation of A_3 is product of two transpositions, we study two cases: $c(1,3,2)$ and $c(2,1,3)$. The case $c(3,1,2)$ is similar to $c(2,1,3)$.

By (4.16) and (4.7), exchange j_1, j_2 gives extra

$$(-1)^{2(j_1-j_2)}(-1)^{j_1-j_2-j_3} = (-1)^{j_1+j_2-3j_3} = (-1)^{j_1+j_2+j_3}$$

To find $c(2,1,3)$, consider a special case

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ j_3-j_2 & j_2 & -j_3 \end{pmatrix} = c(2,1,3)\begin{pmatrix} j_2 & j_1 & j_3 \\ j_2 & j_3-j_2 & -j_3 \end{pmatrix}$$

From the condition in (4.8) and (4.16), the sign of LHS above is

$$(-1)^{j_2-j_3-(j_3-j_2)} = (-1)^{2(j_2-j_3)}$$

the sign of $\begin{pmatrix} j_2 & j_1 & j_3 \\ j_2 & j_3-j_2 & -j_3 \end{pmatrix}$ is the sign of

$$(-1)^{j_1-j_3-j_2}\langle j_2,-j_2|j_1,j_3-j_2;j_3,-j_3\rangle$$

Denote $\langle j_2,-j_2|j_1,j_3-j_2;j_3,-j_3\rangle = \diamondsuit$. By (4.8)

$$\langle j_2, j_1-j_3|j_1,j_1;j_3,-j_3\rangle > 0$$

Write

$$|j_2, j_1-j_3; j_1; j_2\rangle = \square\,|j_1,j_1;j_3,-j_3\rangle + (...)\,|...\rangle + ...$$

$\square = \langle j_2, j_1-j_3|j_1,j_1;j_3,-j_3\rangle$. Applying the lowering operator $j_1+j_2-j_3$ times to above, get

$$\begin{aligned} |j_2,-j_2;j_1;j_2\rangle &= \square\sqrt{...}\sqrt{...}\,|j_1,j_3-j_2;j_3,-j_3\rangle + (...)\,|...\rangle + ... \\ &= \diamondsuit\,|j_1,j_3-j_2;j_3,-j_3\rangle + (...)\,|...\rangle + ... \end{aligned}$$

Hence $\diamondsuit > 0$, so

$$(-1)^{2(j_2-j_3)} = c(2,1,3)(-1)^{j_1-j_3-j_2}$$

so

$$c(2,1,3) = (-1)^{j_1+j_2+j_3}$$

(4.20) is proven.

4.4 Fine Structure (continued)

Pick up from (3.32), let

$$J = L + S$$

then

$$E^{(1)SO}_{n,j,l} = -\frac{(g-1)e^2}{2m^2c^2}\left\langle n,j,l,m_j\left|\frac{\vec{L}\cdot\vec{S}}{r^3}\right|n,j,l,m_j\right\rangle$$

This is 1st order degenerated perturbation for each n, and it is diagonalized in $\left|j, m_j; l; \frac{1}{2}\right\rangle$.

$$\left\langle n,l\left|\frac{1}{r^3}\right|n,l\right\rangle = \frac{1}{a^3}\frac{1}{n^3}\frac{1}{l(l+\frac{1}{2})(l+1)}$$

$$\vec{L}\cdot\vec{S} = \frac{(L+S)^2 - L^2 - S^2}{2}$$

so

$$E^{(1)SO}_{n,j,l} = -\frac{mc^2\alpha^2}{2n^2}\left[1 - \frac{\alpha^2}{n^2}\left(\frac{n}{j+\frac{1}{2}} - \frac{3}{4}\right)\right]$$

Put $l = j \pm \frac{1}{2}$, into (3.29), and add to above, l dependence cancels.

Fine structure has no l dependence. E.g.

$$E_{2,\frac{3}{2}} - E_{2,\frac{1}{2}} = 10,900\text{MHz}$$

Lamb shift has l dependence. Lamb shift deals with e^- interaction with proton and modifies the EM potential.

4.5 Zeeman Effect

Apply a magnetic field $B\hat{z}$.

$$H = \frac{p^2}{2m} - \frac{e^2}{r} - \frac{p^4}{8m^3c^2} + \underbrace{\frac{(g-1)e^2}{2m^2c^2}\frac{\vec{L}\cdot\vec{S}}{r^3}}_{SO} + \underbrace{\frac{e\hbar\vec{B}}{2mc}(\vec{L}+g\vec{S})}_{Zee}$$

The two disagree on what the "good" basis is for the perturbation.

Depending on B,

$$B \ll 5000 \text{ Gauss } \vec{L}\cdot\vec{S} \text{ dominates}$$

$$B \gg 5000 \text{ Gauss } L_z + gS_z \text{ dominates}$$

Strong Field (Paschen-Back Effect)

$$E^{(0)}_{n,l,m_l,m_s} = -\frac{mc^2\alpha^2}{2n^2} + \frac{e\hbar B}{2mc}(m_l + 2m_s)$$

Because B is strong, the degeneracy is lifted, perturbation on $\frac{\vec{L}\cdot\vec{S}}{r^3}$ will converge.

$$\vec{L}\cdot\vec{S} = \frac{(L_x+iL_y)(S_x+iS_y)}{2} + \frac{(L_x-iL_y)(S_x-iS_y)}{2} + L_zS_z$$

First two terms on the right give 0

$$\begin{aligned} E^{(1)}_{n,l,m_l,m_s} &= \left\langle n,l,m_l,m_s \left| \frac{(g-1)e^2}{2m^2c^2}\frac{\vec{L}\cdot\vec{S}}{r^3} \right| n,l,m_l,m_s \right\rangle \\ &= \frac{(g-1)e^2}{2m^2c^2}\frac{1}{n^3}\frac{1}{a^3}\frac{\hbar^2}{l(l+\frac{1}{2})(l+1)}m_lm_s \end{aligned}$$

for $l \neq 0$.

Weak Field

$$E^{(1)}_{n,j,l,m_j} = \left\langle n,j,l,m_j \left| \frac{e\hbar B}{2mc}(L_z+2S_z) \right| n,j,l,m_j \right\rangle \tag{4.21}$$

One could write the states in $|n,l,m_l,m_s\rangle$using CG to evaluate above, but there is a more beautiful way, evolving Wigner-Eckart theorem.

4.6 Wigner-Eckart Theorem

Define an set of $2j+1$ operators $O_m^{(j)}$ as belonging to the j representation of the rotation group s.t.

$$e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}O_m^{(j)}e^{i\vec{J}\cdot\hat{n}\theta/\hbar} = \sum_{m'}\mathcal{D}_{m'm}^{(j)}(\hat{n},\theta)O_{m'}^{(j)}$$

If

$$|v\rangle \to e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}|v\rangle$$

then

$$O|v\rangle \to e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}Oe^{i\vec{J}\cdot\hat{n}\theta/\hbar}e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}|v\rangle = e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}O|v\rangle$$

The combination $O_{m_1}^{(j)}|j_2,m_2\rangle$ transforms in the same way as $|j_1,m_1;j_2,m_2\rangle$. Indeed

$$\begin{aligned} e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}O_{m_1}^{(j_1)}|j_2,m_2\rangle &= e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}O_{m_1}^{(j_1)}e^{i\vec{J}\cdot\hat{n}\theta/\hbar}e^{-i\vec{J}\cdot\hat{n}\theta/\hbar}|j_2,m_2\rangle \\ &= \sum_{m_1',m_2'}\mathcal{D}_{m_1'm_1}^{(j_1)}(\hat{n},\theta)\mathcal{D}_{m_2'm_2}^{(j_2)}(\hat{n},\theta)O_{m_1'}^{(j_1)}|j_2,m_2'\rangle \end{aligned}$$

This is reminiscent of (4.10), from what allows (4.10), we infer that $\left\langle j_3,m_3\middle|O_{m_1}^{(j_1)}\middle|j_2,m_2\right\rangle$ transforms just like CG coefficients. Since we showed the dependence of CG coefficients on m_1, m_2, and m_3 are unique up to some multiplicative constants, thus

$$\left\langle j_1,m_1\middle|O_{m_2}^{(j_2)}\middle|j_3,m_3\right\rangle = \langle j_1 \parallel O^{(j_2)} \parallel j_3\rangle\langle j_1,m_1|j_2,m_2;j_3,m_3\rangle \tag{4.22}$$

the constant $\langle j_1 \parallel O^{(j_2)} \parallel j_3\rangle$, called reduced matrix element, is independent of m_1, m_2, and m_3.

Wigner-Eckart applies to rotation O, so does to any vector operators.

4.7 Zeeman Effect (Continued)

We want to evaluate (4.21). First recognize that by (4.22) both

$$\langle n,j,l,m_j|L_i|n,j,l,m_j\rangle \text{ and } \langle n,j,l,m_j|J_i|n,j,l,m_j\rangle \qquad \text{where } i=x,y,z$$

are proportional to the same CG coefficients, so they are too proportional, i.e.

$$\langle n,j,l,m_j|L_i|n,j,l,m_j\rangle = c_l\,\langle n,j,l,m_j|J_i|n,j,l,m_j\rangle$$

Similarly

$$\langle n,j,l,m_j|S_i|n,j,l,m_j\rangle = c_s\,\langle n,j,l,m_j|J_i|n,j,l,m_j\rangle$$

where c_l, c_s are independent of m_j. So (4.21) becomes

$$E^{(1)}_{n,j,l,m_j} = \frac{e\hbar B}{2mc} m_j (c_l + 2c_s)$$

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We want to find c_l and c_s. The trick is to consider

$$\left\langle n,j,l,m_j\middle|\vec{S}\cdot\vec{J}\middle|n,j,l,m_j\right\rangle = \left\langle n,j,l,m_j\middle|\frac{J^2-\vec{L}^2+\vec{S}^2}{2}\middle|n,j,l,m_j\right\rangle = \hbar^2\frac{j(j+1)-l(l+1)+\frac{3}{4}}{2}$$

because

$$\vec{J}=\vec{L}+\vec{S} \quad \vec{L}\cdot\vec{S}=\frac{J^2-L^2-S^2}{2} \implies \vec{S}\cdot\vec{J}=S^2+\vec{L}\cdot\vec{S}$$

On the other hand

$$\begin{aligned}
\left\langle n,j,l,m_j\middle|\vec{S}\cdot\vec{J}\middle|n,j,l,m_j\right\rangle &= \sum_{i=1}^{3}\sum_{m_j'}\left\langle n,j,l,m_j\middle|S_i\middle|n,j,l,m_j'\right\rangle\left\langle n,j,l,m_j'\middle|J_i\middle|n,j,l,m_j\right\rangle \\
&= \sum_{i=1}^{3}\sum_{m_j'} c_l\left\langle n,j,l,m_j\middle|c_l J_i\middle|n,j,l,m_j'\right\rangle\left\langle n,j,l,m_j'\middle|J_i\middle|n,j,l,m_j\right\rangle \\
&= \sum_{i=1}^{3} c_l\left\langle n,j,l,m_j\middle|J_i^2\middle|n,j,l,m_j\right\rangle = \hbar^2 c_l j(j+1)
\end{aligned}$$

From the second equality to the third equality used the fact that c_s is independent of m_j' and i. Therefore

$$c_s = \frac{j(j+1)-l(l+1)+\frac{3}{4}}{2j(j+1)} \tag{4.23}$$

Similarly find

$$c_l = \frac{j(j+1) + l(l+1) - \frac{3}{4}}{2j(j+1)}$$

In the old days, before QM was fully developed. People used vector model (see Griffiths figure 6.10) and claimed

$$\vec{S} = \frac{\vec{S}\cdot\vec{J}}{J^2}\vec{J}$$

where $\frac{\vec{S}\cdot\vec{J}}{J^2}$ corresponded to our c_s and accidentally agreed the calculation (4.23).

4.8 Hyperfine Structure

$$H = \frac{p^2}{2m} - \frac{e^2}{r} - \frac{p^4}{8m^3c^2} + \frac{(g-1)e^2}{2m^2c^2}\frac{\vec{L}\cdot\vec{S}}{r^3} + H^{hfs}$$

After fine structure, there is hyperfine structure that includes the magnetic field of proton magnetic moment

$$\vec{\mu}_p = \frac{g_p e}{2m_p c}\vec{I}$$

$g_p = 5.58$ gyromagnetic ratio, it has a lot anomalously quark QM motion. $\vec{I}$ spin angular moment of the proton.

From (3.4), (3.5)

$$H^{hfs} = e\frac{\vec{p}\cdot\vec{A}(\vec{r})}{mc} + \frac{ge}{2mc}\vec{S}\cdot\vec{B}(\vec{r})$$

where $\vec{A}$ and $\vec{B}$ are produced by $\vec{\mu}_p$.

Find $\vec{A}$. We know what $\vec{B}$ is, far field, a dipole

$$\vec{B}(\vec{r}) = \frac{3\vec{r}(\vec{\mu}_p\cdot\vec{r})}{r^5} - \frac{\vec{\mu}_p}{r^3} \tag{4.24}$$

which average to 0. We don't know what $\vec{B}$ is at the origin. Try

$$A = \frac{\vec{\mu}_p\times\vec{r}}{r^3}$$

then

$$\nabla \times A = \vec{\mu}_p \underbrace{\vec{\nabla} \cdot \frac{\vec{r}}{r^3}}_{\propto \delta^3(\vec{r})} \underbrace{- (\vec{\mu}_p \cdot \nabla) \frac{\vec{r}}{r^3}}_{(4.24)}$$

The δ function is not too problematic, since for $l \neq 0$ wave function vanishes at $\vec{r} = 0$. And for $l = 0$

$$\vec{p} \cdot \vec{A} = \frac{\vec{r} \times \vec{p}}{r^3} \cdot \vec{\mu}_p = \frac{\vec{L}}{r^3} \cdot \vec{\mu}_p = 0$$

To evaluate the proportionality of the δ function, we put

$$\vec{\nabla} \cdot \frac{\vec{r}}{r^3} = c\delta^3$$

Integral the ith component of $\vec{B}$ over a small ball around the origin

$$\begin{aligned}
\int_{|\vec{r}|<\epsilon} d^3 r B_i(\vec{r}) &= \int_{|\vec{r}|<\epsilon} d^3 r \hat{e}_i \cdot (\vec{\nabla} \times \vec{A}) = \int_{|\vec{r}|<\epsilon} d^3 r \nabla \cdot (\vec{A} \times \hat{e}_i) \\
&= \int_{|\vec{r}|=\epsilon} dS \hat{r} \cdot (\vec{A} \times \hat{e}_i) = \int_{|\vec{r}|=\epsilon} d\Omega \frac{\hat{r} \cdot [(\vec{\mu}_p \times \vec{r}) \times \hat{e}_i]}{r} \\
&= \int_{|\vec{r}|=\epsilon} d\Omega [\mu_{pi} - (\vec{\mu}_p \cdot \hat{r}) \hat{r}_i)] \\
&= 4\pi \vec{\mu}_{pi} - \frac{4\pi}{3} \vec{\mu}_{pi} = \frac{8\pi}{3} \vec{\mu}_{pi} \qquad (4.25)
\end{aligned}$$

because (Griffiths problem 6.27)

$$\int_{|\vec{r}|=\epsilon} d\Omega (\vec{\mu}_p \cdot \hat{r}) \hat{r}_i = \vec{\mu}_{pi} \int_{|\vec{r}|=\epsilon} d\Omega \hat{r}_i \hat{r}_i + \vec{\mu}_{pj} \int_{|\vec{r}|=\epsilon} d\Omega \hat{r}_j \hat{r}_i + \vec{\mu}_{pk} \int_{|\vec{r}|=\epsilon} d\Omega \hat{r}_k \hat{r}_i$$

$$\int_{|\vec{r}|=\epsilon} d\Omega \hat{r}_j \hat{r}_i = 0$$

for $j \neq i$, because for each $|\vec{r}| = \epsilon$, one can find another $\vec{r}'$ s.t. $\hat{r}'_i = \hat{r}_i$ and $\hat{r}'_j = -\hat{r}_j$.

$$\int_{|\vec{r}|=\epsilon} d\Omega \hat{r}_i \hat{r}_i = \frac{4\pi}{3}$$

because of the spherical symmetry, assume $i = z$

$$\int_{|\vec{r}|=\epsilon} d\Omega \hat{r}_i \hat{r}_i = \int_{|\vec{r}|=\epsilon} d\Omega \hat{r}_z \hat{r}_z = \int d\cos\theta \int d\phi \cos^2\theta = 2\pi\frac{2}{3}$$

On the other hand

$$\begin{aligned}
\int_{|\vec{r}|<\epsilon} d^3r \vec{B}(\vec{r}) &= \int_{|\vec{r}|<\epsilon} d^3r \left(\frac{3\vec{r}(\vec{\mu}_p \cdot \vec{r})}{r^5} - \frac{\vec{\mu}_p}{r^3} + c\delta^3(\vec{r}) \right) \\
&= \int_{|\vec{r}|<\epsilon} d^3r c\delta^3(\vec{r}) \\
&= c
\end{aligned}$$

Compare to (4.25),

$$c = \frac{8\pi}{3}$$

Therefore

$$\vec{B}(\vec{r}) = \frac{3\vec{r}(\vec{\mu}_p \cdot \vec{r})}{r^5} - \frac{\vec{\mu}_p}{r^3} + \frac{8\pi}{3}\vec{\mu}_p\delta^3(\vec{r})$$

$$\begin{aligned}
H^{hfs} &= \frac{e}{mc}\frac{\vec{L}}{r^3} \cdot \vec{\mu}_p + \frac{g_e e}{2mc}\vec{S} \cdot \left(\frac{3\vec{r}(\vec{\mu}_p \cdot \vec{r})}{r^5} - \frac{\vec{\mu}_p}{r^3} + \frac{8\pi}{3}\vec{\mu}_p\delta^3(\vec{r}) \right) \\
&= \frac{g_p e^2}{2m_p m_e c^2}\frac{\vec{L} \cdot \vec{I}}{r^3} + \frac{g_p g_e e^2}{4m_p m_e c^2} \left(\frac{3(\vec{S} \cdot \vec{r})(\vec{I} \cdot \vec{r})}{r^5} - \frac{\vec{S} \cdot \vec{I}}{r^3} + \frac{8\pi}{3}\vec{S} \cdot \vec{I}\delta^3(\vec{r}) \right)
\end{aligned}$$

m_I, m_s mix degeneracy. The good basis is F^2, F_z, where $\vec{F}$ the total angular momentum

$$\vec{F} = \vec{L} + \vec{S} + \vec{I}$$

For simplicity, assume s-state $l = 0$, then $\vec{I}$, $\vec{S}$ commute with $\vec{F}$, and

$$F^2 = I^2 + 2\vec{I} \cdot \vec{S} + S^2 = \frac{3}{4}\hbar^2 + 2\vec{I} \cdot \vec{S} + \frac{3}{4}\hbar^2$$

$\frac{3(\vec{S}\cdot\vec{r})(\vec{I}\cdot\vec{r})}{r^5} - \frac{\vec{S}\cdot\vec{I}}{r^3}$ average to 0, thus

$$\begin{aligned}
E^{(1)}_{n,j=\frac{1}{2},l=0,f,m_f} &= \left\langle n, j=\frac{1}{2}, l=0, f, m_f \middle| \frac{g_p g_e e^2}{4 m_p m_e c^2}\frac{8\pi}{3}\vec{S}\cdot\vec{I}\delta^3(\vec{r}) \middle| n, j=\frac{1}{2}, l=0, f, m_f \right\rangle \\
&= \frac{g_p g_e e^2}{4 m_p m_e c^2}\frac{8\pi}{3}\left\langle n, j=\frac{1}{2}, l=0, f, m_f \middle| \frac{F^2 - \frac{3}{2}\hbar^2}{2}\delta^3(\vec{r}) \middle| n, j=\frac{1}{2}, l=0, f, m_f \right\rangle \\
&= \frac{g_p g_e e^2}{m_p m_e c^2}\frac{2\pi}{3}\frac{f(f+1)-\frac{3}{2}}{2}\hbar^2 \underbrace{|\psi_{n,l=0}(0)|^2}_{\frac{4}{4\pi a^3 n^3}} \\
&= \frac{g_e g_p m_e c^2 \alpha^4}{3n^3}\frac{m_e}{m_p}[f(f+1)-\frac{3}{2}]
\end{aligned}$$

shows hyperfine structure is at the order α^4 and the m_e/m_p factor makes it even smaller.

In particular

$$E_{n=1,f=1} - E_{n=1,f=0} = 1420\text{MHz}$$

the famous 21 centimeter line in cosmology.

$l=1\ j=\frac{3}{2}$

$n=2\ l=1$ or 0

$\updownarrow$ 10,900MHz

$l=1$

1057MHz

$l=1\ j=\frac{1}{2}$

$l=0\ j=\frac{1}{2}$

$l=0$

$\uparrow$

$2.45\times 10^{15}\frac{1}{\text{sec}}$

high optical freq

$\downarrow$

$f=1$

1420MHz

$n=1\ l=0$

$f=0$

The 1057MHz is Lamb shift, which will study in QFT.

5 Time Dependent Hamiltonian

We solve

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$$

We will deal with both cases: H change slowly, use approximation from time independent Schrodinger solution; H change quickly, which we discuss first.

The solution can be given by the time development operator $U(t_2, t_1)$ s.t.

$$U(t_2, t_1)|\Psi(t_1)\rangle = |\Psi(t_2)\rangle$$

and U satisfies

$$\begin{aligned} i\hbar\frac{\partial}{\partial t_2}U(t_2, t_1) &= H(t_2)U(t_2, t_1) \\ U(t, t) &= I \end{aligned} \tag{5.1}$$

To solve above, we write

$$U(t_2, t_1) = U^{(0)} + U^{(1)} + U^{(2)} + ...$$

0th order in H + 1st order in H + 2nd order in H...

Put

$$U^{(0)}(t_2, t_1) = I$$

we can solve the irritate equation below

$$i\hbar\frac{\partial}{\partial t}U^{(n)}(t_2, t_1) = H(t)U^{(n-1)}(t_2, t_1)$$

which approximates (5.1). We get

$$
\begin{aligned}
U^{(1)}(t_2, t_1) &= -\frac{i}{\hbar} \int_{t_1}^{t_2} dt H(t) \\
U^{(2)}(t_2, t_1) &= \left(-\frac{i}{\hbar}\right)^2 \int_{t_1}^{t_2} dt H(t) \int_{t_1}^{t_2} dt' H(t')
\end{aligned}
$$

such method is called "time order product".

(to be continued next semester...)